# ON A CLASS OF INITIAL VALUE PROBLEMS IN THE KINETIC THEORY OF DENSE GASES

By

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ABSTRACT

For a one-dimensional hard "sphere" gas, initial value problems are considered of the form where certain particles have specified positions and velocities and the rest have regular distributions at $t = 0$ . A hierarchy equation treatment is used to produce new results in a way that is not critically dependent on the simplified dynamics.

For the case where the background of particles are in equilibrium at $t = 0$ , initial conditions on the reduced distribution functions (r.d.f.) are calculated exactly. An approximate "local" factorization condition is discovered for the r.d.f's which enables approximate kinetic equations to be obtained. A Banach space formulation is found useful in determining rigorous upper bounds on the errors involved. For the general initial value problem outlined above, the existence and uniqueness of the solution are proved using Banach space and countably normed space formulations. The second approach is expected to be applicable to more general systems. For the case of a single specified particle, exact closed equations are obtained for the delta function part of the one-particle r.d.f's for a wide class of initial conditions. These enable the analysis of behaviour thought to be characteristic of more general systems e.g. the weak dependence of the approach to equilibrium on initial spatial inhomogeneities and on the presence of an external potential, the positive nature of the solutions, and the existence of an entropy functional monotonically increasing in time. A more general discussion of irreversibility is also given emphasizing the way in which we

restrict our attention to entropy increasing solutions.

Using and extending Jepsen's technique, exact calculations are performed specifically for the velocity correlation functions associated with finite versions of the above system. A sharp cut-off has been discovered on a time scale associated with the finite size of the system. A stochastic version of one of the above systems has been considered. Boundary effects with regard to the position of the specified particle have been examined. These considerations have been extended to more general systems.

Finally, using a formulation due to Anstis in the grand canonical ensemble, we examine the problem of obtaining an exact expression for certain n-particle r.d.f's in terms of the one-particle r.d.f. for a particle having a specified initial distribution when the background is in equilibrium. For the special system above, a solution is obtained using cluster and graph theoretical techniques. The solution to the corresponding problem in higher dimensions for a general inter-particle potential is obtained more directly by combinatorial methods Contributions to terms in the expansion of the solution are characterized in terms of collision sequences between isolated groups of particles. The range of convergence with respect to time is considered and is expected to be non-zero even for potentials allowing bound states. For hard sphere potentials, a technique is presented for the analysis of the delta-function part of the r.d.f. also satisfying a closed kinetic equation. The aim is that by examining the asymptotic behaviour, we may ascertain the usefulness of the kinetic equation and assess the need for resummation.

# STATEMENT

This thesis contains no material which has been accepted for the award of any other degree, and to the best of my knowledge and belief, contains no material previously published or written by another person except where due reference is made in the text.

James William Evans.

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# CHAPTER 1

# INTRODUCTION

## 1.1 THE DEVELOPMENT AND TECHNIQUES OF KINETIC THEORY

One of the original aims of kinetic theory was to produce an equation describing the time evolution of the one-particle reduced distribution function (r.d.f.) $f(\underline{x},\underline{v};t)$. This is the probability measure for finding some particle of the gas with position $\underline{x}$ and velocity $\underline{v}$ at time $t$. Certain macroscopic quantities pertaining to the fluid flow may be obtained from this function. Also certain transport coefficients may be calculated.

The Boltzmann equation, derived from heuristic reasoning was the first such equation successful for the case of a dilute gas where correlations between particles may be neglected. Hilbert, Chapman and Enskog then showed how to calculate transport coefficients from this equation (see Chapman and Cowling [1]). The introduction of the hierarchy equations through the work of Kirkwood [2], Bogoliubov [3], and Born and Green [4], enabled generalization of Boltzmann's equation to a higher range of densities. H.S. Green [5] demonstrated how Boltzmann's equation may be obtained from the first hierarchy equation if a "molecular chaos" assumption is made. Bogoliubov proposed that in the time evolution of a fluid, a stage would be reached where the higher order r.d.f's may be obtained as time independent functionals of the one-particle r.d.f. A technique was provided for obtaining these functionals from the hierarchy equations. When such an expression for the two-particle r.d.f. is substituted into the first hierarchy equation, the Boltzmann equation is obtained as a first approximation. Retaining the next order term in density results in the Choh Uhlenbeck [6] equation. Extensive calculations have been made by Sengers [7] in 2- and 3- dimensions to determine second order density corrections to the transport coefficients from this equation.

M.S. Green [8] and Cohen [9] have used cluster expansion techniques to obtain the same results as Bogoliubov. Their method indicates the range of validity of the assumption of Bogoliubov's work. In the application of this method, fundamental concepts are introduced common to several methods used in kinetic theory. Among these is the characterization of contributions to the expressions in the resulting operator expansions in terms of collision sequences between isolated groups of particles. Also the concept of resummation is introduced whereby the lowest order terms are modified by contributions from those of higher order. The aim of this scheme is to prevent divergences associated with "isolated" collision sequences over large distances (see Cohen [10, 11]). Van Hove [12] and Prigogine [13] have also derived exact non-Markovian equations for the irreversible evolution of a many body system. More recently Balescu [14] and others have undertaken a program to derive irreversible kinetic equations by starting with the space of all solutions to the Liouville equation and considering only a subspace (subdynamics) of these.

Quite a different method of calculating transport coefficients was developed first by M.S. Green [15]. Here the transport coefficients are obtained as integrals with respect to time over certain correlation functions. These results were re-derived later by Kubo [16], Mori [17] and H.S. Green [18] sometimes in modified form. From the work of Kubo originated the concept of the K.M.S. condition used in algebraic statistical mechanics.

In this area the binary collision expansion (b.c.e.) has proved useful. This method was developed first by Yang and Lee [19] and later in simplified form by Siegert and Teramoto [20]. Zwanzig [21] was first to calculate transport coefficients using correlation formulae and the b.c.e. taking the Laplace transform with respect to time of the operators appearing (the $\varepsilon$-method). Kawasaki and Oppenheim [22] later used the b.c.e. to resum the most divergent (ring) terms appearing in the expansion for the transport coefficients. Weinstock [23] has also used the b.c.e. method to derive non-Markovian equations for the velocity distribution function which were later used to examine transport coefficients. Dorfman and Cohen [24] concentrated on the long time behaviour of the correlation functions. After resumming the most divergent terms they showed that the correlation functions exhibit a slow long time decay of the form $\sim (t_o/t)^{\frac{d}{2}}$ where $t_o$ is the relaxation time and $d$ is the dimension. This agreed with the computer simulations of Alder and Wainwright.[25]

Instead of calculating directly the transport coefficients via the correlation formula method, one may instead focus attention on the initial value problem (i.v.p.) associated with the correlation functions. Here a specified particle (or particles) have given positions and velocities at the initial time and the remainder are in equilibrium. Through the solution of this i.v.p. we may calculate the correlation functions and thus the transport coefficients. Various approaches have been used. Some calculate the correlation functions directly and others determine the linear kinetic equation satisfied by the r.d.f. associated with a specified particle. There are several basic approaches: the mean field approach, hydrodynamical and mode-mode coupling theories, the Mori memory function approach, and a more rigorous approach starting from first principles and using microscopic considerations.

In the mean field approach (Singwi and Sjolander [26] and Kerr [27]), the specified particle is regarded as an external agent. The motion of the rest of the fluid is calculated assuming a known behaviour for the specified particle. This is substituted back into the equation of motion for the specified particle to obtain a self consistent result.

Kadanoff and Martin [28] have related the hydrodynamical variables to the correlation functions in the linear response domain with disturbances from equilibrium slowly varying in space and time. They have shown that the dynamical structure functions related to the correlation functions must exhibit certain asymptotic wave number behaviour in order for the system to have correct hydrodynamics. This provides a check for many methods. Ernst, Hauge and Van Leeuwen [29] were able to derive from hydrodynamical arguments, the same long time dependence for the correlation functions as obtained from computer simulations [25]. They assumed that the decay to local equilibrium of the non-equilibrium distribution functions was faster than the decay of the correlation functions and that the long wavelength components of hydrodynamical quantities satisfy the linearized Navier Stokes equations. Their arguments showed that the long time tail of the correlation functions was due to slowly decaying (long wavelength) hydrodynamical modes i.e. a feedback effect where the hydrodynamical behaviour of the rest of the fluid is effecting the behaviour of the specified particle. Kawasaki [30] has obtained the same results from a mode-mode coupling theory (see Ernst *et al* [31] for a more detailed exposition). Badeaux and Mazur [32] produced a re-normalized hydrodynamical theory by taking into account the dependence of the "bare" diffusion coefficient on e.g. the local density of the fluid. A renormalized wave number and frequency dependent diffusion coefficient is obtained in terms of a "dressed" diffusion propagator.

Zwanzig [33] obtained a non-Markovian equation for the time evolution of the macroscopic state variables. Mori [34] extended this work utilizing projection operators similar to those of Zwanzig. The kernel of the non-Markovian part of the equations is referred to as the Mori memory function. Several authors have used this formulation to derive kinetic equations for correlation functions and r.d.f's. For example, Akcasu and Duderstadt [35] used a continuous parameter representation (in this case momentum) of the Mori type equation to obtain a kinetic equation for the one-particle r.d.f. Several approximations were then made for the memory function based on physical arguments. Lebowitz, Percus and Sykes [36] also used a Mori type equation choosing the memory function so that the short time behaviour of the r.d.f's was described exactly.

Several workers have developed systematic theories starting from first principles. Of these we mention the following. Mazenko's [37] fully renormalized kinetic theory provides a microscopic expression for the memory function valid for all wave numbers and frequencies. The memory function is re-arranged as the sum of an effective two body term and a term representing the rest of the particles. Isolated clusters never appear as in Cohen's Theory or the b.c.e. The equations have been renormalized first. Gross [38] has used a "dressed" particle approach which involves splitting the Liouville operator into parts $L = L_o + L_1$ where $L_o$ is the "dressed" rather than free Liouville operator. This approach enables one to describe screening and backflow effects. Also the interaction of particles or clusters of particles with fluctuations in the fluid is emphasized. Sjögren and Sjölander [39] have developed a treatment of the problem where the physics is rather transparent. The r.d.f's are split into self(specified particle) and distinct (background) parts so the effect of the backflow of the background of particles on the specified particle is emphasized.

## 1.2 OUTLINE OF THE THESIS

Throughout we deal with the class of i.v.p's where a specified particle(or particles) have a given initial distribution (sometimes chosen so as to fix the position and velocity). The background of particles have a smooth distribution often chosen to be the equilibrium distribution. The advantage of studying these problems is that we have well posed initial conditions which ensure that the one-particle r.d.f. for a specified particle satisfies a linear kinetic equation. As mentioned previously, the solution to these equations can be used to calculate correlation functions and transport coefficients.

Most of our analysis is for a one-dimensional hard "sphere" gas where the particles interact elastically and interchange velocities on collision. This system has been studied previously by several authors (e.g. Jepsen [40], Lebowitz and Percus [41], Lebowitz, Percus and Sykes [36], and Anstis, Green and Hoffman [42]) in an attempt to obtain results applicable to 3 dimensional systems.

In Chapter 2 we consider a class of i.v.p's for the above special system (of infinite size) where several particles have specified positions and velocities and the remainder are in equilibrium at $t=0$. We discover an approximate "local" factorization condition for the r.d.f's at the initial time. This is used together with the hierarchy equations derived by Anstis *et al* [42] to obtain approximate kinetic equations. A Banach space technique is used to give a rigorous analysis of the errors involved. This work is extended to more general i.v.p's in Chapter 3. Existence and uniqueness results are obtained using Banach space and countably normed space techniques. For the case of a single specified particle and certain "factorizing" background distributions, exact kinetic equations are obtained for the delta-function part of the one-particle r.d.f. $f_j^{(1)\delta}$. These are used to examine the dependence of the approach to equilibrium on background distribution inhomogeneities the effect of an external potential, and the positive nature of the solutions. Chapter 4 concludes the analysis of this section with a discussion of irreversibility. Where we have exact equations for $f_j^{(1)\delta}$, an entropy functional in terms of $f_j^{(1)\delta}$ is found which has finite and monotonically increasing behaviour in time.

Jepsen's [40] method is used and extended in Chapter 5 to enable an exact calculation of the long time behaviour of the velocity correlation functions (v.c.f.) for various finite one-dimensional hard "sphere" systems. A stochastic version of the system is also treated. The effect on the v.c.f's of the specified particle near the boundary is analyzed and these considerations are extended to higher dimensional systems with more general inter-particle potentials.

In Chapter 6 we implement an elegant method due to Anstis [43,44] using the grand canonical ensemble to obtain a solution to the elimination problem i.e. an expression for a certain n-particle r.d.f. at time t in terms of the one-particle r.d.f. at time t for a specified particle. The initial conditions are such that the specified particle has a given distribution and the rest are in equilibrium. Whereas Anstis only obtained the first few terms in the expansion of the solution by an iterative technique, we develop a systematic scheme for solving the problem obtaining an expression for the general term in the expansion. First we treat the one-dimensional hard "sphere" system where the r.d.f's have a cluster structure and graph theoretical techniques are applicable. Then by more direct combinatorial methods, a solution is obtained for the corresponding problem in higher dimensions with a more general interparticle potential. In Chapter 7 contributions to the terms in the solution involving abstract streaming operators are associated with various collision sequences. This enables convergence considerations to be made. We comment on the usefulness of these expressions for the 2-particle r.d.f. in obtaining kinetic equations including mention of the case where the interparticle potential allows bound states to occur. For hard sphere potentials a method is presented for the analysis of the delta-function part of the r.d.f. essentially by projection of the kinetic equation on to the delta-function component. This method is demonstrated for the one-dimensional case.

# CHAPTER 2

## QUASI-EQUILIBRIUM INITIAL VALUE PROBLEMS

## (ONE-DIMENSIONAL HARD "SPHERE" GAS)

### 2.1 INTRODUCTION

In this chapter we examine the solutions of a special class of initial value problems in kinetic theory. The system considered is an infinite one-dimensional gas of identical particles interacting elastically. The canonical ensemble in the thermodynamic limit (t.l.) is used and a reduced distribution function (r.d.f.) formalism adopted. A similar approach has been used previously for this system by Lebowitz and Percus [4.1] and Anstis et al.[4.2]. We consider only the zero diameter (point particle) case since, as observed by the above authors, general results may easily be obtained from this analysis.

First we give a derivation of the appropriate hierarchy equations for this system. The solutions of these equations are shown to exhibit certain fundamental properties necessary for physical interpretation.

The initial value problems (i.v.p.) considered are of the form where a number of particles have specified positions and velocities at the initial time. The rest are in equilibrium subject to the constraints imposed by the specified particles. For these problems, the initial conditions on the r.d.f.'s may be calculated exactly from the theory of equilibrium statistical mechanics. The case where a single particle is specified and the rest are in equilibrium at $t = 0$ has been treated by Anstis et al.[42] using hierarchy techniques. The problem was solved for the one-particle r.d.f.'s using an exact factorization property of the higher order r.d.f.'s. A periodic analogue of this problem is discussed in detail here and an approximate factorization condition for the r.d.f.'s is obtained. The corresponding approximate kinetic equations for the one-particle r.d.f.'s are derived and their solution obtained. To determine the accuracy of this approximate solution, it is necessary to determine an upper bound on the size of the error terms associated with the factorization of the r.d.f.'s. This necessitates the consideration, on certain "precollision" regions of phase space, of the complete coupled hierarchy of equations satisfied by these error functions. Existence and uniqueness are proved using a Banach space formulation and a rigorous upper bound is obtained on the norm of these error functions. The choice of norm is specifically tailored to suit the problem at hand. In the next chapter, it is shown that other choices are possible.

We conclude by discussing approximate factorization conditions and kinetic equations for the most general i.v.p.'s mentioned above.

## 2.2 THE DISTRIBUTION FUNCTIONS AND THEIR HIERARCHY EQUATIONS

Since we shall be using the canonical ensemble, we must first define the appropriate r.d.f.'s for a finite system of N' particles in a region $\mathcal{L}'$ of size (length) $L' < \infty$. Having done so, we then take the t.l. $N' \to \infty$, $L' \to \infty$ with $N'/L'$ constant.

The particles are labelled at the initial time with an integer index increasing from left to right. Then, since the particles are impenetrable, this ordering is preserved for all times. Let the set of labels be denoted by S, then $|S| = N'$. We introduce the complete distribution function for the finite system at time t:

$$D = D(z_j, j\varepsilon S; t|\mathcal{L}') \tag{2.1}$$

where $z_j = (x_j, v_j)$ denotes the position and velocity of particle j. $D \prod_{j\varepsilon S} dz_j$ gives the probability of finding particle "j" in a region of phase space $dz_j$ about $z_j$. D satisfies the N'-particle Liouville equation and is not assumed to be symmetrical in the arguments $z_j$.

We shall, however, be more interested in the r.d.f.'s. The n-particle r.d.f.'s are defined, for $n \leqslant N'$, by

$$f^{(n)}_{i1\ i2\ \ldots\ in}(z_{i1}; z_{i2}; \ldots; z_{in}; t|\mathcal{L}') = \prod_{j\varepsilon S\setminus\{i1\ldots in\}} \int_{\mathcal{L}'\times R} dz_j\ D(z_k, k\varepsilon S; t|\mathcal{L}') \tag{2.2}$$

which gives the probability measure for finding particle "iα" at $z_{i\alpha}$, $\alpha = 1,2 \ldots n$. Starting from the Liouville equation, we derive the time evolution equations satisfied by the $f^{(n)}_{i1 \ldots in}$. The method used is an adaptation of that described by Bogoliubov [3] for the case of a symmetric complete distribution function. We need the following definitions:

$\Phi_{\mathcal{L}'}(x)$ : external potential with support confined to a suitably small neighbourhood of the boundary where the potential goes smoothly to infinity.

$H(z) = \frac{1}{2}mv^2 + \Phi_{\mathcal{L}'}(x)$ : one-particle Hamiltonian for particles of mass m.

$$[A;B] = \sum_{j\varepsilon S} \left( \frac{\partial}{\partial x_j} A \frac{\partial}{\partial P_j} B - \frac{\partial}{\partial P_j} A \frac{\partial}{\partial x_j} B \right) \quad \text{with } P_j = mv_j$$

: Poisson brackets.

$\phi(|r|)$ : interparticle potential for separation "r".

D satisfies the Liouville equation

$$\frac{\partial}{\partial t} D = \sum_{j\varepsilon S} [H(z_j);D] + \sum_{\substack{i<j \\ i,j\varepsilon S}} [\phi(|x_i - x_j|);D] \qquad (2.3)$$

from which it follows that

$$\frac{\partial}{\partial t} f^{(n)}_{i1\ i2 \ldots in}(z_{i1};\ldots;z_{in};t|\mathcal{L}') =$$

$$\sum_{i\varepsilon S} \prod_{j\varepsilon S\setminus\{i1 \ldots in\}} \int_{\mathcal{L}'\times R} dz_j [H(z_i);D] \qquad (2.4)$$

$$+ \sum_{\substack{i<j \\ i,j\varepsilon S}} \prod_{k\varepsilon S\setminus\{i1 \ldots in\}} \int_{\mathcal{L}'\times R} dz_k [\phi(|x_i - x_j|);D]$$

In (2.4) we write $\sum_{i\in S} = \sum_{i\in\{i1\ldots in\}} + \sum_{i\in S\setminus\{i1\ldots in\}}$ (2.5)

Since from our choice of $\Phi_{\mathcal{L}'}(x)$, D = 0 on the boundaries of $\mathcal{L}'$, integration by parts shows that $\int_{\mathcal{L}'\times R} dz_i [H(z_i);D] = 0$.

So all terms in the second sum of (2.5) vanish. We also write

$$\sum_{\substack{i<j\\ i,j\in S}} = \sum_{\substack{i<j\\ i,j\in\{i1\ldots in\}}} + \sum_{\substack{i\in\{i1\ldots in\}\\ j\in S\setminus\{i1\ldots in\}}} + \sum_{\substack{i<j\\ i,j\in S\setminus\{i1\ldots in\}}} \tag{2.6}$$

Since from integration by parts $\int_{\mathcal{L}'\times R} dz_i \int_{\mathcal{L}'\times R} dz_j$ $[\phi(|x_i-x_j|);D] = 0$, all terms in the third sum of (2.6) vanish (see Bogoliubov [3]). (2.4) may now be rewritten as

$$\frac{\partial}{\partial t} f^{(n)}_{i1\ i2\ \ldots\ in}(z_{i1};\ldots;z_{in};t|\mathcal{L}') \tag{2.7}$$

$$= \Bigg[\sum_{i\in\{i1\ldots in\}} H(z_i) + \sum_{\substack{i<j\\ i,j\in\{i1\ldots in\}}} \phi(|x_i-x_j|);$$

$$f^{(n)}_{i1\ i2\ \ldots\ in}(z_{i1};\ldots;z_{in};t|\mathcal{L}')\Bigg]$$

$$+ \int_{\mathcal{L}'\times R} dz \Bigg[\sum_{i\in\{i1\ldots in\}} \phi(|x_i-x|);$$

$$f^{(n+1)}_{i1\ i2\ldots in}(z_{i1};\ldots;z_{in};z;t|\mathcal{L}')\Bigg]$$

where $f^{(n+1)}_{i1\ i2\ \ldots\ in}(z_{i1};\ldots;z_{in};z;t|\mathcal{L}')$ (2.8)

$$= \sum_{j\neq i1\ldots in} f^{(n+1)}_{i1\ i2\ \ldots\ in\ j}(z_{i1};\ldots;z_{in};z;t|\mathcal{L}')$$

Note that $f^{(N')}_{1\,2\,\ldots\,N'} = D$ and $f^{(N'+r)}_{i\,\ldots} = 0$ for $r > 0$. At this stage we take the t.l. For our i.v.p.'s, all the $f^{(n)}_{i1\;i2\;\ldots\;in}$ exist in this limit and (2.7) becomes an infinite coupled hierarchy where now $H(z) = \frac{1}{2}mv^2$. These equations are identical with those obtained by Anstis et al.[42] using the grand canonical ensemble. This is expected from the equivalence of ensembles in the t.l.

Since we are interested primarily in $f^{(1)}_i$, it will suffice to deal only with the r.d.f.'s

$$f^{(n)}_i = \sum_{\substack{i2\;i3\;\ldots in \\ i\alpha \neq i\beta\;\; \alpha\neq\beta \\ i\alpha \neq i}} f^{(n)}_{i\;i2\;i3\;\ldots\;in} \tag{2.9}$$

From (2.9) $f^{(n)}_i$ is symmetrical in the last "n-1" variables $z_\alpha$. In (2.7), we may sum over i2 i3 ... in to obtain

$$\left(\frac{\partial}{\partial t} + K^{(n)}\right) f^{(n)}_j (z_1;z_2;\ldots;z_n;t) \tag{2.10}$$

$$= \int_{R\times R} dz_{n+1} \sum_{i=1}^{n} \frac{\partial}{\partial x_i} \phi(|x_i - x_{n+1}|)$$

$$\times \frac{\partial}{\partial P_i} f^{(n+1)}_j (z_1;\ldots;z_n;z_{n+1};t)$$

where $K^{(n)}$ is the n-particle Liouville operator. Using (2.10) we may prove the continuity of $f^{(n)}_j$ across the lines $x_\alpha = x_\beta$ $\alpha,\beta \in \{2,3,\ldots,n\}$, $\alpha \neq \beta$. Consider for example the line $x_2 = x_3$ for $v_2 > v_3$. (2.10) may be written as

$$\left(\frac{\partial}{\partial t} + v_2 \frac{\partial}{\partial x_2} + v_3 \frac{\partial}{\partial x_3} - \frac{\partial}{\partial x_2} \phi_{2,3} \frac{\partial}{\partial P_2} - \frac{\partial}{\partial x_3} \phi_{2,3} \frac{\partial}{\partial P_3}\right) f_j^{(n)} = \text{other terms.} \tag{2.11}$$

with $\phi_{m,n} = \phi(|x_m - x_n|)$. In the limit $x_2 - x_3 \to 0$, the delta-function contributions to (2.11) associated with any discontinuity in $f_j^{(n)}$ at $x_2 = x_3$ come along from terms on the l.h.s. These terms have the structure of a Liouville equation in the pair space $(z_2, z_3)$. Since particles interchange velocities upon collision, after integration of (2.11) we obtain

$$\begin{aligned} &\lim_{\in\to 0} f_j^{(n)}(z_1; x-\in, v_2; x, v_3; z_4; \ldots; z_n; t) \\ &= \lim_{\in\to 0} f_j^{(n)}(z_1; x, v_3; x+\in, v_2; z_4; \ldots; z_n; t) \end{aligned} \tag{2.12}$$

From the symmetry of $f_j^{(n)}$ in the variables $z_2$ and $z_3$, we also have

$$\begin{aligned} &f_j^{(n)}(z_1; x, v_3; x+\in, v_2; \ldots; t) \\ &= f_j^{(n)}(z_1; x+\in, v_2; x, v_3; \ldots; t) \end{aligned} \tag{2.13}$$

The continuity result may now be proved taking (2.12) and (2.13) in the limit $\in \to 0$. From (2.10)

$$\begin{aligned} &\left(\frac{\partial}{\partial t} + K_j^{(n)}\right) f_j^{(n)}(z_1; \ldots; z_n; t) \\ &= \int_{R\times R} dz_{n+1} \sum_{i=1}^{n} \frac{\partial}{\partial x_i} \phi_{i,n+1} \frac{\partial}{\partial P_i} f_j^{(n+1)}(z_1; \ldots; z_n; z_{n+1}; t) \end{aligned} \tag{2.14}$$

except on the lines $x_\alpha = x_\beta$ $\alpha,\beta \in \{2,3\ldots n\}$ $\alpha \neq \beta$. Across these lines $f_j^{(n)}$ is continuous. $K_j^{(n)}$ is the n-particle Liouville operator which takes into account only interactions of the $j^{th}$ particle with the unlabelled particles. So to obtain a solution to (2.14), we must integrate along the characteristics of $\frac{\partial}{\partial t} + K_j^{(n)}$ (see Courant and Hilbert[45]). Whenever one of the lines $x_\alpha = x_\beta$ is reached the continuity condition is employed. This produces a result identical to that obtained by assuming (2.14) holds everywhere. Anstis et al.[42] have provided a physical argument to arrive at the same conclusion.

(2.14) is now rewritten so that the r.h.s. does not depend explicitly on the interparticle potential. The only possible contributions to the integral over $x_{n+1}$ are from $x_{n+1}$ in a neighbourhood of $x_i, i = 1,2,\ldots,n$. Let us consider the case where i = 1. If we regard $f_j^{(n)}$ as a function of the variables $x_1 - x_{n+1}$ and $x_1 + x_{n+1}$ rather than $x_1$ and $x_{n+1}$ separately, then (2.14) becomes

$$\left((v_1 - v_{n+1})\frac{\partial}{\partial(x_1 - x_{n+1})} - \frac{\partial}{\partial x_1}\phi_{1,n+1}\frac{\partial}{\partial P_1} - \frac{\partial}{\partial x_{n+1}}\phi_{1,n+1}\frac{\partial}{\partial P_{n+1}}\right)f_j^{(n)}$$

$$= \text{other terms} \tag{2.15}$$

The other terms are regular for $x_1 - x_{n+1} = 0$. This result, when used to evaluate the i = 1 term in the sum in (2.14), yields

$$\lim_{\epsilon\to 0}\int_{-\infty}^{+\infty} dv_{n+1}|v_{n+1}-v_1| \times \Big(f_j^{(n+1)}(z_1;\ldots;z_n;x_1^+,v_{n+1};t) - f_j^{(n+1)}(z_1;\ldots;z_n;x_1^-,v_{n+1};t)\Big) \tag{2.16}$$

where $x_1^{\pm} = x_1 \pm \epsilon\ \mathrm{sgn}(v_{n+1} - v_1)$. Using the continuity of $f_j^{(n+1)}$ across $x_{n+1} = x_i$ $i = 2,3,\ldots,n$, it is clear that the other terms in the sum produce zero contribution to the integral.

Two other properties of the $f_j^{(n)}$ are needed (Appendix A). The first we call an asymptotic Liouville property. This incorporates microscopic reversibility and may be proved from an equation similar to (2.11).

$$\lim_{\epsilon\to 0} f_j^{(n+1)}(z_1;\ldots;z_n;x_1^{\pm},v_{n+1};t) = \lim_{\epsilon\to 0} f_j^{(n+1)}(x_1^{\mp},v_{n+1};z_2;\ldots;z_n;z_1;t) \tag{2.17}$$

The second reflects the impenetrability property of the particles (the $j^{th}$ is always between the $(j+1)^{th}$ and $(j-1)^{th}$):

$$\lim_{\epsilon\to 0} f_j^{(n+1)}(x_1\pm\epsilon,v_{n+1};z_2;\ldots;z_n;z_1;t) = \lim_{\epsilon\to 0} f_{j\mp 1}^{(n+1)}(z_1;\ldots;z_n;x_1\pm\epsilon,v_{n+1};t) \tag{2.18}$$

Setting $(j) = j + \mathrm{sgn}(v_{n+1} - v_1)$ and using (2.17), (2.18) and (2.16), the equations for $f_j^{(n)}$ become (see Anstis et al.[42]).

$$\left(\frac{\partial}{\partial t} + K_j^{(n)}\right) f_j^{(n)}(z_1;\ldots;z_n;t) \tag{2.19}$$

$$= \lim_{\epsilon\to 0} \int_{-\infty}^{+\infty} dv_{n+1}|v_{n+1}-v_1| \times \left( f_{(j)}^{(n+1)}(z_1;x_1^-,v_{n+1};z_2;\ldots;z_n;t) - f_j^{(n+1)}(z_1;x_1^-,v_{n+1};z_2;\ldots;z_n;t)\right)$$

Some basic properties of the solutions of (2.19) are discussed in Appendix A.

## 2.3 INITIAL CONDITIONS ON THE REDUCED DISTRIBUTION FUNCTIONS

The work of this section involves exact equilibrium statistical mechanical calculations. Such calculations may be performed for one-dimensional systems rather more easily than for higher dimensions. Tonks [46] succeeded in calculating the partition function for the hard "sphere" system. Other soluble one-dimensional hard core systems are, for example, nearest neighbour interactions (Takahashi[47]) and some special long range interactions (Bountis and Hellerman[48]). A hierarchy equation approach has been used by Raveche and Stuart[49] for an homogeneous hard "sphere" system to prove uniqueness of equilibrium solutions.

For a particle ("0" say) specified at the origin at $t = 0$ and the remaining particles in equilibrium, the initial conditions on the r.d.f.'s have been calculated by Anstis et al.[42]. They used the grand canonical ensemble in the infinite volume limit. For the one-particle r.d.f.'s, one obtains

$$f_0^{(1)}(z_1;0) = \delta(x_1)\ \delta(v_1-v')$$

$$\text{for } j>0:\ f_j^{(1)}(z_1;0) = H(x_1)\ \frac{\rho(\rho x_1)^{j-1}}{(j-1)!}\ \exp(-\rho x_1)\ h_0(v_1) \tag{3.1}$$

$$\text{for } j<0:\ f_j^{(1)}(z_1;0) = f_{-j}^{(1)}(-x_1,v_1;0)$$

where H( ) is the Heaviside step function, $\rho$ is the mean particle density and $h_0(v) = (2\Pi)^{-\frac{1}{2}}\, v_{th}^{-1} \exp(-\tfrac{1}{2}(v/v_{th})^2)$ with $v_{th} = (m\beta)^{-\frac{1}{2}}$ (the thermal velocity). Higher order r.d.f.'s $f_j^{(n)}$ at t = 0 may be obtained from (3.1) together with the exact factorization condition

$$f_j^{(n)}(z_1;\ldots;z_n;0) = f_{j*}^{(n-1)}(z_1;\ldots;z_{n-1};0)\cdot h(z_n) \tag{3.2}$$

where

$$\begin{aligned} j^* &= j-1\ ,\ 0 < x_n < x_1 \\ &= j+1\ ,\ x_1 < x_n < 0 \\ &= j \quad \text{otherwise} \end{aligned} \tag{3.3}$$

and $h(z) = \rho h_0(v) + \delta(x)\cdot\delta(v-v')$. When considering points where specified particles are situated, e.g. $x_i = x_j = 0$ in the above example, we must adopt suitable limit procedures because of the possibility of discontinuities in the regular part of the r.d.f.'s and because of the delta-function dependence. If $v_i,\ v_j \neq v'$, then we may consider the limits $x_i = 0 \pm \epsilon$, $x_j = 0 \pm \epsilon'$ as $\epsilon, \epsilon' \rightarrow 0$. If $v_i = v'$, $v_j \neq v'$, then we may also consider $x_i = 0$, $x_j = 0 \pm \epsilon \rightarrow 0$. If $v_i = v_j = v'$, then as well as the above limits we may also consider $x_i = 0 \pm \epsilon$ as $\epsilon \to 0$, $x_j = 0$. We shall always work in a function space for the r.d.f.'s where these limits exist. None involve the product of delta-functions. These considerations should, for example, be applied to the interpretation of (3.2). If we set $f^{(n)} = \sum_{j=-\infty}^{+\infty} f_j^{(n)}$, then we may sum over j in (3.3) to obtain:

$$f^{(n)}(z_1;\ldots;z_n;0) = f^{(n-1)}(z_1;\ldots;z_{n-1};0)\cdot h(z_n;0) \qquad (3.4)$$

Let us now consider the initial conditions on the r.d.f.'s for the periodic analogue of the above problem. We first examine the problem of determining the r.d.f.'s for P particles in a hard walled box of length L (a Tonks gas). L is chosen so that the particle density $\frac{P}{L} = \rho$. Calculation of the r.d.f.'s involves a simple adaptation of methods used to calculate the partition function in the canonical ensemble (see Thompson[50]). The canonical ensemble average is defined here by

$$\langle G(z^1;\ldots;z^P)\rangle_{c.e.} =$$

$$\frac{\left(\prod_{i=1}^{P}\int dv^i h_0(v^i)\right)\left(\prod_{i=1}^{P}\int_{0\leqslant x^1\leqslant x^2\leqslant\ldots\leqslant x^P\leqslant L} dx^i\right) G(z^1;\ldots;z^P)}{Z_{c.e.}} \qquad (3.5)$$

where $Z_{c.e.}$ is the canonical partition function for the system defined by $\langle 1\rangle_{c.e.} = 1$ so $Z_{c.e.} = \frac{L^P}{P!}$. The one-particle r.d.f.'s are defined by

$$f_j^{(1)}(z_1)_L = \langle\delta(z_1 - z^j)\rangle_{c.e.} \tag{3.6}$$

More generally, the n-particle r.d.f.'s are defined by

$$f^{(n)}_{j1\ j2\ \ldots\ jn}(z_1;z_2;\ldots;z_n)_L =$$

$$\langle\delta(z_1 - z^{j1})\ \delta(z_2 - z^{j2})\ \ldots\ \delta(z_n - z^{jn})\rangle_{c.e.} \tag{3.7}$$

for $n \leqslant P$ and $\{j1, j2, \ldots, jn\} \subseteq \{1, 2, \ldots, P\}$. These expressions may be calculated exactly. We give a few examples for the lowest orders before stating general results.

$\underline{f_j^{(1)}}$: $$f_j^{(1)}(z_1)_L = \left(\frac{(L-x_1)^{P-j}}{(P-j)!} \quad \frac{x_1^{\ j-1}}{(j-1)!}\right) h_0(v_1)\chi_{[0,L]}(x_1)/\frac{L^P}{P!} \tag{3.8}$$

where $\chi_A(\ )$ is the characteristic function for region A. From (3.8) and the binomial theorem

$$\sum_{j=1}^{P} f_j^{(1)}(z_1)_L = \rho\ h_0(v_1)\ \chi_{[0,L]}(x_1) \tag{3.9}$$

$\underline{f_{jk}^{(2)}}$: Consider the case $0 < x_2 < x_1 < L$. For $1 \leqslant k < j \leqslant P$,

$$f_{jk}^{(2)}(z_1;z_2)_L = \left(\frac{(L-x_1)^{P-j}}{(P-j)!} \quad \frac{(x_1-x_2)^{j-k-1}}{(j-k-1)!} \quad \frac{x_2^{\ k-1}}{(k-1)!}\right) h_0(v_1)h_0(v_2)$$

$$\times\ \chi_{[0,L]}(x_1)\ \chi_{[0,L]}(x_2)/\frac{L^P}{P!} \tag{3.10}$$

For $1 \leqslant j < k \leqslant P$, $f_{jk}^{(2)}(z_1;z_2)_L = 0$

For $0 < x_1 < x_2 < L$, use $f_{m,n}^{(2)}(z;z')_L = f_{n,m}^{(2)}(z';z)_L$

Our primary interest is in the 2-particle r.d.f.'s of the form $f_j^{(2)}$. From (3.10), for $0 < x_2 < x_1 < L$

$$f_j^{(2)}(z_1;z_2)_L = \sum_{k=1}^{j-1} f_{jk}^{(2)}(z_1;z_2)_L$$

$$= \frac{(L-x_1)^{P-j}}{(P-j)!} \frac{x_1^{j-2}}{(j-2)!} h_0(v_1)h_0(v_2)\chi_{[0,L]}(x_1)\chi_{[0,L]}(x_2)/\frac{L^P}{P!}$$

$$\text{for } j \geq 2 \qquad (3.11)$$

$= 0$ otherwise

where again the binomial theorem has been used. A similar calculation may be performed for the case $0 < x_1 < x_2 < L$ where

$$f_j^{(2)}(z_1;z_2)_L = \sum_{k=j+1}^{P} f_{jk}^{(2)}(z_1;z_2)_L \qquad (3.12)$$

$f_{jk\ell}^{(3)}$: We consider only the case $0 < x_3 < x_2 < x_1 < L$ (the other cases follow easily from this).

$$f_{jk\ell}^{(3)}(z_1;z_2;z_3)_L = \frac{(L-x_1)^{P-j}}{(P-j)!} \frac{(x_1-x_2)^{j-k-1}}{(j-k-1)!} \frac{(x_2-x_3)^{k-\ell-1}}{(k-\ell-1)!} \frac{x_3^{\ell-1}}{(\ell-1)!}$$

$$\times\, h_o(v_1)h_o(v_2)h_o(v_3)\chi_{[o,L]}(x_1)\chi_{[o,L]}(x_2)\chi_{[o,L]}(x_3)/\frac{L^P}{P!}$$

$$\text{for } 1 \leq \ell < k < j \leq P, \quad = 0 \text{ otherwise} \qquad (3.13)$$

and $$f_j^{(3)}(z_1;z_2;z_3)_L = \sum_{k=2}^{j-1} \sum_{\ell=1}^{k-1} f_{jk\ell}^{(3)}(z_1;z_2;z_3)_L$$

$$= \frac{(L-x_1)^{P-j}}{(P-j)!} \frac{x_1^{j-3}}{(j-3)!} h_0(v_1)h_0(v_2)h_0(v_3)\chi_{[0,L]}(x_1)\chi_{[0,L]}(x_2)\chi_{[0,L]}(x_3)/\frac{L^P}{P!}$$

$$\text{for } j \geq 3 \qquad (3.14)$$

$= 0$ otherwise

$f_j^{(n)}$: Only the expressions for the $f_j^{(n)}$ are given here as those for the general n-particle r.d.f.'s are not needed. Suppose $0 < x_\alpha < x_1 < x_\beta < L$ for $\alpha \in S_1$, $\beta \in S_2$ with $S_1 \dot{\cup} S_2 = \{2,3,\ldots,n\}$ and $|S_1| = \Lambda_1$, $|S_2| = \Lambda_2$. Then

$$f_j^{(n)}(z_1;\ldots;z_n)_L = \frac{(L-x_1)^{P-j-\Lambda_2}}{(P-j-\Lambda_2)!} \frac{x_1^{j-1-\Lambda_1}}{(j-1-\Lambda_1)!} \prod_{i=1}^{n} h_0(v_i)\chi_{[0,L]}(x_i) / \frac{L^P}{P!}$$

$$\text{for } \Lambda_1 < j \text{ and } \Lambda_2 < P-j+1 \tag{3.15}$$

= 0 otherwise.

From (3.15), $\sum_{j=1}^{P} f_j^{(n)}(z_1;\ \ldots;z_n)_L$

$$= \sum_{j=\Lambda_1+1}^{P-\Lambda_2} f_j^{(n)}(z_1;\ldots;z_n)_L \tag{3.16}$$

$$= \frac{P-1}{P} \cdot \frac{P-2}{P} \cdots \frac{P-n+1}{P} \prod_{i=1}^{n} \rho h_0(v_i)\chi_{[0,L]}(x_i)$$

(3.16) shows that the symmetrized equilibrium distribution function factorizes as in the semi-infinite case (3.4). The numerical factor $\frac{P-1}{P} \cdot \frac{P-2}{P} \cdots \frac{P-n+1}{P}$ just takes account of normalization.

It is instructive to show how the initial conditions for the semi-infinite problem may be obtained from (3.8) - (3.16) taking the t.l. $P,L \to \infty$, $\frac{P}{L} = \rho$. Equivalence of canonical and grand canonical ensembles in this limit again guarantees consistency with those results obtained by Anstis et al.[42].

From (3.8)

$$f_j^{(1)}(z_1)_L = \frac{P}{P-1} \cdot \frac{P}{P-2} \cdots \frac{P}{P-j+1} \cdot \frac{1}{\left(1-\frac{\rho x_1}{P}\right)^j}$$

$$\times \chi_{[0,L]}(x_1) \frac{\rho(\rho x_1)^{j-1}}{(j-1)!} \left(1-\frac{\rho x_1}{P}\right)^P h_0(v_1) \tag{3.17}$$

It is now clear that we recover (3.1) upon taking the t.l..
From (3.10) in the t.l. for $0 < x_2 < x_1$ and $1 \leqslant k < j$,

$$f^{(2)}_{jk}(z_1;z_2) = \frac{(\rho(x_1-x_2))^{j-k-1}}{(j-k-1)!} \frac{(\rho x_2)^{k-1}}{(k-1)!} \exp(-\rho x_1) \times h_0(v_1)\, h_0(v_2) \cdot H(x_1)H(x_2) \qquad (3.18)$$

and from (3.15) in the t.l. for $0 < x_\alpha < x_1 < x_\rho, \alpha \varepsilon S_1$,
$\beta \;\varepsilon\; S_2$ (as defined previously) and $j > \Lambda_1$

$$f^{(n)}_{j}(z_1;\ldots;z_n) = \frac{(\rho x_1)^{j-1-\Lambda_1}}{(j-1-\Lambda_1)!} \cdot \exp(-\rho x_1) \cdot \prod_{i=1}^{n} h_0(v_i)\;\; H(x_i) \qquad (3.19)$$

Having made these remarks, we return to the consideration of the periodic problem. The particle specified to be at $x = mL$ initially with velocity $v'$ will be labelled "m(P+1)" so the particles in the cell [mL,(m+1)L] initially will be labelled m(P+1)+1, m(P+1)+2,...,m(P+1)+P. The initial conditions on the r.d.f.'s $f^{(n)}_{j1j2\ldots jn}(\quad;0)$ for the periodic problem shall be specified in terms of the $f^{(m)}_{k1\ldots km}(\quad)_L$ calculated above. In particular if j1, j2,...,jn ε {1,2,...,P} then

$$f^{(n)}_{j1\;j2\ldots jn}(z_1;\ldots;z_n;0) = f^{(n)}_{j1\;j2\ldots jn}(z_1;\ldots;z_n)_L \qquad (3.20)$$

and $f^{(1)}_0(z_1;0) = \delta(x_1)\delta(v_1-v')$

In order for the specification to be complete, the following results are needed. Since particles in different cells [mL,(m+1)L] do not interact at the initial time, there is a factorization condition on the r.d.f.'s of the following form : make the decomposition

$$\{1,2,\ldots,n\} = \dot{\bigcup}_{K=-\infty}^{+\infty} \Gamma_K \,\dot{\cup}\, \Gamma \qquad (3.21)$$

where $\alpha \varepsilon \Gamma_K$ if $j\alpha \ \varepsilon \ \{K(P+1)+1,\ldots,K(P+1)+P\}$ and $\alpha \varepsilon \Gamma$ if $j\alpha = 0 \pmod{P+1}$, then

$$f^{(n)}_{j1j2\ldots jn}(z_1;\ldots;z_n;0) =$$

$$\prod_{K=-\infty}^{+\infty} f^{(|\Gamma_K|)}_{j\alpha\,:\,\alpha\varepsilon\Gamma_K}(z_\alpha : \alpha \ \varepsilon \ \Gamma_K; 0) \ . \prod_{\beta\varepsilon\Gamma} f^{(1)}_{j\beta}(z_\beta;0) \qquad (3.22)$$

setting $f^{(0)} = 1$. Finally we mention a periodicity constraint (valid for all $t \geqslant 0$) :

$$f^{(m)}_{k1k2\ldots km}(x_1,v_1;\ldots;x_m,v_m;t) = f^{(m)}_{k1+K(P+1)\ k2+K(P+1)\ldots km+K(P+1)}(x_1+KL, v_1;\ldots;x_m+KL,v_m;t) \qquad (3.23)$$

In the treatment of the periodic problem, we shall always deal with a periodic version of the r.d.f.'s :

$$\bar{f}^{(n)}_j(z_1;\ldots;z_n;t) = \sum_{j'\equiv j(\mathrm{mod}P+1)} f^{(n)}_{j'}(z_1;\ldots;z_n;t) \qquad (3.24)$$

j should now be regarded as an index modulo P+1. The initial conditions on $\bar{f}^{(1)}_j$, for example, are

$$\bar{f}^{(1)}_0(z_1;0) = \sum_{K=-\infty}^{+\infty} \delta(x_1-KL)\ \delta\ (v_1-v')$$

for $1 \leqslant j \leqslant P$ : $\bar{f}^{(1)}_j(z_1;0) = f^{(1)}_j(z_1)_L$ for $x_1 \ \varepsilon \ [0,L]$ and

$\bar{f}^{(1)}_j$ is extended periodically in $x_1$, outside this interval.

## 2.4 FACTORIZATION OF THE REDUCED DISTRIBUTION FUNCTIONS AT t = 0.

The situation for the periodic problem is not as simple as for the semi-infinite problem. Instead of an exact factorization (3.2) of initial conditions, we only obtain an approximate factorization (again of the form (3.2) ). In this section, we determine the error in this factorization approximation.

First we consider the factorization of the regular part of the r.d.f.'s. Since the functions considered are periodic in the variable $x_1$ of period L, we restrict $x_1$ here to [0,L]. The approximate factorization condition shall be accurate in the high density limit $\frac{1}{P} \to o$ and for $\bar{f}_j^{(n)}$ with $n = O(1)$. The result obtained depends primarily on the fact that for $\frac{1}{P} = \epsilon \ll 1$ and $n = O(1)$, the $\bar{f}_j^{(n)}$ are strongly localized with respect to $x_1$. Let $\bar{f}_j^{(n)s}$ denote the spatial part of $\bar{f}_j^{(n)}$ and set $\xi_i = \frac{x_i}{L}$. Then from (3.15) for $\Lambda_1 < j$, $\Lambda_2 < P-j+1$ and $o < \xi_i < 1$

$$\bar{f}_j^{(n)s}(x_1;\ldots;x_n;o) = \bar{f}_j^{(n)s}(\xi_{1max}^n;\xi_2;\ldots;\xi_n;o) \times \left(\frac{1-\xi_1}{1-\xi_{1max}^n}\right)^{P-j-\Lambda_2} \left(\frac{\xi_1}{\xi_{1max}^n}\right)^{j-1-\Lambda_1} \tag{4.1}$$

where $\xi_{1max}^n = \xi_{1max}^n(\Lambda_1,\Lambda_2,j)$ is the value of $\xi_1$ which maximizes $\bar{f}_j^{(n)s}$ for a given choice of $\Lambda_1,\Lambda_2$. The function of $\xi_1$ appearing in (4.1) has a sharp peak at $\xi_1 = \xi_{1max}^n$ where

$$\xi_{1max}^n = \frac{j-1-\Lambda_1}{P-\Lambda_1-\Lambda_2-1} = \frac{j-1-\Lambda_1}{P-n} \quad (\approx \frac{j}{P} \text{ for } n = O(1)) \tag{4.2}$$

as one would expect on physical grounds. Equivalently, setting $x_{1max}^n = L\xi_{1max}^n$,

$$\frac{P-j-\Lambda_2}{L-x_{1max}^n} = \frac{j-1-\Lambda_1}{x_{1max}^n} = \frac{P-\Lambda_1-\Lambda_2-1}{L} \approx \rho \text{ for } n = O(1) \tag{4.3}$$

An estimate of the width of this peak can be obtained (for both cases of stationary and non-stationary maxima) by determining the root(s) of the expression

$$\frac{d}{d\xi_1}\left[\left(\xi_1-\xi^n_{1max}\right)\left(\frac{1-\xi_1}{1-\xi^n_{1max}}\right)^{P-j-\Lambda_2}\left(\frac{\xi_1}{\xi^n_{1max}}\right)^{j-1-\Lambda_1}\right] = 0 \tag{4.4}$$

The root(s) of (4.4) satisfy the equation

$$(1-\xi_1)\ \xi_1 = (P-\Lambda_1-\Lambda_2-1)\ (\xi_1-\xi^n_{1max})^2 \tag{4.5}$$

from which we conclude that the root(s) satisfy

$$|\ \xi_1-\xi^n_{1max}| \leqslant E(n,j) \tag{4.6}$$

where for $j - \Lambda_1 \neq O(1)$, $P-j-\Lambda_2 \neq O(1)$

$$E(n,j) = O\left(\frac{\epsilon^{\frac{1}{2}}}{\sqrt{1-\frac{n}{P}}}\right) \quad \text{for } n < P \tag{4.7}$$

$$= O(1) \qquad \text{otherwise}$$

and for $j - \Lambda_1 = O(1)$ or $P-j-\Lambda_2 = O(1)$

$$E(n,j) = O\left(\frac{\epsilon}{1-\frac{n}{P}}\right) \quad \text{for } n < P \tag{4.8}$$

$$= O(1) \quad \text{otherwise}$$

This gives an estimate of the width of the peak.

Let us now derive an approximate factorization condition for the $\bar{f}^{(n)}_j$s. There are many different cases (ranges and orderings of spatial arguments) to be considered. First we make the restriction $o < x_j < L$ and consider the cases where the polynomial expression (4.1) is valid i.e. $\Lambda_1 < j$, $\Lambda_2 \leq P-j+1$ for $j \in \{1,2,\ldots,P\}$. Simple manipulation of (4.1) leads to the following results:

(i) $o < x_1 < x_n < \frac{L}{2}$ :

$$\bar{f}_j^{(n)s}(x_1;\ldots;x_n;o) = \bar{f}_j^{(n-1)s}(x_1;\ldots;x_{n-1};o)\cdot\frac{P-j-\Lambda_2+1}{L-x_1} \qquad (4.9)$$

For $P-j \neq O(1)$ and $n \leqslant \frac{P}{2}$ , $\bar{f}_j^{(n-1)s}$ has a sharp peak at

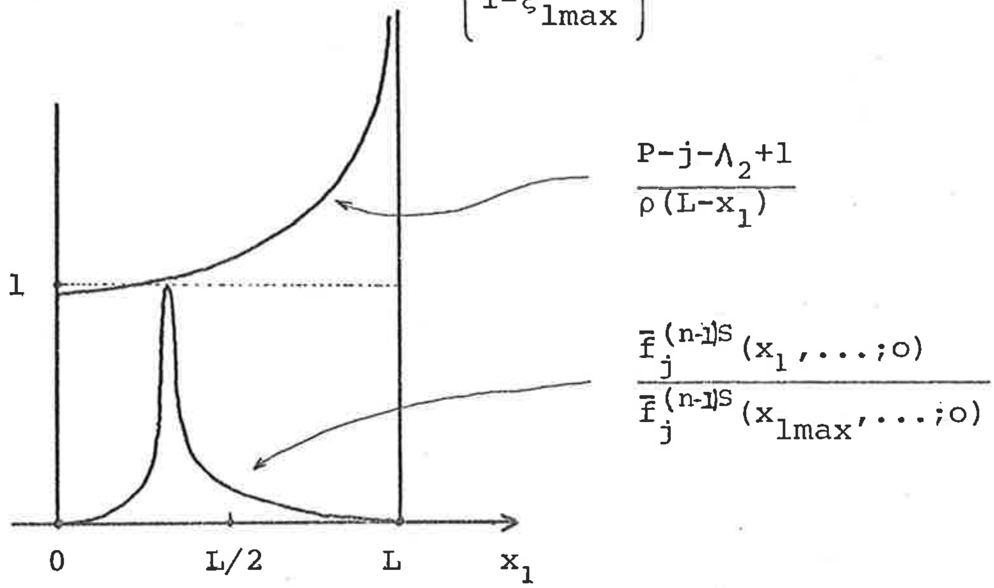
$$\xi_1 = \xi_{1max}^{n-1} = \frac{j-1-\Lambda_1}{P-n+1} \text{ for which } \frac{P-j-\Lambda_2+1}{L-x_{1max}^{n-1}} = \rho(1+O(n\epsilon))$$

Since $P-j-\Lambda_2 \neq O(1)$ so $L-x_{1max}^{n-1} = O(L)$, we expand $\frac{P-j-\Lambda_2+1}{L-x_1}$

about $x_1 = x_{1max}^{n-1}$ giving

$$\bar{f}_j^{(n)s}(x_1;\ldots;x_n;o) \approx \bar{f}_j^{(n-1)s}(x_1;\ldots;x_{n-1};o)\ \rho(1+O(n\epsilon)) \qquad (4.10)$$

$$+\ \bar{f}_j^{(n-1)s}(x_1;\ldots;x_{n-1};o)\left(\frac{\xi_1-\xi_{1max}^{n-1}}{1-\xi_{1max}^{n-1}}\right)\ \rho(1+O(n\epsilon))$$




The second expression on the r.h.s. of (4.10) has the same form as the function differentiated in (4.4). From the results of the analysis of (4.4) we conclude that, under the stated conditions,

$$\bar{f}_j^{(n)s}(x_1;\ldots;x_n;o) = \bar{f}_j^{(n-1)s}(x_1;\ldots;x_{n-1};o).\rho + \bar{f}_j^{(n-1)s}(x_{1max}^{n-1};\ldots;o)\ \rho\ E'(n,j) \tag{4.11}$$

where $E'(n,j) = (O(n\epsilon) + E(n,j))$ for $n < P$

$= O(1)$ otherwise.

For the case $P-j-\Lambda_2 = O(1)$, $n < \frac{P}{2}$, since $\xi_{1max}^{n-1} \approx 1$

$\bar{f}_j^{(n)s}$ and $\bar{f}_j^{(n-1)s}$ will be extremely small for $o < x_1 < \frac{L}{2}$.

Again (4.11) is valid (but for different reasons). For the other cases, the corresponding results are stated below.

(ii) $o < x_n < x_1 < \frac{L}{2}$ :

$$\bar{f}_j^{(n)s}(x_1;\ldots;x_n;o) = \bar{f}_{j-1}^{(n-1)s}(x_1;\ldots;x_{n-1};o)\ \frac{P-j-\Lambda_2+1}{L-x_1} \tag{4.12}$$

$$= \bar{f}_{j-1}^{(n-1)s}(x_1;\ldots;x_{n-1};o)\ \rho + \bar{f}_{j-1}^{(n-1)s}(x_{1max}^{n-1};\ldots;o)\ \rho\ E'(n,j)$$

(iii) $o < x_1 < \frac{L}{2} < x_n < L$ : (4.9) and (4.11) are again valid.

(iv) $\frac{L}{2} < x_n < x_1 < L$ :

$$\bar{f}_j^{(n)s}(x_1;\ldots;x_n;o) = \bar{f}_j^{(n-1)s}(x_1;\ldots;x_{n-1};o)\ .\ \frac{j-\Lambda_1}{x_1} \tag{4.13}$$

$$= \bar{f}_j^{(n-1)s}(x_1;\ldots;x_{n-1};o)\ \rho + \bar{f}_j^{(n-1)s}(x_{1max}^{n-1};\ldots;o)\ \rho\ E'(n,j)$$

(v) $\frac{L}{2} < x_1 < x_n < L$ :

$$\bar{f}_j^{(n)s}(x_1;\ldots;x_n;o) = \bar{f}_{j+1}^{(n-1)s}(x_1;\ldots;x_{n-1};o)\ \frac{j-\Lambda_1}{x_1} \tag{4.14}$$

$$= \bar{f}_{j+1}^{(n-1)s}(x_1;\ldots;x_{n-1};0)\ \rho + \bar{f}_{j+1}^{(n-1)s}(x_{1max}^{n-1};\ldots;o)\,\rho E'(n,j)$$

(vi) $o < x_n < \frac{L}{2} < x_1 < L$ : (4.13) is again valid .

Under the constraints mentioned, the above results may be summarized in the following form:

$$\bar{f}_j^{(n)s}(x_1;\ldots;x_n;o) = \bar{f}_{j*}^{(n-1)s}(x_1;\ldots;x_{n-1};o)\rho + \bar{f}_{j*}^{(n-1)s}(x_{1max}^{n-1};\ldots;o)\ \rho\ E'(n,j) \qquad (4.15)$$

where j* takes values $j, j\pm1$ as determined by (i)-(vi). For $\Lambda_1 \geq j$ or $\Lambda_2 \geq P-j+1$, $\bar{f}_j^{(n)s}$ is identically zero. If $n \lesssim \frac{P}{2}$, $\bar{f}_{j*}^{(n-1)s}$ is either identically zero or very small. Again (4.15) is valid.

We next extend our considerations to the case where $o < x_1 < L$ and $x_i$ for $i \neq 1$ may be in any of the open cells $(KL, (K+1)L)$. (3.22) and (3.23) may be used to determine the behaviour of the $\bar{f}_j^{(n)s}$. (4.15) is again valid with $j* = j$.

Finally, we shall obtain results with no restrictions on the arguments. In particular, this means that we must examine the delta-function dependence of the r.d.f.'s at t=o. As discussed in section 2.3, a suitable limit interpretation must be adopted for the evaluation of r.d.f.'s where there is delta-function behaviour. Suppose that $x_n \varepsilon (KL,(K+1)L)$ and so are $n_K-1$ other $x_i$. Then from (3.16)

$$\bar{f}_o^{(n)}(z_1;\ldots;z_n;o) = \bar{f}_o^{(n-1)}(z_1;\ldots;z_{n-1};o) \times \left[\frac{P-n_K+1}{P}\cdot\rho h_o(v_n) + \sum_{k=-\infty}^{+\infty}\delta(x_n-kL)\,\delta(v_n-v')\right] \qquad (4.16)$$

If $\bar{f}_o^{(n-1)}$ is replaced by $\bar{f}_{o*}^{(n-1)}$ in (4.16), a knowledge of the support and behaviour of $\bar{f}_{o*}^{(n-1)}$ shows that the errors introduced are extremely small and regular. (3.22) supplies the required information as to the delta-function behaviour of $\bar{f}_j^{(n)}$ for $j \not\equiv o \bmod (P+1)$.

Combining all the results of this section and choosing $x_1 \in [-\frac{L}{2},+\frac{L}{2}]$ gives

$$\begin{aligned} \bar{f}_j^{(n)} (z_1;\ldots;z_n;o) &= \bar{f}_{j*}^{(n-1)} (z_1;\ldots;z_{n-1};o) \\ &\times \left[ \rho h_o(v_n) + \sum_{k=-\infty}^{+\infty} \delta(x_n-kL)\,\delta(v_n-v') \right] \qquad (4.17) \\ &+ (1-\delta_{j*,o}^{P+1})\, \bar{f}_{j*}^{(n-1)} (x_{1max}^{n-1};\ldots;o)\ \rho\, h_o(v_n)\ E'(n,j) \\ &+ \delta_{j,o}^{P+1}\ \delta(x_1)\ \delta(v_1-v')\ \bar{f}^{(n-2)}(z_2;\ldots;z_{n-1};o)\,\rho h_o(v_n) \\ &\times \min\{O(1), O(n\epsilon)\} \end{aligned}$$

where now

$$\begin{aligned} j^* &= j-1 \text{ for } o < x_n - v_n t < x_1 - v_1 t < \tfrac{L}{2} \\ &= j+1 \text{ for } -\tfrac{L}{2} < x_1 - v_1 t < x_n - v_n t < o \\ &= j \quad \text{otherwise} \qquad (4.18) \end{aligned}$$

(t=o here)

and

$$\begin{aligned} \delta_{j,k}^{P+1} &= 1 \text{ if } j-k \equiv o \ (\text{mod } P+1) \\ &= o \text{ otherwise} \qquad (4.19) \end{aligned}$$

(4.17) for the periodic problem is the analogue of (3.2) for the semi-infinite problem. In fact (4.17) is not quite strong enough for the required analysis of the hierarchy equations. It is necessary to consider the factorization properties of the expressions $\bar{f}_{j\pm1}^{(n)} - \bar{f}_j^{(n)}$. The reason why (4.17) is inadequate here is that, for some j, the size of $\bar{f}_{j\pm1}^{(n)} - \bar{f}_j^{(n)}$

is comparable with the "error" terms in (4.17). This is the case for $j-\Lambda_1 \neq O(1)$, $P-j-\Lambda_2 \neq O(1)$, $n=O(1)$. The maximum of $\bar{f}^{(n)}_{j\pm1} - \bar{f}^{(n)}_j$ is of the order of $\bar{f}^{(n-1)}_j (x^{n-1}_{1max}, \ldots)\ O(\epsilon^{\frac{1}{2}})$.

We shall give an example of the analysis of this factorization condition for just one case and then state the general result. Consider $o < x_n < x_1 < \frac{L}{2}$, $o < x_i < L$ otherwise, $n=O(1)$

Simple manipulation of (4.1) shows that for

(i) $\Lambda_1 < j, \Lambda_2 < P-j$, $j \neq O(1)$, $P-j \neq O(1)$

$$\left(\bar{f}^{(n)s}_{j+1}(x_1;\ldots;x_n;o) - \bar{f}^{(n)s}_j(x_1;\ldots;x_n;o)\right) - \left(\bar{f}^{(n-1)s}_{j^*+1}(x_1;\ldots;x_{n-1};o) - \bar{f}^{(n-1)s}_{j^*}(x_1;\ldots;x_{n-1};o)\right)\rho$$

$$= -\bar{f}^{(n-1)s}_{j^*+1}(x_1;\ldots;x_{n-1};o)\frac{1}{L-x_1} + \bar{f}^{(n-1)s}_{j^*}(x_1;\ldots;x_{n-1};o)\frac{P-\Lambda_2-\Lambda_1-1}{(j^*-\Lambda_2)(P-j^*-1-\Lambda_2)}\left(x_1 - L\left(\frac{j^*-\Lambda_1}{P-\Lambda_1-\Lambda_2-1}\right)\right)\left(\frac{P-j-\Lambda_2}{L-x_1} - \rho\right) \tag{4.20}$$

The second term on the r.h.s. has the form

$$\bar{f}^{(n-1)s}_{j^*}(\xi^{n-1}_{1max};\ldots;o)\left(\frac{1-\xi_1}{1-\xi^{n-1}_{1max}}\right)^{P-j^*-\Lambda_2}\left(\frac{\xi_1}{\xi^{n-1}_{1max}}\right)^{j^*-\Lambda_1}(\xi_1-\xi^{n-1}_{1max})^2 \tag{4.21}$$

neglecting errors $O(\epsilon)\ \bar{f}^{(n-1)s}_{j^*}(\xi^{n-1}_{1max};\ldots;o)$ The maxima of (4.21) occur for $\xi_1$ satisfying

$$2(1-\xi_1)\xi_1 = (P-\Lambda_1-\Lambda_2)\ (\xi_1-\xi^{n-1}_{1max})^2 \tag{4.22}$$

from which we conclude that $|\xi_1-\xi^{n-1}_{1max}| \approx O(\epsilon^{\frac{1}{2}})$. So the r.h.s. of (4.20) has the order of magnitude

$$\bar{f}^{(n-1)s}_{j^*}(\xi^{n-1}_{1max};\ldots;o)\ \rho\ O(\epsilon).$$

ii) $j = O(1)$ or $P-j = O(1)$

Since $E'(n,j) = O(\epsilon)$ in this case, it suffices for our purposes to apply the factorization approximation (4.17) to $\bar{f}^{(n)s}_{j+1}$ and $\bar{f}^{(n)s}_{j}$ separately.

The general result is , for $x_1 \varepsilon [-\frac{L}{2}, +\frac{L}{2}]$ ,

$$\bar{f}^{(n)}_{j\pm1}(z_1;\ldots;z_n;o) - \bar{f}^{(n)}_{j}(z_1;\ldots;z_n;o) \quad (4.23)$$

$$= \bar{f}^{(n-1)}_{j*\pm1}(z_1;\ldots;z_{n-1};o) - \bar{f}^{(n-1)}_{j*}(z_1;\ldots;z_{n-1};o)$$

$$\times \left( \rho h_o(v_n) + \sum_{k=-\infty}^{+\infty} \delta(x_n-kL)\delta(v_n-v') \right)$$

$$+ \max_{k=-1,0,+1} (1 - \delta^{P+1}_{j*+k,o}) \bar{f}^{(n-1)}_{j*+k} (x^{n-1}_{1max},\ldots;o)\rho h_o(v_n)\underset{\sim}{E}(n,j)$$

$$+ (\delta^{P+1}_{j,o} + \delta^{P+1}_{j,\pm1}) \delta(x_1)\delta(v_1-v') \bar{f}^{(n-2)}(z_2;\ldots;z_{n-1};o)\rho h_o(v_n)$$

$$\times \min(O(1),O(n\epsilon))$$

where $j^*$ is given by (4.18) and

$$\underset{\sim}{E}(n,j) = O(n\epsilon) + O\left[\frac{\epsilon}{1-\frac{n}{P}}\right] \text{ for } n<P \quad (4.24)$$
$$= O(1) \quad \text{otherwise}$$

This is the result that shall be used in the analysis of the hierarchy equations.

## 2.5 EQUATIONS FOR THE ONE-PARTICLE REDUCED DISTRIBUTION FUNCTIONS.

For the sem-infinite problem, Anstis et al.[42] have used a factorization condition derived from (3.2) to obtain exact closed kinetic equations for the one-particle r.d.f.'s. These equations are

$$\left(\frac{\partial}{\partial t} + v_1 \frac{\partial}{\partial x_1}\right) f^{(1)}_{j}(z_1;t) = \gamma(x_1,v_1;t)\,[f^{(1)}_{j-1}(z_1;t) - f^{(1)}_{j}(z_1;t)]$$
$$+ \beta(x_1,v_1;t)\,[f^{(1)}_{j+1}(z_1;t) - f^{(1)}_{j}(z_1;t)] \quad (5.1)$$

except on the line $x_1 = v't$ where the $f_j^{(1)}$ are discontinuous and satisfy

$$\lim_{\xi \to o} f_j^{(1)}(v't-\xi, v_1; t) = \lim_{\xi \to o} f_{j+1}^{(1)}(v't+\xi, v_1; t) \qquad (5.2)$$

$$\text{and } \gamma(x_1; v_1; t) = \rho \int_{-\infty}^{x_1/t} dw\,(v_1-w)\,h_o(w)$$

$$(5.3)$$

$$\beta(x_1, v_1; t) = \rho \int_{x_1/t}^{+\infty} dw\,(w-v_1)\,h_o(w)$$

We shall now derive the corresponding equations for the periodic case. They contain an error term associated with the error in factorization of the r.d.f.'s at t = o. In the next section a rigorous determination shall be made of an upper bound on this error term.

The equations for $\bar{f}_j^{(n)}$ are obtained from (2.19) by summing over equal j (mod P+1). They are identical to (2.19) :

$$\left(\frac{\partial}{\partial t} + K_j^{(n)}\right) \bar{f}_j^{(n)}(z_1; \ldots; z_n; t) \qquad (5.4)$$

$$= \lim_{\epsilon \to o} \int dv_{n+1} |v_{n+1}-v_1| \times \left(\bar{f}_{(j)}^{(n+1)}(z_1; x_1^-, v_{n+1}; z_2; \ldots; z_n; t)\right.$$

$$\left. - \bar{f}_j^{(n+1)}(z_1; x_1^-, v_{n+1}; z_2; \ldots; z_n; t)\right)$$

It is convenient to define a new hierarchy of functions to describe the error in factorization. These are defined for $n \geqslant 2$ by

$$\bar{g}_j^{(n)}(z_1; \ldots; z_n; t) \qquad (5.5)$$

$$= \bar{f}_j^{(n)}(z_1; \ldots; z_n; t) - \bar{f}_{j*}^{(n-1)}(z_1; \ldots; z_{n-1}; t)\,\left(\rho h_o(v_n) + \sum_{k=-\infty}^{+\infty} \delta(x_n - v_n t - kL)\,\delta(v_n - v_n')\right)$$

adopting a suitable limit procedure at points $x_i - v_i t = kL$ and where j* is given by (4.18). We now confine our attention to precollision regions of phase space. These regions, at time t denoted $R_p^t$, consist of those points $(z_1, z_2, \ldots z_n, t)$ such that the particle at $z_1$ at time t has not interacted with the particles at $z_2, \ldots, z_n$ at time t under n-particle dynamics in the time interval (o,t). In these regions $\bar{g}_j^{(n)}$ satisfy the same set of equations as $\bar{f}_j^{(n)}$ and $\frac{\partial}{\partial t} + K_j^{(n)}$ reduces to $\frac{\partial}{\partial t} + \sum_{i=1}^{n} v_i \frac{\partial}{\partial x_i}$. These equations may be integrated

along the characteristics of $\frac{\partial}{\partial t} + \sum_{i=1}^{n} v_i \frac{\partial}{\partial x_i}$ in regions $\bigcup_{o \leq t \leq \tau} (R_p^t, t)$ for any $\tau > o$. From (4.23), $\bar{g}_j^{(n)}$ is regular in the variable $z_n$ at $t = o$. From the hierarchy equations, it easily follows that $\bar{g}_j^{(n)}$ is regular in $z_n$ for all points in precollision regions of phase space. In particular $\bar{g}_j^{(2)}(z_1; x_1^-, v_2; t)$ is

regular in the variables $x_1^-$ and $v_2$ for all times.

To obtain equations for the $\bar{f}_j^{(1)}$, we substitute (5.5) for n = 2 into (5.4) for n = 1. After determining values of (j) and j* for $v_2$ in the appropriate ranges, this equation becomes, for $-\frac{L}{2} < x_1 - v_1 t < +\frac{L}{2}$,

$$
\begin{aligned}
\left(\frac{\partial}{\partial t} + v_1 \frac{\partial}{\partial x_1}\right) \bar{f}_j^{(1)}(z_1;t) &= \gamma(x_1, v_1; t) \cdot \left\{ \bar{f}_{j-1}^{(1)}(z_1;t) - \bar{f}_j^{(1)}(z_1;t) \right\} \\
&+ \beta(x_1, v_1; t) \cdot \left\{ \bar{f}_{j+1}^{(1)}(z_1;t) - \bar{f}_j^{(1)}(z_1;t) \right\} \\
&+ \lim_{\xi \to o} \sum_{k=-\infty}^{+\infty} \delta(x_1^{=} - v' t - kL) \left[ \begin{array}{c} H(v'-v_1)(v'-v_1) \left\{ \bar{f}_{j+1}^{(1)}(z_1;t) - \bar{f}_j^{(1)}(z_1;t) \right\} \\ + \\ H(v_1-v')(v_1-v') \left\{ \bar{f}_{j-1}^{(1)}(z_1;t) - \bar{f}_j^{(1)}(z_1;t) \right\} \end{array} \right] \\
&+ \lim_{\epsilon \to o} \int_{-\infty}^{+\infty} dv_2 |v_2 - v_1| \left\{ \bar{g}_{(j)}^{(2)}(z_1; x_1^-, v_2; t) - \bar{g}_j^{(2)}(z_1; x_1^-, v_2; t) \right\}
\end{aligned}
\qquad (5.6)
$$

where $x_1^{=} = x_1 - \xi \operatorname{sgn}(v'-v_1)$ and $\gamma(\ )$, $\beta(\ )$ are defined in (5.3). Because of the term explicitly exhibiting the delta-function on the r.h.s. of (5.6), the $\bar{f}_j^{(1)}$ are discontinuous across the lines $x_1 = v't + kL$. Integrating along a small segment of the characteristic crossing these lines and noting that the last term in (5.6) is regular in $x_1^-$ yields the jump conditions

$$\lim_{\xi\to o} \bar{f}_j^{(1)} (v't + kL - \xi, v_1; t) = \lim_{\xi\to o} f_{j+1}^{(1)} (v't + kL + \xi, v_1; t) \qquad (5.7)$$

These conditions are expected since the particle on the above-mentioned segment of the characteristic must always undergo a collision with another particle at the point where the characteristic crosses the line $x_1 = v't + kL$. So (5.6) becomes

$$\left(\frac{\partial}{\partial t} + v_1 \frac{\partial}{\partial x_1}\right) \bar{f}_j^{(1)}(z_1;t) = \bar{\gamma}(x_1,v_1;t) \cdot \left[\bar{f}_{j-1}^{(1)}(z_1;t) - \bar{f}_j^{(1)}(z_1;t)\right]$$

$$+ \bar{\beta}(x_1,v_1;t) \cdot \left[\bar{f}_{j+1}^{(1)}(z_1;t) - \bar{f}_j^{(1)}(z_1;t)\right]$$

$$+ \bar{\zeta}_j(z_1;t) \qquad (5.8)$$

except on the lines $x_1 = v't + kL$ where (5.7) must be applied. $\bar{\gamma}$ ($\bar{\beta}$) is the periodic extension of $\gamma$ ($\beta$) outside the interval $x_1 \in [-\frac{L}{2}+v_1t, +\frac{L}{2}+v_1t]$ and

$$\bar{\zeta}_j(z_1;t) = \lim_{\epsilon\to o} \int_{-\infty}^{+\infty} dv_2 (v_2-v_1) \cdot \left[\bar{g}_{(j)}^{(2)}(z_1;x_1^-,v_2;t) - \bar{g}_j^{(2)}(z_1;x_1^-,v_2;t)\right] \qquad (5.9)$$

We obtain approximate kinetic equations for $\bar{f}_j^{(1)}$ by neglecting this term in (5.8). Although $\bar{\gamma}$ and $\bar{\beta}$ are discontinuous at points $x_1 - v_1t = kL$, we indicate why the r.h.s. of the approximate equations only has a discontinuity

$$O(\epsilon) \max_{k=-1,o,+1} (1-\delta^{P+1}_{j+k,o}) \; \bar{f}^{(1)}_{j+k} \; (x^1_{1max}, v_1; o) \; \max_{\pm} \bar{\beta} \; (\pm\frac{L}{2}+v_1 t, v_1; t) \tag{5.10}$$

To see this, the r.h.s. is rewritten as

$$\rho v_1 \left[\bar{f}^{(1)}_{j-1} - \bar{f}^{(1)}_{j}\right] + \bar{\beta}\left[\bar{f}^{(1)}_{j+1} + \bar{f}^{(1)}_{j-1} - 2\,\bar{f}^{(1)}_{j}\right] \tag{5.11}$$

The first term in (5.11) is continuous and it is possible to show that the second term produces the $O(\epsilon)$ factor in (5.10).

In the analysis of (5.8), we first convert these equations to a set of ordinary differential equations, by introducing a parameter "s" along the characteristics $\{(x_1,t) : x_1 = v_1 s + x_{1,0},\ t = s, s \in R\}$ of $\frac{\partial}{\partial t} + v_1 \frac{\partial}{\partial x_1}$. Then $\frac{\partial}{\partial t} + v_1 \frac{\partial}{\partial x_1} = \frac{d}{ds}$ in (5.8) and functions of $(x_1, v_1; t)$ are regarded as functions of $(x_{1,o}, v_1, s)$. (5.8) may also be expressed in matrix form so that the jump conditions (5.7) are automatically accounted for. Define regions $E_K$ of the $(x_1,t)$ plane as follows :

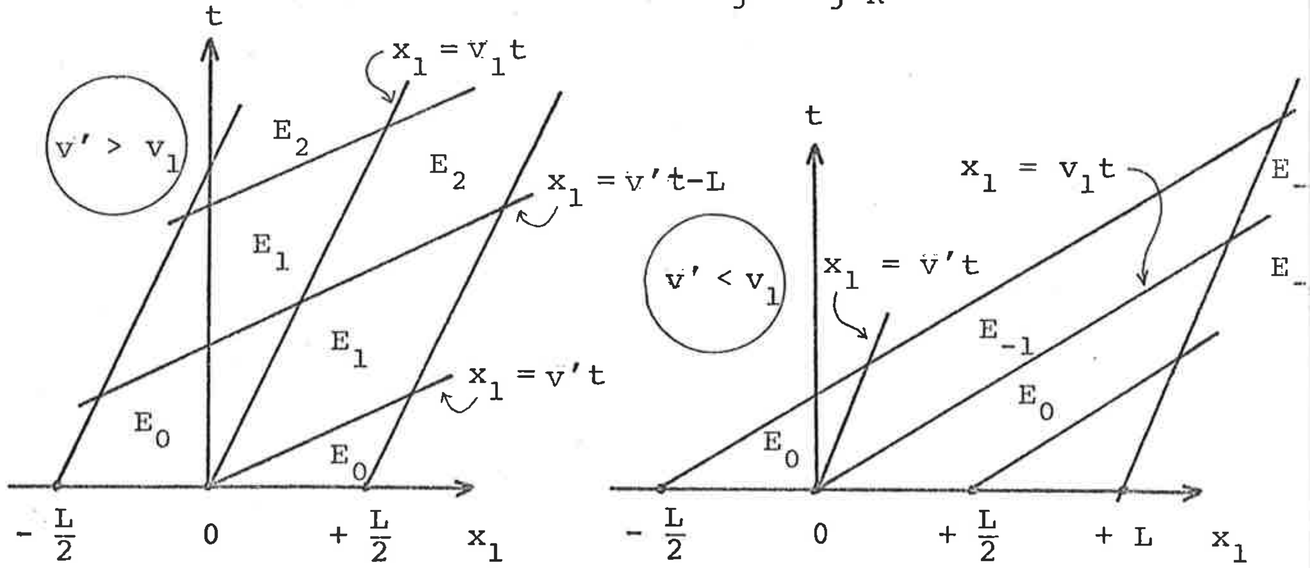
$$E_K = \{(x_1,t) : o < x_1 - v_1 t < \frac{L}{2} \text{ and } v' t - KL < x_1 < v' t - (K-1)L\}$$

$$\dot{U}\ \{(x_1,t) : -\frac{L}{2} < x_1 - v_1 t < o \text{ and } v' t - (K+1)L < x_1 < v' t - KL\} \tag{5.12}$$

For $-\frac{L}{2} < x_1 - v_1 t = x_{1,0} < \frac{L}{2}$, the "P+1" dimensional column vectors $\underset{\sim}{\bar{f}}^{(1)}$ and $\underset{\sim}{\bar{\zeta}}$ are defined by

$$\underset{\sim}{\bar{f}}^{(1)}(x_{1,0}, V_1; s) = \begin{bmatrix} \bar{f}^{(1)}_{0-K} \\ \bar{f}^{(1)}_{1-K} \\ \vdots \\ \bar{f}^{(1)}_{P-K} \end{bmatrix} \quad \text{and} \quad \underset{\sim}{\bar{\zeta}}(x_{1,0}, v_1; s) = \begin{bmatrix} \bar{\zeta}_{0-K} \\ \bar{\zeta}_{1-K} \\ \vdots \\ \bar{\zeta}_{P-K} \end{bmatrix} \tag{5.13}$$

for $(x_1,t) \varepsilon E_K$ (choosing $K = 0$ for $x_{1,0} = 0$) i.e. if $\left(\bar{\underset{\approx}{f}}^{(1)}\right)_j$ the $j^{th}$ component of $\bar{\underset{\approx}{f}}^{(1)}$, then $\left(\bar{\underset{\approx}{f}}^{(1)}\right)_j = \bar{f}^{(1)}_{j-K}$.




Using this notation, (5.7) and (5.8) become

$$\frac{d}{ds} \bar{\underset{\approx}{f}}^{(1)}(x_{1,0},v_1;s) = \underset{\approx}{C}^P(x_{1,0},v;s) \cdot \bar{\underset{\approx}{f}}^{(1)}(x_{1,0},v_1;s) + \bar{\underset{\approx}{\zeta}}(x_{1,0},v_1;s) \quad (5.14)$$

where $\underset{\approx}{C}^P$ is a $(P+1)\times(P+1)$ matrix with entries

$$C^P_{i\,j} = \bar{\beta}\ \delta^{P+1}_{j-1,i} + \bar{\gamma}\ \delta^{P+1}_{j+1,i} - (\bar{\gamma}+\bar{\beta})\ \delta^{P+1}_{i,j} \quad (5.15)$$

To solve (5.14), we need the propagator $\underset{\approx}{U}^P$ associated with $\underset{\approx}{C}^P$. $\underset{\approx}{U}^P$ satisfies the equation

$$\frac{d}{ds} \underset{\approx}{U}^P(x_{1,0},v_1;s) = \underset{\approx}{C}^P(x_{1,0},v_1;s) \cdot \underset{\approx}{U}^P(x_{1,0},v_1;s) \quad (5.16)$$

where $\underset{\approx}{U}^P(x_{1,0},v_1;0) = \underset{\approx}{I}$ (the identity matrix)

Using the commutation property (verified by direct calculation)

$$[\underset{\approx}{C}^P(s), \underset{\approx}{C}^P(s')]_- = o \text{ for all } s,s' \geqslant o \quad (5.17)$$

and the Baker-Campbell-Hausdorff theorem, it follows that

$$\underset{\approx}{U}^P(x_{1,0},v_1;s) = \exp\left(\int_o^s ds' \underset{\approx}{C}^P(x_{1,0},v_1;s')\right) \quad (5.18)$$

Now $\int_0^s ds' \underset{\approx}{C}^P(s') = \bar{\gamma}_{av}(s)\ \underset{\approx}{\Delta}^- + \bar{\beta}_{av}(s)\underset{\approx}{\Delta}^+ - (\bar{\gamma}_{av}+\bar{\beta}_{av})\ \underset{\approx}{I}$

where $\Delta^-_{ij} = \delta^{P+1}_{j+1,i}$, $\Delta^+_{ij} = \delta^{P+1}_{j-1,i}$, $\bar{\gamma}_{av}(s) = \int_0^s ds' \bar{\gamma}(s')$

and $\bar{\beta}_{av}(s) = \int_0^s ds'\ \bar{\beta}(s')$. Since $\underset{\approx}{\Delta}^-$ and $\underset{\approx}{\Delta}^+$ commute and have non-degenerate eigenvalues, simultaneous eigenvectors may be constructed for these matrices (see Ziock[51]), for example $\{\underset{\sim}{e}^n : n = 0,\ldots,P\}$ where $e^n_j = (P+1)^{-\frac{1}{2}}\ \exp\left(\frac{2\pi \hat{i} nj}{P+1}\right)$

The corresponding eigenvalues of $\int_0^s ds' \underset{\approx}{C}^P(s')$ are given by

$$\lambda_n\ (x_{1,0},v_1;s) = (\bar{\gamma}_{av}+\bar{\beta}_{av})\left(\cos\left(\frac{2\pi n}{P+1}\right) - 1\right) + \hat{i}\ (\bar{\gamma}_{av}-\bar{\beta}_{av})\ \sin\left(\frac{2\pi n}{P+1}\right) \qquad (5.19)$$

and the projection operator corresponding to the $n^{th}$ eigenspace by $\underset{\approx}{E}^n = (\underset{\sim}{e}^n)(\underset{\sim}{e}^n)^H$ where $(\ )^H$ is the Hermitian transpose. The following spectral representation applies (see Dunford and Schwartz[52])

$$\underset{\approx}{U}^P(x_{1,0},v_1;s) = \sum_{n=o}^{P} \exp\ \left(\lambda_n(x_{1,0},v_1,s)\right)\ \underset{\approx}{E}^n \qquad (5.20)$$

(5.14) has the solution

$$\bar{\underset{\sim}{f}}^{(1)}(x_{1,0},v_1;s) = \underset{\approx}{U}^P(x_{1,0},v_1;s).\bar{\underset{\sim}{f}}^{(1)}(x_{1,0},v_1;0) \qquad (5.21)$$

$$+ \int_0^s ds'\ \ \underset{\approx}{U}^P(x_{1,0},v_1;s-s')\ .\ \bar{\underset{\approx}{\zeta}}(x_{1,0},v_1;s')$$

$\bar{\underset{\sim}{f}}^{(1)}$ and $\bar{\underset{\approx}{\zeta}}$ may be decomposed into delta- and regular function components as follows. For $-\frac{L}{2} \leqslant x_1-v_1t = x_{1,0} \leqslant +\frac{L}{2}$

$$\bar{\underset{\sim}{f}}^{(1)}(x_{1,0},v_1;s) = \delta(x_{1,0})\delta(v_1-v')\ \bar{\underset{\sim}{f}}^{(1)\delta}(v';s) + \bar{\underset{\sim}{f}}^{(1)}_{reg}(x_{1,0},v_1;s)$$

$$(5.22)$$

$$\bar{\underset{\approx}{\zeta}}(x_{1,0},v;s) = \delta(x_{1,0})\delta(v_1-v')\ \bar{\underset{\approx}{\zeta}}^{\delta}(v';s) + \bar{\underset{\approx}{\zeta}}^{\delta}_{reg}(x_{1,0},v_1;s)$$

$\bar{\underset{\sim}{f}}^{(1)\delta}$ and $\bar{\underset{\sim}{f}}^{(1)}_{reg}$ satisfy closed equations which may be obtained by substitution of (5.22) into (5.21).

We must now ask under what conditions can the second term in (5.21) be neglected. We will require its components to be small compared with those of $(\underset{\approx}{U}^P(x_{1,0},v_1;s) - \underset{\approx}{I})\underset{\sim}{\bar{f}}^{(1)}(s=0)$

and $\underset{\approx}{U}^P(x_{1,0};v_1;s)\ \underset{\sim}{\bar{f}}^{(1)}(s=o) - \underset{\sim}{\bar{f}}^{(1)}(s=\infty)$. To facilitate this analysis, norms are introduced appropriate to the delta- and regular function parts of $\underset{\sim}{\bar{f}}^{(1)}$. The choice of these norms is motivated by the nature of the error term $\bar{\zeta}$ at s=0. From (4.23)

$$\bar{\zeta}^{\delta}_j(s=0) = (\delta^{P+1}_{j,o} + \delta^{P+1}_{j,-1})\ \rho\ \left(\int_{v'}^{+\infty} dw(w-v')h_o(w)\right)\ O(\in)$$

$$+ (\delta^{P+1}_{j,o} + \delta^{P+1}_{j,+1})\ \rho\ \left(\int_{-\infty}^{v'} dw(v'-w)h_o(w)\right)\ O(\in) \qquad (5.23)$$

For the delta-function part of $\underset{\sim}{\bar{f}}^{(1)}$, an appropriate norm is

$$\|\underset{\sim}{\bar{f}}^{(1)\delta}\|_\delta = \sum_{i=o}^{P} |\bar{f}_i^{(1)\delta}| \qquad (5.24)$$

Also from (4.23)

$$\bar{\zeta}_{regj}(s=o) = \max_{k=-1,o,+1} (1-\delta^P_{j+k,o})\ \bar{f}^{(1)}_{j+k}(x^1_{1max},v_1;o)\ \rho\ \alpha(v_1)\ O(\in) \qquad (5.25)$$

where $\alpha(v) = \int_{-\infty}^{+\infty} dw\ |w-v|\ h_o(w)$. So an analysis of the dependence of $\bar{f}^{(1)}_j(x^1_{1max},v_1;o)$ on j is appropriate. From (3.8) and Stirling's formula, for k = O(1) and large P

$$\bar{f}^{(1)s}_{P+1-k}(x^1_{1max};o) = \bar{f}^{(1)s}_k(x^1_{1\ max};o) \sim \bar{f}^{(1)s}_1(x^1_{1max};o)\ (2\Pi)^{-\frac{1}{2}} e^1 (1-\tfrac{1}{k})^k \tfrac{k^{\frac{1}{2}}}{k-1}$$

and $\bar{f}^{(1)s}_{\frac{P}{2}}(x^1_{1max};o) \sim \bar{f}^{(1)s}_1(x^1_{1max};o)\ (2\Pi)^{\frac{1}{2}} e^{-1} \in^{\frac{1}{2}}$ for large P. (5.26)

This type of behaviour is expected since the width of the peak of $\bar{f}^{(1)s}_j$ for $j \approx \frac{P}{2}$ is $O(\in^{\frac{1}{2}})$ compared with a width $O(\in)$ for j or P-j = O(1) and each of the $\bar{f}_j^{(1)}$s are normalized to one. This appreciable variation in $\bar{f}_j^{(1)}$s$(x^1_{1max}, v_1; o)$ is incorporated in the choice of norm for the regular part of $\bar{\underset{\sim}{f}}^{(1)}$. Let $\bar{\underset{\sim}{h}}_{reg}(x_{1,0}, v_1; s)$ be a "P+1"-dimensional vector valued function, periodic in $x_{1,0}$ of period L and continuous except possibly at $x_{1,0} = kL$. Define

$$||\bar{\underset{\sim}{h}}reg(\text{——}; s)||_{reg} = \max_{o \leq j \leq P} \quad \underset{-\frac{L}{2} \leq x_{1,0} \leq +\frac{L}{2}}{\text{ess sup}} \left| \frac{(\bar{\underset{\sim}{h}}reg)_j(x_{1,0}, v_1; s)}{\bar{f}^{(1)}_{j+\delta j}(x^1_{1max}, v_1; o)} \right| \qquad (5.27)$$

where $(\bar{\underset{\sim}{h}}reg)_j$ is the $j^{th}$ component of the column vector $\bar{\underset{\sim}{h}}_{reg}$

and $$\bar{f}^{(1)}_{j+\delta j}(x^1_{1max}, v_1; 0) = \max_{|k| \leq \delta j} (1 - \delta^{P+1}_{j+k,o}) \; \bar{f}^{(1)}_{j+k} \; (x^1_{1max}, v_1; o) \qquad (5.28)$$

So from (5.25) $$||\bar{\underset{\sim}{\zeta}}reg(s=o)||_{reg} = \rho\alpha(v_1) \; O(\in) \qquad (5.29)$$

In sections 2.6/7 an upper bound is obtained on $\bar{\underset{\sim}{\zeta}}^{\delta}$ and $\bar{\underset{\sim}{\zeta}}reg(s)$ for $s \geq o$ in terms of the appropriate norms.

## 2.6 ANALYSIS OF THE HIERARCHY EQUATIONS FOR $\bar{g}_j^{(n)}$.

It is possible to show that the r.d.f.'s $\bar{f}_j^{(n)}(z_1; \ldots; z_n; t)$ (or $\bar{g}_j^{(n)}$) may be completely determined by another hierarchy of functions regular in all variables except possibly $z_1$. This reduction is a consequence of the following property. If for $i\alpha \in \{2,3,\ldots,m\}$, $\alpha = 1,\ldots,K$ $x_{i\alpha} - v_{i\alpha}t = k_\alpha L (k_\alpha \neq k_\beta; \alpha \neq \beta)$ and $v_{i\alpha} = v'$, then

$$\bar{f}_j^{(m)}(z_1; \ldots; z_m; t) = \bar{f}_j^{(m-K)}(z_1; \ldots; \hat{z}_{i1}; \ldots; \hat{z}_{iK}; \ldots; z_m; t) \prod_{\alpha=1}^{K} \delta(z_{i\alpha} - Z^{k\alpha}(t)) \qquad (6.1)$$

where $$Z^{k\alpha}(t) = (k_\alpha L + v't, v') \text{ and } \delta(z_{i\alpha} - Z^{k\alpha}(t)) = \delta(x_{i\alpha} - v't - k_\alpha L)\,\delta(v_\alpha - v') \qquad (6.2)$$

Using (6.1) and the regularity of $\bar{g}_j^{(n)}(z_1;\ldots;z_n;t)$ in the variable $z_n$, we make the decomposition

$$\bar{g}_j^{(n)}(z_1;\ldots;z_n;t)$$

$$= \sum_{q=o}^{n-2} \sum_{\substack{k\alpha \,\varepsilon\, \{2,\ldots,n-1\}\ \alpha = 1,\ldots,q \\ k\alpha < k\beta \text{ for } \alpha < \beta}} \bar{g}^{(n-q)}_{regl'j} (z_1;\ldots;\hat{z}_{k1};\ldots;\hat{z}_{kq};\ldots;z_n;t)$$

$$\times \prod_{\alpha=1}^{q} \left[ \sum_{k=-\infty}^{+\infty} \delta(z_{k\alpha}-Z^k(t)) \right] \qquad (6.3)$$

where a suitable limit procedure must be adopted for points where there is delta-function or discontinuous behaviour. $\bar{g}^{(m)}_{regl'_j}$ is regular in all variables except possibly $z_1$. If we substitute (6.3) into the equations satisfied by $\bar{g}_j^{(m)}$ in precollision regions and equate coefficients of

$\prod_{\alpha=1}^{q} \left[ \sum_{k=-\infty}^{+\infty} \delta(z_{k\alpha}-Z^k(t)) \right]$, we obtain

$$\left( \frac{\partial}{\partial t} + \sum_{i=1}^{m} v_i \frac{\partial}{\partial x_i} \right) \bar{g}^{(m)}_{regl'j} (z_1;\ldots;z_m;t)$$

$$= \lim_{\epsilon \to o} \int_{-\infty}^{+\infty} dv_{m+1} |v_{m+1}-v_1| \cdot \left( \bar{g}^{(m+1)}_{regl'_{(j)}} (z_1;x_1^-,v_{m+1};z_2;\ldots;z_m;t) - \bar{g}^{(m+1)}_{regl'_j} (z_1;x_1^-,v_{m+1};z_2;\ldots;z_m;t) \right)$$

$$+ \lim_{\xi \to o} \sum_{k=-\infty}^{+\infty} \delta(x_1^{=}-v't + kL) \times$$

$$\left[ \begin{array}{c} H(v'-v_1)(v'-v_1)\ [\bar{g}^{(m)}_{regl'_{j+1}} (z_1;\ldots;z_m;t) - \bar{g}^{(m)}_{regl'_j} (z_1;\ldots;z_m;t)] \\ + \\ H(v_1-v')(v_1-v')\ [\bar{g}^{(m)}_{regl'_{j-1}} (z_1;\ldots;z_m;t) - \bar{g}^{(m)}_{regl'_j} (z_1;\ldots;z_m;t)] \end{array} \right] \qquad (6.4)$$

where $x_1^- = x_1 - \epsilon \operatorname{sgn}(v_{m+1}-v_1)$ and $x_1^{=} = x_1 - \xi \operatorname{sgn}(v'-v_1)$.

By comparison with (5.6), the last term on the r.h.s. of (6.4) may be replaced by a jump condition of the form

$$\lim_{\xi\to o} \bar{g}^{(m)}_{regl'_j}(v't + kL - \xi,\ v_1;z_2;\ldots;z_m;t)$$

$$= \lim_{\xi\to o} \bar{g}^{(m)}_{regl'_{j+1}}(v't + kL + \xi, v_1;z_2;\ldots;z_m;t) \qquad (6.5)$$

across the lines $x_1 = v't + kL$. It is clear that it suffices to determine just the $\bar{g}^{(m)}_{regl'_j}$. In fact $\bar{g}^{(2)}_{regl'_j} = \bar{g}^{(2)}_j$.

To exhibit explicitly the delta-function dependence, we make the further decomposition, for $x_1 - v_1t \ \varepsilon\ [-\frac{L}{2} + \frac{L}{2}]$.

$$\bar{g}^{(m)}_{regl'_j}(z_1;\ldots;z_m;t) = \delta(x_1-v_1t)\,\delta(v_1-v')\ \bar{g}^{(m)\,\delta}_j(v';z_2;\ldots;z_m;t)$$

$$+ \bar{g}^{(m)}_{reg_j}(z_1;\ldots;z_m;t) \qquad (6.6)$$

As indicated in section 2.5, we are primarily interested in expressions of the form

$$\bar{G}^{(n)}_{regl'_j} = \bar{g}^{(n)}_{regl'_{j+1}} - \bar{g}^{(n)}_{regl'_j} \qquad (6.7)$$

If $\bar{G}^{(n)}_{regl'_j}$ is decomposed into components $\bar{G}^{(n)\,\delta}_j$ and $\bar{G}^{(n)}_{reg_j}$ (c.f. (6.6)), then these satisfy the equations (in precollision regions)

$$\left(\frac{\partial}{\partial t} + \sum_{i=1}^{n} v_i\frac{\partial}{\partial x_i}\right)\bar{G}^{(n)\,\delta}_j(v';z_2;\ldots;z_n;t)$$

$$= \lim_{\varepsilon\to o} \int_{-\infty}^{+\infty} dv_{n+1}\ |v_{n+1}-v'| \times \Big( \bar{G}^{(n+1)\delta}_{(j)}(v';(v't)^-,v_{n+1};z_2;\ldots;z_n;t)$$

$$- \bar{G}^{(n+1)\delta}_j(v';(v't)^-,v_{n+1};z_2;\ldots;z_n;t)\Big) \qquad (6.8)$$

with no jump condition and

$$\left(\frac{\partial}{\partial t} + \sum_{i=2}^{n} v_i \frac{\partial}{\partial x_i}\right) \bar{G}^{(n)}_{reg_j} (z_1;\ldots;z_n;t) \tag{6.9}$$

$$= \lim_{\epsilon \to o} \int_{-\infty}^{+\infty} dv_{n+1} |v_{n+1} - v_1| \times \left[\bar{G}^{(n+1)}_{reg_{(j)}} (z_1;x_1^-,v_{n+1};z_2;\ldots;z_n;t) - \bar{G}^{(n+1)}_{reg_j} (z_1;x_1^-,v_{n+1};z_2;\ldots;z_n;t)\right]$$

except on $x_1 = v't + kL$ where

$$\lim_{\xi \to o} \bar{G}^{(n)}_{reg_j} (v't + kL - \xi, v_1;z_2;\ldots;z_n;t) = \lim_{\xi \to o} \bar{G}^{(n)}_{reg_{j+1}} (v't + kL + \xi, v_1;z_2;\ldots;z_n t) \tag{6.10}$$

Let $\bar{G}_j^{(n)\delta ext} \left(\bar{G}^{(n)ext}_{reg_j}\right)$ have the same initial conditions as $\bar{G}_j^{(n)\delta} \left(\bar{G}^{(n)}_{reg_j}\right)$ and satisfy the corresponding hierarchy equations throughout the entire phase space. Since these functions must agree on precollision regions of phase space, we solve for the extended functions and then apply the results to precollision regions.

As we shall be working in an abstract vector space formulation, the governing equations are rewritten in a suggestive vector from which automatically accounts for the jump conditions (6.10). For $-\frac{L}{2} < x_1 - v_1 t = x_{1,0} < +\frac{L}{2}$ , the "P+1" dimensional column vector $\underset{\sim}{\bar{G}}{}^{(n)\ ext}_{regl}$ is defined by

(c.f. 5.13)

$$\underset{\sim}{\bar{G}}^{(n)ext}_{regl'} = \begin{pmatrix} \bar{G}^{(n)ext}_{regl'}{}_{O-K} \\ \vdots \\ G_{regl'}{}_{P-K} \end{pmatrix} \quad \text{for } (x_1,t) \in E_K \tag{6.11}$$

An infinite dimensional vector is constructed from the $\underset{\sim}{\bar{G}}^{(n)ext}_{regl'}$ by setting

$$\underset{\sim}{\bar{G}}^{ext}_{regl'} = \begin{pmatrix} \bar{G}^{(2)ext}_{regl'} \\ \bar{G}^{(3)ext}_{regl'} \\ \vdots \end{pmatrix} \tag{6.12}$$

where $\underset{\sim}{\bar{G}}^{ext}_{regl'} = \underset{\sim}{\bar{G}}^{\,ext}\delta(x_1-v_1t)\delta(v_1-v') + \underset{\sim}{\bar{G}}^{ext}_{reg}$ for $-\frac{L}{2}<x_1-v_1t<+\frac{L}{2}$

Evolution Equation for $\underset{\sim}{\bar{G}}^{\delta ext}$ : The time evolution equations have the form of a partial differential operator equation, formally

$$\left(\frac{\partial}{\partial t} + \sum_i v_i \frac{\partial}{\partial x_i}\right)\cdot\underset{\sim}{\bar{G}}^{\delta ext}(z_i;t) = \underset{\approx}{C}\cdot\underset{\sim}{\bar{G}}^{\delta ext}(z_i;t) \tag{6.13}$$

where the structure of $\underset{\approx}{C}$ is obtained from (6.8). In the natural presentation, $\underset{\approx}{C}$ is an off-diagonal matrix with entries $C_{ij} = \delta_{i,j-1}\, C_{ij}$ , $i,j \geq 2$ where the $C_{ij}$ are themselves $(P+1) \times (P+1)$ matrices whose entries are integral operators. To convert (6.13) to an ordinary differential operator equation, we introduce a parameter "s" along the characteristics $\{(x_i,t) : x_i = v_i s + x_{i,o},\ t = s\}$ of the partial differential operator $\frac{\partial}{\partial t} + \sum_i v_i \frac{\partial}{\partial x_i}$ . (6.13) becomes

$$\frac{d}{ds}\ \bar{\underset{\sim}{G}}^{\delta ext}(x_{i,o},v_i;s) = \underset{\approx}{C}(x_{i,o},v_i;v';s)\ \bar{\underset{\approx}{G}}^{\delta ext}(x_{i,o},v_i;s) \tag{6.14}$$

The norm for the space of vectors $\bar{\underset{\sim}{G}}^{\delta ext}$ is constructed so as to be compatible with that chosen for $\bar{\underset{\approx}{\zeta}}^{\delta}$ and $\bar{\underset{\sim}{f}}^{(1)\delta}$ in (5.24). Let $\bar{\underset{\sim}{H}}^{(n)\delta}$, regarded either as a function of the variables $(z_i,t)$ or of the variables $(x_{i,o},v_i;s)$, be continuous except possibly at $X_{i,o} = kL$. Define for $n \geqslant 2$

$$\left\|\bar{\underset{\sim}{H}}^{(n)\delta}\right\|_n^{\delta} = \sum_{j=o}^{P}\ \underset{x_{i,o},v_i}{\text{ess sup}}\ \left|\frac{\bar{\underset{\sim}{H}}_j^{(n)\delta}(v';z_2;\ldots;z_n;t)}{\prod_{i=2}^{n}\rho h_o(v_i)}\right| \tag{6.15}$$

or equivalently we may take the ess sup over $x_i$. Next define

$$\left\|\bar{\underset{\sim}{H}}^{\delta}\right\|_{\beta,1}^{\delta} = \sum_{n=2}^{\infty}\frac{1}{n^{\beta}}\left\|\bar{\underset{\sim}{H}}^{(n)\delta}\right\|_n^{\delta} \quad : \quad \beta > 2 \tag{6.16}$$

and

$$\left\|\bar{\underset{\sim}{H}}^{\delta}\right\|_{\beta,\infty}^{\delta} = \sup_{n\geqslant 2}\frac{1}{n^{\beta}}\left\|\bar{\underset{\sim}{H}}^{(n)\delta}\right\|_n^{\delta} \quad : \quad \beta \geqslant 1$$

Let $D^{\delta}_{\beta,1(\infty)}$ be the spaces of functions of the above type with finite $\|-\|^{\delta}_{\beta,1(\infty)}$ norms, then $D^{\delta}_{\beta,1(\infty)}$ are Banach spaces (Appendix B). From (4.23), it is immediate that

$$\left\|\underset{\sim}{G}^{\delta ext}(-\ ;\ 0)\right\|_{\beta,1(\infty)}^{\delta} = O(\epsilon) \tag{6.17}$$

for the ranges of $\beta$ specified in (6.16).

To obtain a solution to (6.14), an analysis of the properties of the linear operator $\underset{\approx}{C}$ is necessary. It is clear that $\underset{\approx}{C} : D^{\delta}_{\beta,1(\infty)} \to D^{\delta}_{\beta,1(\infty)}$. We show that $\underset{\approx}{C}$ is bounded. Suppose $\bar{\underset{\sim}{H}}^{\delta} \in D^{\delta}_{\beta,1(\infty)}$ and set

$$\bar{\underset{\sim}{F}}^{\delta} = \underset{\approx}{C}\ .\ \bar{\underset{\sim}{H}}^{\delta} \tag{6.18}$$

then
$$\operatorname*{ess\ sup}_{\substack{x_{i,o},v_i\\ i=2,\dots,n}} \left| \frac{\bar{F}_j^{(n)\delta}(v';z_2;\dots;z_n;t)}{\prod_{i=2}^{n} \rho h_o(v_i)} \right|$$

$$\leqslant \left(\rho\int_{-\infty}^{v'} dv_{n+1}\left|v_{n+1}-v'\right|h_o(v_{n+1})\right) \operatorname*{ess\ sup}_{\substack{x_{i,o},v_i\\ i=2,\dots,n+1}} \left| \frac{\bar{H}_{j-1}^{(n+1)\delta}(v';z_{n+1};z_2;\dots;z_n;t)}{\prod_{i=2}^{n+1} \rho h_o(v_i)} \right|$$

$$+ \left(\rho\int_{v'}^{+\infty} dv_{n+1}\left|v_{n+1}-v'\right|h_o(v_{n+1})\right) \operatorname*{ess\ sup}_{\substack{x_{i,o},v_i\\ i=2,\dots,n+1}} \left| \frac{\bar{H}_{j+1}^{(n+1)\delta}(v';z_{n+1};z_2;\dots;z_n;t)}{\prod_{i=2}^{n+1} \rho h_o(v_i)} \right|$$

$$+ \left(\rho\int_{-\infty}^{+\infty} dv_{n+1}\left|v_{n+1}-v'\right|h_o(v_{n+1})\right) \operatorname*{ess\ sup}_{\substack{x_{i,o},v_i\\ i=2,\dots,n+1}} \left| \frac{\bar{H}_{j}^{(n+1)\delta}(v';z_{n+1};z_2;\dots;z_n;t)}{\prod_{i=2}^{n+1} \rho h_o(v_i)} \right| \tag{6.19}$$

From (6.15) and (6.19)

$$\|\bar{\underset{\sim}{F}}^{(n)\delta}\|_n^\delta \leqslant 2\,\alpha\,(v')\,\|\bar{\underset{\sim}{H}}^{(n+1)\delta}\|_{n+1}^\delta \tag{6.20}$$

with $\alpha(\ \ )$ as in (5.25). Finally from (6.16) and (6.20)

$$\|\bar{\underset{\sim}{F}}^\delta\|_{\beta,1(\infty)}^\delta \leqslant 2\left(\frac{3}{2}\right)^\beta \alpha\,(v')\,\|\bar{\underset{\sim}{H}}^\delta\|_{\beta,1(\infty)}^\delta \tag{6.21}$$

So $\underset{\approx}{C}$ is bounded and

$$\|\underset{\approx}{C}(\text{—};v';s)\|_{\beta,1(\infty)}^\delta \leqslant 2\left(\frac{3}{2}\right)^\beta \alpha\,(v') \tag{6.22}$$

Consequently (6.14) has a unique solution which may be written formally as

$$\bar{\underset{\sim}{G}}^{\delta ext}(x_{i,o},v_i;s) = \sum_{m=o}^{\infty}\left(\int_o^s ds_m \underset{\approx}{C}(x_{i,o},v_i;v';s_m)\int_o^{s_m} ds_{m-1}\underset{\approx}{C}(x_{i,o},v_i;v';s_{m-1})\cdots\right.$$

$$\left.\cdots\int_o^{s_2} ds_1\underset{\approx}{C}(x_{i,o},v_i;v';s_1)\right)\bar{\underset{\sim}{G}}^{\delta ext}(x_{i,o},v_i;o) \tag{6.23}$$

The explicit form of the components is not needed here, but this is given in Appendix C for a more general case treated in the next chapter. The following upper estimate on the norm of $\bar{\underset{\sim}{G}}^{\delta ext}$ is obtained from (6.23) :

$$\| \bar{\underset{\sim}{G}}^{\delta ext}(\text{—};s) \|^{\delta}_{\beta,1(\infty)} \leqslant \exp\left[\sup_{0\leqslant s'\leqslant s} \| \underset{\approx}{C}(s') \|^{\delta}_{\beta,1(\infty)}\right] \tag{6.24}$$

$$\times \; \| \bar{\underset{\sim}{G}}^{\delta ext}(\text{—};\, 0) \|^{\delta}_{\beta,1(\infty)}$$

$$\leqslant \exp\left[2.\left(\tfrac{3}{2}\right)^{\beta} \alpha(v')s\right].\; O(\epsilon)$$

In particular,

$$\| \bar{\underset{\sim}{G}}^{(2)\,\delta ext}(\text{—};s) \|^{\delta}_{2} \leqslant 2^{\beta} \exp\left[2\left(\tfrac{3}{2}\right)^{\beta} \alpha(v')s\right].O(\epsilon) \tag{6.25}$$

This last result is used in the analysis of the size of the delta-function part of the error term in (5.21).

<u>Evolution Equation for $\bar{\underset{\sim}{G}}^{ext}_{reg}$</u> : If we again set $x_i = x_{i,o} + v_i s$ and $t = s$, then the evolution equations for $\bar{\underset{\sim}{G}}^{ext}_{reg}$ formally become

$$\frac{d}{ds}\; \bar{\underset{\sim}{G}}^{ext}_{reg}(x_{i,o},v_i;s) = \underset{\approx}{C}(x_{i,o},v_i;s)\;.\; \bar{\underset{\sim}{G}}^{ext}_{reg}\;(x_{i,o},v_i;s) \tag{6.26}$$

The norm for the space of vectors $\bar{\underset{\sim}{G}}^{ext}_{reg}$ is constructed to be compatible with that chosen for $\bar{\underset{\sim}{G}}_{reg}$ and $\bar{\underset{\sim}{f}}^{(1)}_{reg}$ in (5.27).

Let $\bar{\underset{\sim}{H}}^{(n)}_{reg}$, regarded either as a function of the variables $(z_i,t)$ or $(x_{i,o},v_i;s)$, be continuous except possible at $x_{i,o} = kL$. Define for $n \geqslant 2$

$$\| \bar{\underset{\sim}{H}}^{(n)}_{reg} \|^{reg}_{n} = \max_{0\leqslant j\leqslant P}\; \operatorname*{ess\,sup}_{\substack{x_{i,o}\; i\geqslant 1\\ v_i\; i\geqslant 2}} \left| \frac{\left(\bar{H}^{(n)}_{reg}\right)_j (z_1;\ldots;z_n;t)}{\bar{f}^{(1)}_{j+\delta j}(x^{1}_{1max},v_1;o)\,.\, \prod_{i=2}^{n} \rho h_o(v_i)} \right| \tag{6.27}$$

where $\left(\bar{H}^{(n)}_{\sim reg}\right)_j$ is the $j^{th}$ component of the column vector $\bar{H}^{(n)}_{\sim reg}$, $\bar{f}^{(1)}_{j+\delta j}$ is defined as in (5.28) and again we may equivalently take the ess sup over $x_i$ rather than $x_{i,o}$.

Next define

$$\|\bar{H}_{\sim reg}\|^{reg}_{\beta,1} = \sum_{n=2}^{\infty} \frac{1}{n^{\beta}} \|\bar{H}^{(n)}_{\sim reg}\|^{reg}_{n} \quad : \quad \beta > 2 \tag{6.28}$$

$$\text{and } \|\bar{H}_{reg}\|^{reg}_{\beta,\infty} = \sup_{n\geq 2} \left(\frac{1}{n^{\beta}} \|\bar{H}^{(n)}_{\sim reg}\|^{reg}_{n}\right) \quad : \quad \beta \geq 1$$

The spaces $D^{reg}_{\beta,1(\infty)}$ corresponding to $\|-\|^{reg}_{\beta,1(\infty)} < \infty$ are Banach (Appendix B). From (4.23),

$$\|\bar{G}^{ext}_{\sim reg}(\text{———};o)\|^{reg}_{\beta,1(\infty)} = O(\epsilon) \tag{6.29}$$

for the ranges of $\beta$ specified in (6.28). We may show that the linear operator $\underset{\approx}{C} : D^{reg}_{\beta,1(\infty)} \to D^{reg}_{\beta,1(\infty)}$ is bounded with

$$\|\underset{\approx}{C}(\text{———};s)\|^{reg}_{\beta,1(\infty)} \leq 2\left(\frac{3}{2}\right)^{\beta} \alpha\,(v_1) \tag{6.30}$$

(6.26) has a unique solution which may be written formally as

$$\bar{G}^{ext}_{\sim reg}(x_{i,o},v_i;s) = \sum_{m=o}^{\infty} \left\{\int_o^s ds_m \, \underset{\approx}{C}(x_{i,o},v_i;s_m) \int_o^{s} ds_{m-1} \, \underset{\approx}{C}(x_{i,o},v_i;s_{m-1}) \right.$$
$$\left. \cdots\cdots \int_o^{s_2} ds_1 \, \underset{\approx}{C}(x_{i,o},v_i;s_1)\right\} \cdot \bar{G}_{\sim reg}(x_{i,o},v_i;o) \tag{6.31}$$

From (6.31) we may obtain an upper bound on $\bar{G}^{ext}_{\sim reg}$ in terms of the norm $\|-\|^{reg}_{\beta,1(\infty)}$ which may in particular be used to show that

$$\|\bar{G}^{(2)ext}_{reg}(\text{———};s)\|^{reg}_{2} \leq 2^{\beta} \exp\left[2\left(\frac{3}{2}\right)^{\beta} \alpha(v_1)s\right] O(\epsilon) \tag{6.32}$$

This is used in the analysis of the size of the regular part of the error term in (5.21).

## 2.7 ANALYSIS OF EQUATIONS FOR ONE-PARTICLE REDUCED DISTRIBUTION FUNCTIONS.

From (5.9) $\bar{\underset{\approx}{\zeta}}$ depends only on $\bar{\underset{\sim}{G}}^{(2)}$ in precollision regions of phase space. Using the norm upper bounds (6.25) (resp. (6.32)) on $\bar{\underset{\sim}{G}}^{(2)\delta ext}$ (resp. $\bar{G}^{(2)ext}_{\sim reg}$) to provided corresponding upper bounds on $\bar{\underset{\sim}{G}}^{(2)\delta}$ (resp. $\bar{G}^{(2)}_{\sim reg}$) in precollision regions, we obtain

$$\begin{aligned} \| \bar{\underset{\approx}{\zeta}}^{\delta}(v';s) \|_{\delta} &\leqslant \alpha(v') \, \| \bar{\underset{\sim}{G}}^{(2)\delta ext} (-;s) \|_2^{\delta} \\ &\leqslant 2^{\beta} \alpha(v') \exp\left[ 2 (\tfrac{3}{2})^{\beta} \alpha(v') s \right] \; O(\epsilon) \end{aligned} \tag{7.1}$$

and

$$\begin{aligned} \| \bar{\zeta}_{\approx reg}(-;s) \|^{reg} &\leqslant \alpha(v_1) \, \| \bar{G}^{(2)ext}_{\sim reg}(-;s) \|_2^{reg} \\ &\leqslant 2^{\beta} \alpha(v_1) \exp\left[ 2 (\tfrac{3}{2})^{\beta} \alpha(v_1) s \right] O(\epsilon) \end{aligned} \tag{7.2}$$

An upper estimate of the norms of the (P+1) × (P+1) matrices $\underset{\approx}{U}^P(o,v_1;s)$ and $\underset{\approx}{U}^P(x_{1,0},v_1;s)$ is obtained from

$$\| \underset{\approx}{U}^P(x,v;s) \| \leqslant \exp\left( \int_o^s ds' \, \| \underset{\approx}{C}^P(x,v;s') \| \right)$$

$$\leqslant \exp\left( \bar{\gamma}_{av}(x,v;s) \; (1+\| \underset{\approx}{\Delta}^- \|) + \bar{\beta}_{av}(x,v,s) \; (1+\| \underset{\approx}{\Delta}^+ \|) \right) \tag{7.3}$$

Now $\| \underset{\approx}{\Delta}^- \| = \| \underset{\approx}{\Delta}^+ \|$ for the norms that we consider and

$$\sup_x \left( \bar{\gamma}_{av}(x,v;s) + \bar{\beta}_{av}(x,v;s) \right) \leqslant \alpha(v) s \tag{7.4}$$

So $$\| \underset{\approx}{U}^P(x;v;s) \| \leqslant \exp\left( \alpha(v) \; (1+\| \underset{\approx}{\Delta}^+ \|) s \right) \tag{7.5}$$

From (5.1/2/5), the following size estimates of the "error" terms in (5.21) may be made where β lie in the ranges specified:

$$\left\| \int_o^s ds' \underset{\approx}{U}^P(o,v';s-s').\bar{\underset{\approx}{\zeta}}^\delta(s') \right\|_\delta$$

$$\leqslant \int_o^s ds' \left\| \underset{\approx}{U}^P(o,v',s-s') \right\|_\delta \left\| \bar{\underset{\approx}{\zeta}}^\delta(s') \right\|_\delta \tag{7.6}$$

$$\leqslant \frac{2^{\beta-1}}{(\frac{3}{2})^\beta - 1} \left\{ \exp\left[ 2\left((\tfrac{3}{2})^\beta - 1\right)\alpha(v')s \right] - 1 \right\} \exp\left(\alpha(v')s\right) . O(\in)$$

and similarly

$$\left\| \int_o^s ds' \underset{\approx}{U}^P(x_{1,0},v_1;s-s').\bar{\underset{\approx}{\zeta}}_{reg}(s') \right\|_{reg} \tag{7.7}$$

$$\leqslant \frac{2^\beta}{2(\frac{3}{2})^\beta - 1 - \|\Delta^+\|_{reg}} \left\{ \exp\left[ \left(2(\tfrac{3}{2})^\beta - 1 - \|\underset{\approx}{\Delta}^+\|_{reg}\right)\alpha(v_1)s \right] - 1 \right\} \exp\left(\alpha(v_1)s\right) \; O(\in)$$

These will be O(1) for times t such that

$$\rho v_{th} t \approx \frac{\ln P}{2\hat{\alpha}(\frac{w}{v_{th}})} = \tau(w) \text{ choosing } \beta=1 \tag{7.8}$$

with $w = v'$ in (7.6), $w = v_1$ in (7.7) and $\hat{\alpha}(\frac{w}{v_{th}}) = (\rho v_{th})^{-1}\alpha(w)$

Using the estimate (7.2) of $\bar{\underset{\approx}{\zeta}}_{reg}$, we may verify that the intial growth rate of each component of $\int_o^s ds' \underset{\approx}{U}^P(x_{1,0},v_1;s-s').\bar{\underset{\sim}{\zeta}}_{reg}(s')$ is smaller by a factor of at least $\in^{\frac{1}{2}}$ than the corresponding component of $\left(\underset{\approx}{U}^P(x_{1,0},v_1;s) - \underset{\approx}{I}\right)\cdot\bar{\underset{\sim}{f}}^{(1)}_{reg}(o)$. We therefore expect that the components of $\left(\underset{\approx}{U}^P(x_{1,0},v_1;s) - \underset{\approx}{I}\right)\bar{\underset{\sim}{f}}^{(1)}_{reg}(o)$ will be large compared with those of $\int_o^s ds \; \underset{\approx}{U}^P(x_{1,0},v_1;s-s').\bar{\underset{\approx}{\zeta}}_{reg}(s')$ for times $o < \rho v_{th} s << \tau(v_1)$ (where size is measured in terms of a suitably weighted ess sup norm c.f. (i) of Appendix B).

Using a power series expansion of $\underset{\approx}{U}^P(o,v',s)$ and (4.23), a simple calculation shows that the growth rate of each component of $\int_o^s ds' \underset{\approx}{U}^P(o,v';s-s')\cdot \bar{\zeta}^{\delta}(s')$ is smaller by a factor of $\epsilon^{\frac{1}{2}}$ than the corresponding component of $\left(\underset{\approx}{U}^P(o,v';s) - \underset{\approx}{I}\right)\underset{\sim}{\bar{f}}^{(1)\delta}(o)$ for $\epsilon^{\frac{1}{2}} \leqslant \rho v_{th}s \lesssim 1$. Also from (7.6) the norm of the first expression is much smaller than the second for $\rho v_{th}s << \tau(v')$. Although this does not tell us anything directly about the individual components, we expect that the corresponding inequalities are true for $\epsilon^{\frac{1}{2}} \lesssim \rho v_{th}s << \tau(v')$.

It remains to determine those times for which the components of $\int_o^s ds' \underset{\approx}{U}^P(x_{1,0},v_1;s-s')\cdot\bar{\zeta}(s')$ are "smaller" than those of $\underset{\approx}{U}^P(x_{1,0},v_1;s)\cdot \underset{\sim}{\bar{f}}^{(1)}_{(o)} - \underset{\sim}{\bar{f}}^{(1)}_{(s=\infty)}$. For the regular part, rough results may be obtained by noting that the second term decays no faster than $\sim K \exp\left[-2\hat{\alpha}(\frac{v_1}{v_{th}})\rho v_{th}s\right]$ since the points of $\left[\int_o^s ds\ \underset{\approx}{C}^P(\ldots,s')\right]$ have real part greater than $-2\ \hat{\alpha}\ (\frac{v_1}{v_{th}})\cdot\rho v_{th}s$. An upper bound on the first term is obtained from (7.7). Using these two estimates, we expect that the above condition is satisfied for $o \leqslant \rho v_{th}s << \frac{1}{2}\ \tau(v_1)$. Again there are problems with the delta-function part since a norm approach is not suited to a componentwise analysis. However a similar analysis to that for the regular part suggests that the appropriate componentwise inequalities are true for $\epsilon^{\frac{1}{2}} \leqslant \rho v_{th}\ s << \frac{1}{2}\ \tau(v')$.

In conclusion

$$\bar{\underset{\sim}{f}}^{(1)\delta}(v';s) \approx \underset{\approx}{U}^{P}(o,v';s) \cdot \bar{\underset{\sim}{f}}^{(1)\delta}(v';o) \quad \text{for } \epsilon^{\frac{1}{2}} \lesssim \rho v_{th} s \ll \tfrac{1}{3}\tau(v')$$

$$\bar{\underset{\sim}{f}}^{(1)}_{reg}(x_{1,0},v_1;s) \approx \underset{\approx}{U}^{P}(x_{1,0},v_1;s) \cdot \bar{f}^{(1)}_{reg}(x_{1,0},v_1;o) \quad \text{for}$$

$$o \lesssim \rho v_{th} s \ll \tfrac{1}{3}\tau(v_1) \qquad (7.9)$$

For $v'$, $v_1 = O(v_{th})$, these ranges include times of the order of many mean free times ($t_{th}$). Such times are of most interest in the study of relaxation phenomena.

## 2.8. THE GENERAL INITIAL VALUE PROBLEM.

At the initial time we suppose the particle, labelled $n_i$, has specified position $X_i$ and velocity $V_i$ $(i=1,2,\ldots,N)$ where $n_i < n_j$ (and so $X_i < X_j$) for $i < j$. For convenience we set $n_o = X_o = -\infty$ and $n_{N+1} = X_{N+1} = +\infty$. The distances between the specified particles are $L_i = X_{i+1} - X_i$. The remaining particles in each cell $(X_i, X_{i+1})$ are assumed to be in equilibrium at $t = o$ with mean density $\rho_i$.

Initial conditions on the one-particle r.d.f.'s are therefore of the form

$$f^{(1)}_{ni}(z_1;o) = \delta(x_1-X_i)\,\delta(v_1-V_i) \qquad i=1,2,\ldots,N.$$

$f^{(1)}_j(z_1;o)$ are regular for all other $j$ and such that

$$f^{(1)}_j(z_1;o) = f^{(1)s}_j(x_1;o)\; h_o\,(v_1) \text{ with}$$

$$\sum_{n_i<j<n_{i+1}} f^{(1)s}_j(x_1;o) = \rho_i \chi_{[X_i,X_{i+1}]}(x_1) \qquad (8.1)$$

Expressions for these and higher order r.d.f.'s may be written down explicitly from the work of the previous sections.

In order to obtain approximate kinetic equations for the one-particle r.d.f.'s, we need an approximate factorization condition giving the n-particle r.d.f.'s in terms of the (n-1)-particle r.d.f.'s in precollision regions (at least for the case n=2). A detailed analysis of the error terms is not given. However by comparison with previous work, it would be clear that these are "small" in the high density regime $\varepsilon_i = \frac{1}{P_i} << 1$ where $P_i = n_{i+1}-n_i$, $i = 1,2,\ldots,N-1$, with $\rho_o$ and $\rho_N$ arbitrary. A rigorous analysis could again be made using Banach space techniques.

In precollision regions and for $x_1-v_1 t \in [X_i - \frac{L_{i-1}}{2}, X_i + \frac{L_i}{2}]$, the factorization condition has the form

$$f_j^{(n)}(z_1;\ldots;z_n;t) = f_{j*}^{(n-1)}(z_1;\ldots;z_{n-1};t)\; h'(z_n;t) + g_j^{(n)}(z_1;\ldots;z_n;t) \qquad (8.2)$$

where $g_j^{(n)}$ is the "small" error term,

$$\begin{aligned} j^* &= j-1 \text{ for } X_i < x_n-v_n t < x_1-v_1 t \\ &= j+1 \text{ for } x_1-v_1 t < x_n-v_n t < X_i \\ &= j \text{ otherwise} \end{aligned}$$

and $$h'(z;t) = \sum_{i=1}^{N} \delta(x-vt-X_i)\,\delta(v-V_i) + \left(\sum_{i=-1}^{N} \chi[X_i,X_i+1](x-vt)\,\rho_i\right) h_o(v)$$

A suitable limit procedure must be adopted for the evaluation of the r.d.f.'s and interpretation of (8.2) at points where there is delta-function or discontinuous behaviour. In (8.2) $g_j^{(n)}$ is regular in the variable $z_n$ and if $\varepsilon_i << 1$, $n = O(1)$, it is "small" for t extending over a range of many relaxation times. For

$x_1 - v_1 t \,\varepsilon\, [X_i - \frac{L_{i-1}}{2},\ X_i + \frac{L_i}{2}]$, the corresponding equations for $f_j^{(1)}$ are

$$\left(\frac{\partial}{\partial t} + v_1 \frac{\partial}{\partial x_1}\right) f_j^{(1)}(z_1;t) = \gamma_i(x_1,v_1;t) \left[f_{j-1}^{(1)}(z_1;t) - f_j^{(1)}(z_1;t)\right]$$

$$+ \beta_i(x_1,v_1;t)\left[f_{j+1}^{(1)}(z_1;t) - f_j^{(1)}(z_1;t)\right]$$

$$+ \hat{\zeta}_j(z_1;t) \qquad (8.3)$$

where

$$\hat{\zeta}_j(z_1;t) = \int_{-\infty}^{+\infty} dv_2 |v_2 - v_1| \cdot \left(g_{(j)}^{(2)}(z_1;x_1^-,v_2;t) - g_j^{(2)}(z_1;x_1^-,v_2;t)\right) \qquad (8.4)$$

except on the lines $x_1 = X_i + V_i t$ where $f_j^{(1)}$ are discontinuous and satisfy the jump conditions

$$\lim_{\epsilon \to o} f_j^{(1)}(Z_i^+,t^+) = \lim_{\epsilon \to o} f_{j+1}^{(1)}(Z_i^-,t^-) \text{ for } v_1 < V_i$$

$$\lim_{\epsilon \to o} f_j^{(1)}(Z_i^+,t^+) = \lim_{\epsilon \to o} f_{j-1}^{(1)}(Z_i^-,t^-) \text{ for } v_1 > V_i \qquad (8.5)$$

where $(Z_i^{\pm},t^{\pm}) = (X_i + V_i t \pm \epsilon v_1 \ , t \pm \epsilon)$

In (8.3), we have set

$$\gamma_i(x_1,v_1;t) = \int_{-\infty}^{\frac{x_1-X_i}{t}} dv_2(v_1-v_2)h_o(v_2) \cdot \sum_{i=o}^{N} \chi_{[X_i,X_{i+1}]}(x_1-v_2 t)\rho_i$$

$$\beta_i(x_1,v_1;t) = \int_{\frac{x_1-X_i}{t}}^{+\infty} dv_2(v_2-v_1)h_o(v_2) \cdot \sum_{i=o}^{N} \chi_{[X_i,X_{i+1}]}(x_1-v_2 t)\rho_i \qquad (8.6)$$

The partial solution of (8.3) is written most conveniently in vector form. Suppose that the straight line in the $(x',t')$-phase between $(x_1-v_1t,o)$ and $(x_1,t)$ crosses $K^+$ of the lines $\{(X_i+V_it,t): t \in R\}$ where $v_1 < V_i$ and $K^-$ of these lines where $v_1 > V_i$. Set $K(x_1,v_1;t) = K^+(x_1,v_1;t) - K^-(x_1,v_1;t)$ and define the infinite dimensional vector $\underset{\sim}{f}^{(1)}(z_1;t)$ (resp. $\underset{\sim}{\hat{\zeta}}(z_1;t)$) to have a $j^{th}$ component given by $f^{(1)}_{j-K(x_1,v_1;t)}(z_1;t)$ (resp. $\hat{\zeta}_{j-K(x_1,v_1;t)}(z_1;t)$). Using this notation (8.3) may be integrated along the characteristics $\{(x_1,t) : x_1 = v_1s+x_{1,0}t = s \in R\}$ of $\frac{\partial}{\partial t} + v_1 \frac{\partial}{\partial x_1}$ to yield for $x_{1,0} \in [X_i-\frac{L_{i-1}}{2}, X_i + \frac{L_i}{2}]$

$$\underset{\sim}{f}^{(1)}(x_{1,0},v_1;s) = \underset{\approx}{U}(x_{1,0},v_1;s) \cdot \underset{\sim}{f}^{(1)}(x_{1,0},v_1;o) + \int_o^s ds' \, \underset{\approx}{U}(x_{1,0},v_1;s-s') . \underset{\sim}{\hat{\zeta}}(x_{1,0},v_1;s') \qquad (8.7)$$

where $$\underset{\approx}{U}(x_{1,0},v_1;s) = \exp\{\int_o^s ds' \, \underset{\approx}{C}(x_{1,0},v_1;s')\} \qquad (8.8)$$

and $\underset{\approx}{C}$ is an infinite matrix with components

$$c_{ij} = \gamma_i(x_1,v_1;t)(\delta_{i-1,j}-\delta_{i,j}) + \beta_i(x_1,v_1,t)(\delta_{i+1,j}-\delta_{i,j}) \qquad (8.9)$$

$\underset{\approx}{C}$ is bounded with respect to the appropriate norms, so a power series expansion of (8.8) is valid (convergent in norm in the appropriate Banach space).

If $\underset{\sim}{f}^{(1)}$ is decomposed into regular and delta-function parts as

$$f_j^{(1)}(z_1;t) = \sum_{i=1}^{N} f_j^{(1)\delta i}(t)\ \delta\ (x_1-(X_i+V_it))\ \delta\ (v_1-V_i) + f^{(1)}_{reg\,j}(z_1;t) \qquad (8.10)$$

then separate equations are satisfied by each of the $f_j^{(1)\delta i}$

and the $f^{(1)}_{reg_j}$. The equation for $f^{(1)}_{reg_j}$ and the solution are identical in form with that for $f^{(1)}_j$ ($\hat{\zeta}$ is just replaced by $\hat{\zeta}_{reg}$). For $f^{(1)\delta i}_j$, we have

$$\frac{d}{dt} f^{(1)\delta i}_j(t) = \gamma_i(X_i+V_it,V_i;t) \cdot [f^{(1)\delta i}_{j-1}(t) - f^{(1)\delta i}_j(t)]$$

$$+ \beta_i(X_i+V_it,V_i;t) \cdot [f^{(1)\delta i}_{j+1}(t) - f^{(1)\delta i}_j(t)]$$

$$+\hat{\zeta}^{\delta i}_j(t) \qquad (8.11)$$

($\hat{\zeta}^{\delta i}_j$ is the appropriate delta-function component of $\hat{\zeta}_j$)

except for $t = t_{i,k}$ where $t_{i,k} > o$ (if they exist) are the solutions of $X_i + V_it_{i,k} = X_k+V_kt_{i,k}$. For such t, $f^{(1)\delta i}_j$ are discontinuous and satisfy the jump conditions

$$\lim_{\epsilon\to o} f^{(1)\delta i}_j(t_{i,k}+) = \lim_{\epsilon\to o} f^{(1)\delta i}_{j+1}(t_{i,k}-) \text{ if } v_1 < V_i$$

$$\lim_{\epsilon\to o} f^{(1)\delta i}_j(t_{i,k}+) = \lim_{\epsilon\to o} f^{(1)\delta i}_{j-1}(t_{i,k}-) \text{ if } v_1 > V_i$$

(8.12)

The solution of these equations has the same form as (8.7) with $U(x_{1,0},v_1;s)$ replaced by $U(X_i,V_i;s)$ and $\hat{\zeta}$ by $\hat{\zeta}^{\delta}$.

The periodic problem may be treated as a special case of the above. To recover previous equations, we must set periodic initial conditions and sum over equal j (modulo P+1).

# CHAPTER 3

## GENERAL INITIAL VALUE PROBLEMS

## (ONE-DIMENSIONAL HARD "SPHERE" GAS)

### 3.1 INTRODUCTION

Whereas in the last chapter only quasi-equilibrium initial conditions were considered, here we examine more general inhomogeneous initial value problems (i.v.p.) for the same hard "sphere" system. Again a number of particles have specified positions and velocities at the initial time, but now the remainder may be distributed inhomogeneously and have non-Maxwellian velocity distribution functions (of sufficiently fast decrease). There are a number of physical constraints which we must impose such as finite local particle number, energy and momentum and the existence of the means of these quantities. The spaces we work in shall guarantee the finite local behaviour of the above quantities and existence of means at $t = 0$ shall guarantee their existence for $t > 0$ (Appendix A).

First we prove the existence and uniqueness of a particular reduced distribution function (r.d.f.) $f_j^{(n)}(z_1;\ldots;z_n;t)$ where $(z_1;\ldots;z_n;t)$ is an arbitrary point in phase space. A Banach space formulation similar to that of section 2.6 is adopted. Such techniques have been used previously in statistical mechanics, for example by Ruelle[53] in the equilibrium theory of virial expansions for correlation functions. This approach does not, however, enable us to give a unified treatment of the solutions $\underset{\sim}{f}$ of the hierarchy equations throughout phase space. For this, it is found convenient to use a formulation in terms of a countably normed space. By so doing, we avoid problems arising from the unbounded nature (with respect to $v_1$) of the operators

$$\lim_{\epsilon \to 0} \int_{-\infty}^{+\infty} dv_{n+1} |v_{n+1} - v_1| x \ \ldots$$

appearing in the hierarchy equations. The above approach is somewhat different from that of algebraic statistical mechanics in obtaining a rigorous theory. Marchioro et al.[54] have used the algebraic approach to treat a one-dimensional hard core system with a $C^{\infty}$ interparticle potential.

An advantage in dealing with the hard "sphere" system is that, being able to calculate initial values for the r.d.f.'s (at least for the quasi-equilibrium case), we have insight into the appropriate choice of norm(s) for the Banach or countably normed spaces. In fact we can tailor the choice of norm to suit the problem with which we are dealing (as seen in Chapter 2). Also, for this system, the hierarchy equations reduce to a particularly simple form. However, we expect that the countably normed space approach should be extendable to more general systems.

Next we consider the special class of i.v.p.'s where a single particle has specified position and velocity and the rest have regular r.d.f.'s at t = 0. For a class of initial values including quasi-equilibrium and inhomogeneous cases, Evans[55] has shown that it is possible to obtain exact closed kinetic equations for the delta-function part of the one-particle r.d.f.'s $f_j^{(1)\delta}$. This work is presented here. The spectral properties of these equations are analyzed. Under certain conditions, it is shown that their asymptotic form depends only on the mean particle number (and velocity distribution) rather than on the details of the inhomogeneous initial distribution. The asymptotic behaviour of the solutions is analyzed. Exact kinetic equations for the $f_j^{(1)\delta}$ are derived for the corresponding problem with an external potential for a range of velocities of the specified particle which avoid bound states. For the general i.v.p.'s mentioned above, we may write down approximate closed equations for the delta-function part of the one-particle r.d.f.'s. These equations for the periodic case are compared with the above exact case.

Returning to the problem with a single specified particle we show that, given $f_j^{(1)\delta}(t=0) \geq 0$ $(\neq 0)$, then under time evolution governed by the exact closed kinetic equations, $f_j^{(1)\delta}(t) > 0$ for all $t > 0$.

## 3.2 EXISTENCE AND UNIQUENESS OF SOLUTIONS OF THE HIERARCHY EQUATIONS : BANACH SPACE FORMULATION.

As in the last chapter, we prescribe that the specified particles at t = 0 should be labelled $n_i$, i=2,...,N where particle $n_i$ has initially position $X_i$ and velocity $V_i$. On physical grounds, we know that the delta-function behaviour of the r.d.f.'s must be of the form

$$f_j^{(m)}(z_1;\ldots;z_m;t)$$

$$= \sum_{r=0}^{m-1} \sum_{\substack{k\alpha \in \{2,\ldots,m\}\ \alpha=1,\ldots,r \\ k\alpha < k\beta \text{ for } \alpha<\beta}} f^{(m-r)}_{regl'_j}(z_1;\ldots;\hat{z}_{k1};\ldots;\hat{z}_{kr};\ldots;z_m;t)$$

$$\times \sum_{\substack{\ell\gamma \in \{1,2,\ldots,N\}\ \gamma=1,\ldots,r \\ \ell\gamma \neq \ell\delta \text{ for } \gamma\neq\delta}} \prod_{\eta=1}^{r} \delta(z_{k\eta}-Z_{\ell\eta}(t)) \qquad (2.1)$$

where $Z_i(t) = (X_i+V_it,V_i)$ and $\delta(z-Z_i(t)) = \delta(x-(X_i+V_it))\delta(v-V_i)$ (2.2)

and $f^{(p)}_{regl'_j}$ is regular in all variables except possibly the first. The initial conditions chosen must necessarily be of this form. In fact, if the constraint (2.1) is imposed on the initial conditions, then under time evolution governed by the hierarchy equations, it can be verified that (2.1) is valid for all time. $f^{(p)}_{regl'_j}$ may be further decomposed into regular and delta-function components as

$$f^{(p)}_{regl'_j}(z_1;\ldots;z_p;t) = \sum_{i=1}^{N} f_j^{(p)\delta i}(z_2;\ldots;z_p;t)\cdot\delta(z_1-Z_i(t))$$

$$+ f^{(p)}_{reg_j}(z_1;\ldots;z_p;t) \qquad (2.3)$$

It is possible to write down equations for the components of $f_j^{(m)}$. In particular, for $f^{(m)}_{reg_j}$

$$\left(\frac{\partial}{\partial t} + K_j^{(m)}\right) f^{(m)}_{reg_j} \quad (z_1;\ldots;z_m;t) \tag{2.4}$$

$$= \lim_{\epsilon\to o} \int_{-\infty}^{+\infty} dv_{m+1} \, |v'_{m+1}-v_1| \times \left( f^{(m+1)}_{reg_{(j)}} \quad (z_1;x_1^-,v_{m+1};z_2;\ldots;z_m;t) - f^{(m+1)}_{reg_j} (z_1;x_1^-,v_{m+1};\ldots;z_m;t)\right)$$

with $x_1^- = x_1-\epsilon\,\mathrm{sgn}(v_{m+1}-v_1)$

except on the lines $x_1 = X_i+V_it$ where $f^{(m)}_{reg_j}$ is discontinuous and satisfies

$$\lim_{\epsilon\to o} f^{(m)}_{reg_j} \quad (Z_i^+;\ z_2;\ldots;z_m;t^+) = \lim_{\epsilon\to o} f^{(m)}_{reg_{j+1}} \quad (Z_i^-;z_2;\ldots;z_m;t^-) \text{ for } v_1<V_i$$

$$\lim_{\epsilon\to o} f^{(m)}_{reg_j} \quad (Z_i^+;z_2;\ldots;z_m;t^+) = \lim_{\epsilon\to o} f^{(m)}_{reg_{j-1}} \quad (Z_i^-;z_2;\ldots;z_m;t^-) \text{ for } v_1>V_i$$

(2.5)

where $\left(Z_i^{\pm},t^{\pm}\right) = (X_i+V_it\pm v_1\epsilon,t\pm\epsilon)$

If we group together terms with a factor $\delta(z_i-Z_p(t))$, then it follows that

$$f_j^{(m)\,\delta p} \quad (z_2;\ldots;z_m;t)\delta(z_1-Z_p(t)) + \sum_{i=2}^{m} f^{(m-1)}_{reg_j}(z_1;\ldots;\hat{z}_i;\ldots z_m;t)\delta(z_i-Z_p(t)) \tag{2.6}$$

satisfies an equation of the form (2.4) and jump condition of the form (2.5).

The Banach space formulation of the last chapter is modified to prove the existence and uniqueness of the r.d.f. $f_j^{(n)}(z'_1;\ldots;z'_n;t')$ for a specific i.v.p. Here $(z'_1;\ldots;z'_n;t')$ is fixed and need not be in a precollision region of phase space. We first consider the regular part of $f_j^{(n)}$. Existence and uniqueness for the delta-function part depends on the corresponding analysis for the regular part and this will be considered later. (2.4) for $m \geqslant n$ must be used. The partial differential operators $\left(\frac{\partial}{\partial t} + K_j^{(m)}\right)$ in (2.4) may be converted to ordinary differential operators using the following technique (Courant and Hilbert[45]). We parameterize the characteristics of $\left(\frac{\partial}{\partial t} + K_j^{(m)}\right)$ as follows. Set

$$z_i = z_i^m\,(s, z_{k,o}^m)\ i,j = 1,\dots,m;\ t = s$$

$$\text{where } z_i^m\ (o, z_{k,o}^m) = z_{i,o}^m \tag{2.7}$$

Also $z_i^n\,(t', z_{k,o}^n) = z_i'$ are fixed

For $m \geqslant n$ (2.4) be rewritten in the form (using symmetry of the r.d.f.'s)

$$\frac{d}{ds}\ f_{reg_j}^{(m)}\ (z_i^m(s, z_{k,o}^m); s)$$

$$= \lim_{\epsilon \to o} \int_{-\infty}^{+\infty} dv_{m+1} \left| v_{m+1} - v_1^m\ (s, z_{k,o}^m) \right| \ \times \tag{2.8}$$

$$\Big\{ f_{reg_{(j)}}^{(m+1)} \left(z_1^m(s,z_{k,o}^m); \dots; z_n^m(s,z_{k,o}^m); x_1(s,z_{k,o}^m)^-, v_{m+1}; z_{n+1}^m(s,z_{k,o}^m); \dots; z_m^m(s,z_{k,o}^m); s\right)$$

$$- f_{reg_j}^{(m+1)} \left(z_1^m\ (s, z_{k,o}^m);\ \dots \qquad \dots;\ s\right)\Big\}$$

except on the lines $x_1^m = X_i + V_i s$ where $f_{regj}^{(m)}$ are discontinuous and satisfy the jump conditions (2.5).

In order to determine $f_{regj}^{(n)}(z_1, \dots, z_n; t)$ it is not necessary to consider (2.8) on the entire phase space but only on the following restricted domain:

(i) n-particle configurations of the form $z_i^n(s^1, z_{k,o}^n)$ $i=1, \ldots, n; o \leqslant s^1 \leqslant t'$.

(ii) (n+1)-particle configurations $z_i^{n+1}(s^2, z_{k,o}^{n+1})$ $i=1,\ldots, n+1; o \leqslant s^2 \leqslant s^1$

where $z_i^{n+1}(s^1, z_{k,o}^{n+1}) = z_i^n(s^1, z_{k,o}^n)$ $i=1,\ldots,n$

and $z_{n+1}^{n+1}(s^1, z_{k,o}^{n+1}) = (x_1^n(s^1, z_{k,o}^n) - \epsilon \operatorname{sgn}(v_{n+1}-v_1), v_{n+1})$

(iii) (n+2)-particle configurations $z_i^{n+2}(s^3, z_{k,o}^{n+2})$ $i=1,\ldots, n+2;\ o \leqslant s^3 \leqslant s^2$

where $z_i^{n+2}(s^2, z_{k,o}^{n+2}) = z_i^{n+1}(s^2, z_{k,o}^{n+1})$ $i=1,\ldots,n+1$

and $z_{n+2}^{n+2}(s^2, z_{k,o}^{n+2}) = (x_1^{n+1}(s^1, z_{k,o}^{n+1}) - \epsilon \operatorname{sgn}(v_{n+2}-v_1), v_{n+2})$

(iv) (m)-particle configurations for $m \geqslant n+3$ are defined by a natural extension of the above procedure.

Consequently for each time $s : o \leqslant s \leqslant t'$, we confine our attention to those m-particle configurations which are of the above form for some $s^{m-n} : s \leqslant s^{m-n} \leqslant t'$. These may be specified in terms of the corresponding initial phase points $z_{k,o}^m$ associated with the m-particles i.e. $(z_{i,o}^m, \ldots, z_{m,o}^m) \in C_m(s)$. Then $C_m(s') \subseteq C_m(s'')$ for $s' \geqslant s''$.

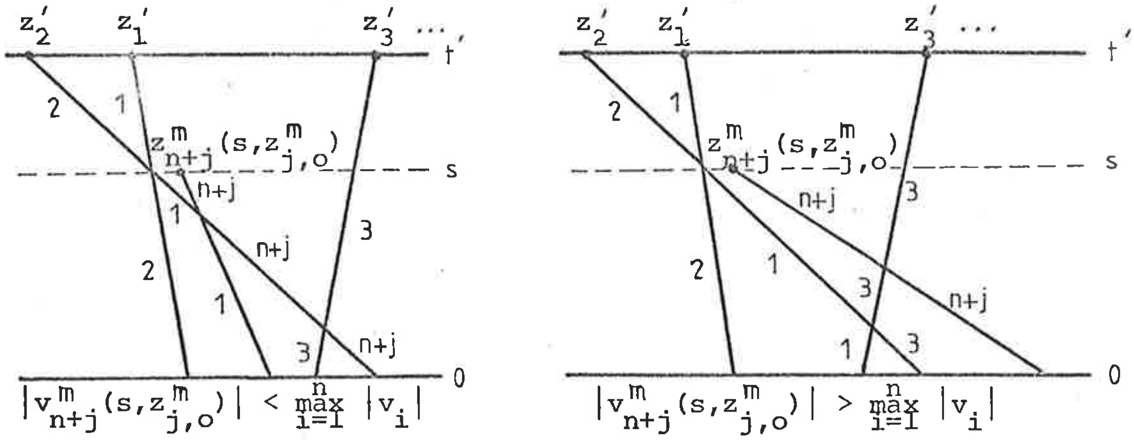
The advantage of the restriction to such a domain is that the time evolution operator will become bounded primarily as a result of the following property which bounds $v_1^m(s, z_{k,o}^m)$ on $C_m(s)$.

If $|v_m| \geqslant \max_{i=o}^{n} |v_i|$, then

$$z_m^m(s^{m-n+1}, z_{k,o}^m) = \left\{x_1^{m-1}(s^{m-n}, z_{k,o}^{m-1}) - v_m(s^{m-n}-s^{m-n+1}), v_m\right\}$$

$$\text{so } v_1^m(s^{m-n+1}, z_{k,o}^m) \neq v_m \qquad (2.9)$$

i.e. in (2.9) the particle at $z_m^m$ does not interact with the particle at $z_1^m$ for $o \leqslant s^{m-n+1} \leqslant s^{m-n}$ under the m-particle motion where only the interaction between the particle at $z_1^m$ and the other particles is taken into account. This will not necessarily be valid when $|v_m| \leqslant \max_{i=1}^{n} | v_i|$.




In the following analysis we first prove the boundedness of the time evolution operator from (2.9) and this is then used to obtain an existence and uniqueness proof for $f_j^{(n)}$.

If we define the vectors

$$\underset{\sim}{f}_{reg}^{(m)}(s) = \begin{bmatrix} \vdots \\ f_{reg-1}^{(m)}(s) \\ f_{reg\ 0}^{(m)}(s) \\ f_{reg+1}^{(m)}(s) \\ \vdots \end{bmatrix} \text{ and } \underset{\sim}{f}_{reg}(s) = \begin{bmatrix} \underset{\sim}{f}_{reg}^{(n)}(s) \\ \underset{\sim}{f}_{reg}^{(n+1)}(s) \\ \vdots \end{bmatrix} \qquad (2.10)$$

then (2.8) becomes formally

$$\frac{d}{ds}\underset{\sim}{f}_{reg}(s) = \underset{\approx}{C}(z_{k,o}^m;s).\underset{\sim}{f}_{reg}(s) \qquad (2.11)$$

together with a jump condition across the lines of discontinuity.

Existence and uniqueness of the solution for the abstract Cauchy problem corresponding to (2.11) are proved. The form of the solution given here is similar to that of the abstract Cauchy-Kovalevska Theorem (see Treves[56]). Consider a bounded, piecewise continuous vector valued function (whose discontinuities are fixed w.r.t. $x^m_{k,o}$) denoted by $\underset{\sim}{h}_{reg}(s)$. The components $h^{(m)}_{reg_j}(z^m_i(s,z^m_{k,o});s)$, $m\geq n$, are defined for $z^m_{k,o} \in C_m(s)$. For $t' \geq s' \geq s$, set

$$\left\| \underset{\sim}{h}^{(m)}_{reg}(s) \right\|^{reg}_{m;s'} = \sup_j \operatorname*{ess\,sup}_{z^m_{k,o} \in C_m(s')} \left| \frac{h^{(m)}_{reg_j}(z^m_i(s,z^m_{k,o});s)}{\rho^{m-1} \prod_{k=1}^{m} h(v^m_{k,o})} \right| \qquad (2.12)$$

where $h(\ \ ) > o$ is a continuous function normalized to unity and such that $\int_{-\infty}^{+\infty} dv\, h(v)\, v^2 < \infty$. Next define

$$\left\| \underset{\sim}{h}_{reg}(s) \right\|^{reg}_{\beta,1;s'} = \sum_{m=n}^{\infty} \frac{1}{m^\beta} \left\| \underset{\sim}{h}^{(m)}_{reg} \right\|^{reg}_{m;s'} \quad : \quad \beta > 1$$

and $$\left\| \underset{\sim}{h}_{reg}(s) \right\|^{reg}_{\beta,\infty;s'} = \sup_{m\geq n} \frac{1}{m^\beta} \left\| \underset{\sim}{h}^{(m)}_{reg} \right\|^{reg}_{m;s'} \quad : \quad \beta \geq o \qquad (2.13)$$

The spaces $D^{reg}_{\beta,1(\infty);s'}$ corresponding to $\|-\|^{reg}_{\beta,1(\infty);s'} < \infty$ are Banach. An element of the space $D^{reg}_{\beta,1(\infty);s'}$ may, by restriction of domain, be regarded also as an element of the space $D^{reg}_{\beta,1(\infty);s''}$ for $s' \leq s'' \leq t$.

We now undertake an analysis of the linear operator

$\underset{\approx}{C}(z^m_{k,o};s)$. Clearly for $s' \geqslant s$, $\underset{\approx}{C}(z^m_{k,o};s) : D^{reg}_{\beta,1(\infty);s} \to D^{reg}_{\beta,1(\infty);s'}$

Suppose $\underset{\sim}{h}_{reg}(s) \varepsilon D^{reg}_{\beta,1(\infty);s}$ and set $\underset{\sim}{g}_{reg}(s) = \underset{\approx}{C}(z^m_{k,o};s).\underset{\sim}{h}_{reg}(s)$,

then using the inequality

$$\underset{\substack{z^m_{k,o}\varepsilon C_m(s') \\ v_{m+1}\varepsilon R}}{\text{ess sup}} \left| \frac{h^{(m+1)}_{reg_j}(z^m_1(s,z^m_{k,o});\ldots;z^m_n(s,z^m_{k,o});x^m_1(s,z^m_{k,o})^-,v_{m+1};z_{n+1}(s,z^m_{k,o});\ldots;s)}{\rho^m \prod_{k=1}^{m} h(v^m_{k,o}) \,.\, h(v_{m+1})} \right|$$

$$\leqslant \underset{z^{m+1}_{k,o}\varepsilon C_{m+1}(s)}{\text{ess sup}} \left| \frac{h^{(m+1)}_{reg_j}(z^{m+1}_i(s,z^{m+1}_{k,o});s)}{\rho^m \prod_{k=1}^{m+1} h(v^{m+1}_{k,o})} \right| \quad \text{for } s' \geqslant s, \qquad (2.14)$$

it follows that

$$\left\|g^{(m)}_{reg}(s)\right\|^{reg}_{m;s'} \leqslant \underset{z^m_{k,o}\varepsilon C_m(s)}{\text{ess sup}} \left(2\int_{-\infty}^{+\infty} dv_{m+1}(v_{m+1}-v^m_1(s,z^m_{k,o}))\,h(v_{m+1})\right)$$

$$\times \left\|h^{(m+1)}_{reg}(s)\right\|^{reg}_{m+1;s}$$

$$\leqslant 2\alpha_h(v^*) \left\| h^{(m+1)}_{reg}(s) \right\|^{reg}_{m+1;s} \qquad (2.15)$$

where $v^* = \max_{i=1}^{n} |v_i|$ and $\alpha_h(v) = \int_{-\infty}^{+\infty} dw|w-v|h(w)$

In (2.15), we have used that $\underset{z^m_{k,o}\varepsilon C_m(s)}{\text{ess sup}} |v^m_1(s,z^m_{k,o})| \leqslant v^*$

which is a consequence of (2.9). From (2.13) and (2.15)

$$\| g_{reg}(s) \|^{reg}_{\beta,1(\infty);s'} \leqslant 2\left(\frac{n+1}{n}\right)^{\beta} \alpha_h(v^*) \,.\, \| \underset{\sim}{h}_{reg}(s) \|^{reg}_{\beta,1(\infty);s} \qquad (2.16)$$

So $\sup_{o \leq s \leq s' \leq t'} \| \underset{\approx}{C}(s) \|^{reg}_{\beta,1(\infty);s,s'} \leq 2\left(\frac{n+1}{n}\right)^{\beta} \alpha_h(v^*)$ (2.17)

From (2.17), we deduce that there exists a solution to the Cauchy problem for $o \leq s \leq t'$ in $\underset{o \leq s \leq t'}{U}(C_m(s),s)$ given formally by

$$\underset{\sim}{f}_{reg}(s) = \wp\left[\sum_{m=o}^{\infty}\left(\int_o^s ds_m \underset{\approx}{C}(s_m)\int_o^{s_m} ds_{m-1}\underset{\approx}{C}(s_{m-1})\ldots\int_o^{s_2} ds_1 \underset{\approx}{C}(s_1)\right).f_{reg}(s=o)\right] \quad (2.18)$$

where $\wp$ takes account of the jump conditions and is defined as follows $\wp(\underset{\sim}{h}_{reg})^{(m)}_j(s) = (\underset{\sim}{h}^{(m)}_{reg})_{j-K(x_1,v_1;s)}(s)$ where

K( ) is defined in section 2.8. The precise meaning of the integral part of this expression is given in Appendix C. Convergence of the r.h.s. of (2.18) and its derivative with respect to "s" may be proved using (2.17).

To prove uniqueness of bounded solutions, suppose that $\underset{\sim}{f}^o_{reg}(s)$ is such a solution of (2.13) with $\underset{\sim}{f}^o_{reg}(s=o) = \underset{\sim}{o}$ and where, for convenience, we neglect the jump conditions. We show that $\underset{\sim}{f}^o_{reg}(s) = \underset{\sim}{o}$, $o \leq s \leq t'$. From integration of (2.11)

$$\underset{\sim}{f}^o_{reg}(s) = \int_o^s ds' \underset{\approx}{C}(s') \cdot \underset{\sim}{f}^o_{reg}(s') \quad (2.19)$$

(2.19) may be iterated to yield

$$\underset{\sim}{f}^o_{reg}(s) = \left(\int_o^s ds_m \underset{\approx}{C}(s_m)\int_o^{s_m} ds_{m-1}\underset{\approx}{C}(s_{m-1})\ldots\int_o^{s_2} ds_1 \underset{\approx}{C}(s_1)\right) \underset{\sim}{f}^o_{reg}(s_1)$$

for m = 1,2,3,... (2.20)

From (2.16) and (2.20)

$$\|f^o_{reg}(s)\|^{reg}_{\beta,1(\infty);s} \leq \frac{\left[2\left(\frac{n+1}{n}\right)^{\beta}\alpha_h(v^*)s\right]^m}{m!} \sup_{o \leq s_1 \leq s} \|f^o_{reg}(s_1)\|^{reg}_{\beta,1(\infty);s_1}$$

$$\to o \text{ as } m \to \infty \quad (2.21)$$

so $\| \underset{\sim}{f}^o_{reg}(s) \|^{reg}_{\beta,1(\infty);s} = o$, $o \leq s \leq t'$, as required.

To obtain the complete solution to the problem, we must determine the existence and uniqueness of the delta-function part $f_j^{(n)\delta p}(z_2;\ldots;z_n;t)$. The construction of the solution shall be similar to that for the regular part except that here the initial data is not specified at s = o. We confine our attention to m-particle configurations $C_m(s)$ where $z_1 = (X_p+V_p t', V_p)$ at $s = t'$. Let $t_k$ be the solution (if it exists) of

$$X_p + V_p t_k = x_k - v_k t_k, \quad o<t_k<t'; \; k=2,\ldots n \tag{2.22}$$

where $z_k = (x_k, v_k)$ at $s = t'$. If $t_{k*} = \max_{k=2,\ldots,n} t_k$, then for $t_{k*} \leqslant s \leqslant t'$, the particle at $z_1$ at $s = t'$ has not interacted with any other particle for all configurations in $C_m(s)$. So if we consider the equations for

$$f_j^{(m)\delta p}\left(z_2(s);\ldots;z_m(s);s\right)\delta\left(z_1(s)-Z_p(s)\right) + \sum_{i=2}^{n} f_{regj}^{(m-1)}\left(z_1(s);\ldots;\hat{z}_i(s);\ldots\right.$$
$$\left.\ldots;z_m(s);s\right)\delta\left(z_i(s)-Z_p(s)\right) \tag{2.23}$$

in $C_m(s)$ for $t_{k*} \leqslant s \leqslant t'$, only the first term in (2.23) is non-zero and the equations for $f_j^{(m)\delta p}$ take the simplified form

$$\frac{d}{ds} f_j^{m\delta p}(x_2-v_2(t'-s),v_2;\ldots;x_m-v_m(t'-s),v_m;s)$$
$$= \lim_{\epsilon\to o}\int_{-\infty}^{+\infty} dv_{m+1}|v_{m+1}-v_1| \quad \times$$
$$\left[f_{(j)}^{(m+1)\delta p}\left(x_2-v_2(t'-s),v_2;\ldots;x_n-v_n(t'-s),v_n;(X_p+V_p s)^-;v_{m+1};x_{n+1}-v_{n+1}(t'-s),\right.\right.$$
$$\left.v_{n+1};\ldots;x_m-v_m(t'-s),v_m;s\right)$$
$$\left. - f_j^{(m+1)\delta p}\left(x_2-v_2(t'-s);v_2; \;\ldots\; \ldots;s\right)\right] \tag{2.24}$$

where $X^- = X - \epsilon\, \mathrm{sgn}(v_{m+1}-v_1)$

(2.24) may be written in the usual vector form as

$$\frac{d}{ds}\underset{\sim}{f}^{\delta p}(s) = \underset{\approx}{C}(s) \cdot \underset{\sim}{f}^{\delta p}(s) \qquad t_{k*} \leq s \leq t' \tag{2.25}$$

It is necessary to specify the value of the function $\underset{\sim}{f}^{\delta p}(s)$ at $s = t_{k*}^{+}$ To do this, we must reconsider the equations for (2.23) in a neighbourhood of $s = t_{k*}$ :

$$\left(\frac{\partial}{\partial s} + K_j^{(m)}\right)\Big[f_j^{(m)\,\delta p}\big(z_2(s);\ldots;z_m(s);s\big)\ \delta\ \big(z_1(s)-Z_p(s)\big)$$
$$+ \sum_{i=2}^{n} f_{reg_j}^{(m-1)}\big((z_1(s);\ldots;\hat{z}_i(s);\ldots;z_m(s);s\big)\ \delta\ \big(z_i(s)-Z_p(s)\big)\Big]$$
$$= \text{other terms} \tag{2.26}$$

Integrating (2.26) over such a neighbourhood gives

$$\lim_{\epsilon\to o} f_j^{(m)\,\delta p}\left[z_2(t_{k*});\ldots;z_{k*}(t_{k*})^{+};\ldots;z_m(t_{k*});t_{k*}^{+}\right] \tag{2.27}$$
$$= \lim_{\epsilon\to o} f_{reg_j}^{(m-1)}\left[z_1(t_{k*})^{-};z_2(t_{k*});\ldots;z_{k*}(t_{k*});\ldots;z_m(t_{k*});t_{k*}^{-}\right]$$

where $z_{k*}(t_{k*})^{+} = \big(x_{k*}(t_{k*})+v_{k*}\epsilon, v_{k*}\big)$ and $z_1(t_{k*})^{-} = \big(x_1(t_{k*})-v_{k*}\epsilon, v_{k*}\big)$ and $x_1(t_{k*}) = x_{k*}(t_{k*}) = X_p+V_p t_{k*}$. So we must solve (2.25) with initial condition (2.27) in $C_m(s)$ for $t_{k*} \leq s \leq t'$.

The solutions are found in the space of bounded, piece-wise-continuous vector valued functions (whose discontinuities are fixed w.r.t. $x_i$) denoted by $\underset{\sim}{h}^{\delta p}(s)$. The components $h_j^{(m)\,\delta p}\big(x_i-v_i(t'-s);v_i;s\big)$, $m \geq n$ are defined on $C_m(s)$. This space is Banach under the norms given, for $t_{k*} \leq s \leq s' \leq t'$, by

$$\left\|\underset{\sim}{h}^{(m)\,\delta p}(s)\right\|_{m;s'}^{\delta} = \sup_j \ \underset{z_i \epsilon C_m(s')}{\text{ess sup}} \left|\frac{h_j^{(m)\,\delta p}\big(x_i-v_i(t'-s),v_i;s\big)}{\rho^{m-1}\prod_{i=2}^{m} h(v_i)}\right| \tag{2.28}$$

or $\sup_j$ esssup replaced by esssup $\sum_j$

$$\text{and } \|\underset{\sim}{h}^{\delta p}(s)\|^{\delta}_{\beta,1;s'} = \sum_{m=n}^{\infty} \frac{1}{m^{\beta}} \|\underset{\sim}{h}^{(m)\,\delta p}(s)\|^{\delta}_{m,s'} \;:\; \beta > 1$$

(2.29)

$$\|\underset{\sim}{h}^{\delta p}(s)\|^{\delta}_{\beta,\infty;s'} = \sup_{m\geq n}\left(\frac{1}{m^{\beta}} \|\underset{\sim}{h}^{(m)\,\delta p}(s)\|^{\delta}_{m,s'}\right) : \beta \geq 0$$

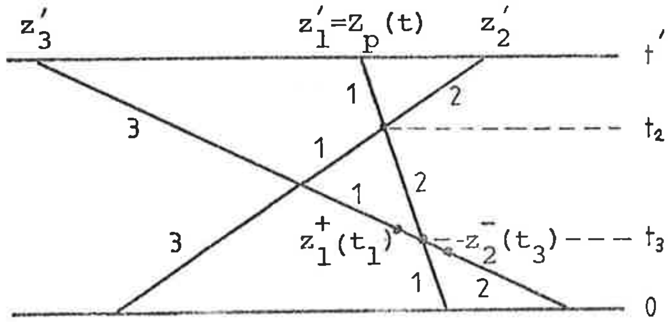
Denote the corresponding spaces by $D^{\delta}_{\beta,1(\infty);s'}$ for $\beta$ as in (2.29). With respect to these norms $\underset{\approx}{C}(s)$ is a bounded linear operator from $D^{\delta}_{\beta,1(\infty);s'}$ for $s \leq s'$. The unique bounded solution to (2.25/7) is given formally by

$$\underset{\sim}{f}^{\delta p}(s) = \sum_{m=0}^{\infty} \int_{t_{k*}}^{s} ds_m \underset{\approx}{C}(s_m) \int_{t_{k*}}^{s_m} ds_{m-1} \underset{\approx}{C}(s_{m-1}) \ldots \int_{t_{k*}}^{s_2} ds_1 \underset{\approx}{C}(s_1) . \underset{\sim}{f}^{\delta p}(s=t^{+}_{k*})$$

$$\text{for } t_{k*} \leq s \leq t' \qquad (2.30)$$

noting that $\underset{\sim}{f}^{\delta p}(s=t^{+}_{k*}) \in D^{\delta}_{\beta,1(\infty);\, t^{+}_{k*}}$.

It is instructive to test the consistency of the above approach, for example, with $n = 3$ and $(z_1', z_2', z_3'; t')$ as shown in the diagram.




Only the first term in (2.23) gives a non-zero contribution for $t_{k*} = t_2 < s \leq t'$. Here $f_j^{(m)\,\delta p}$ satisfy equations (2.24) with the jump conditions (2.27) employed at $t_{k*} = t_2$. For $t_3 < s < t_2$, only $f^{(m-1)}_{reg_j}\left(z_1(s); z_3(s); \ldots; z_m(s); s\right)\delta(z_2(s) - Z_p(s))$ gives a non-zero contribution in (2.23). However $f^{(m-1)}_{reg_j}$ has been previously determined by independent analysis.

The equations here for $t_3 < s < t_2$ are identical with those used previously. It is necessary however to check the consistency of the jump conditions at $s = t_3$. From (2.26)

$$\lim_{\epsilon \to o} f^{(m-1)}_{reg_j} (z_1^+(t_3);\ z_3(t_3);\ldots;z_m(t_3);\ t_3^+) \tag{2.31}$$

$$= \lim_{\epsilon \to o} f_j^{(m)\,\delta p}(z_2^-(t_3);z_3(t_3);\ldots;z_m(t_3);\ t_3^-)$$

with $z_1^+(t_3) = \left[x_3 - v_3\left(t-(t_3+\epsilon)\right), v_3\right], z_2^-(t_3) = \left[x_3 - v_3\left(t-(t_3-\epsilon)\right), v_3\right]$

But from (2.5), since $v_3 < V_p$,

$$\lim_{\epsilon \to o} f^{(m-1)}_{reg_j}\left[z_1^+(t_3);z_3(t_3);\ldots;z_m(t_3);t_3^+\right]$$
$$= \lim_{\epsilon \to o} f^{(m-1)}_{reg_{j+1}}\left[z_2^-(t_3);z_3(t_3);\ldots;z_m(t_3);t_3^-\right] \tag{2.32}$$

That (2.31) and (2.32) are compatible follows from the impenetrability condition (2.18) of Chapter 2.

## 3.3. COUNTABLY NORMED SPACE FORMULATION.

The existence and uniqueness results of the last section are derived in a somewhat more unified fashion here by working in the topology of a countably normed space (see Gelfand and Shilov[57]). The countable set of norms is chosen so that operators of the form $\lim_{\epsilon \to o} \int_{-\infty}^{+\infty} dv_{n+1} |v_{n+1} - v_1| \times \ldots$ are bounded on the entire phase space. The unbounded behaviour of this operator is similar to that of the multaplicative operator $v_1$ so we must ensure that an element of the function space when multiplied by $v_1$ also lies in the space. This is achieved by including a $v_1{}^p$ weighting in the countable set of norms. A similar problem arises in quantum mechanics where the countable set of norms is chosen to make the multaplicative operator "x" bounded (see Böhm[58]). The structure of these norms is similar to those discussed above. Boundedness of the time evolution operator shall make the existence and uniqueness proof much easier.

Again we parameterize the characteristics of $\left(\frac{\partial}{\partial t} + K_j^{(n)}\right)$ by $z_i = z_i^n(s, z_{k,o}^n)$ and $t = s$ where $z_i^n(o, z_{k,o}^n) = z_{i,o}^n$. $f_{regj}^{(n)}(z_i; t) = f_{regj}^{(n)}\left(z_i^n(s, z_{k,o}^n); s\right)$ satisfy the equations (2.8) together with jump conditions (2.5). The following countable set of norms is chosen for the space of vectors $\underset{\sim}{h}_{reg}$ with bounded piecewise-continuous components $h_{reg_j}^{(n)}\left(z_i^n(s, z_{k,o}^n); s\right)$ where the discontinuities are fixed w.r.t. $x_{k,o}^n$.

$$\| \underset{\sim}{h}_{reg}^{(n)} \|_{n;p}^{reg} = \max_{o \leq p' \leq p} \sup_{j} \operatorname{esssup}_{z_{k,o}^n} \left| \frac{\left(\dfrac{v_1^n(s, z_{k,o}^n)}{v_{th}}\right)^{p'} h_{regj}^{(n)}\left(z_i^n(s, z_{k,o}^n); s\right)}{\prod_{k=1}^{n} \rho h(v_{k,o}^n)} \right| \tag{3.1}$$

and
$$\| \underset{\sim}{h}_{reg} \|_{\beta,1;p}^{reg} = \sum_{n=1}^{+\infty} \frac{1}{n^\beta} \left\| \underset{\sim}{h}_{reg}^{(n)} \right\|_{n;p}^{reg} \quad : \quad \beta > 1 \tag{3.2}$$

$$\| \underset{\sim}{h}_{reg} \|_{\beta,\infty;p}^{reg} = \sup_{n \geq 1} \left( \frac{1}{n^\beta} \left\| \underset{\sim}{h}_{reg}^{(n)} \right\|_{n;p}^{reg} \right) \qquad \beta \geq o$$

where
$$h(v) = O\left( \frac{K}{v_{th}} \cdot e^{-c\left(\frac{v}{v_{th}}\right)^{\gamma}} \right) \text{ as } |v| \to \infty \text{ for } \gamma > 1 \text{ and } \int_{-\infty}^{+\infty} dv\, h(v) = 1 \tag{3.3}$$

These norms are compatible and comparable (c.f. Böhm[58]) and thus may be used to define the topology of complete countably normed spaces (denoted $D^{reg\ c.n.}_{\beta,1(\infty)}$).

The hierarchy equations are written formally in vector notation as

$$\frac{d}{d\hat{s}} \underset{\sim}{f}_{reg}(\hat{s}) = \hat{\underset{\approx}{C}}(\hat{s}).\underset{\sim}{f}_{reg}(\hat{s}) \text{ where } \hat{s} = \rho v_{th} s,\ \hat{\underset{\approx}{C}} = (\rho v_{th})^{-1}\underset{\approx}{C} \tag{3.4}$$

together with the usual jump conditions. We show that $\hat{\underset{\approx}{C}}(\hat{s})$ is a bounded operator in the topology of $D^{reg\ c.n.}_{\beta,1(\infty)}$. Clearly $\hat{\underset{\approx}{C}} : D^{reg\ c.n.}_{\beta,1(\infty)} \to D^{reg\ c.n.}_{\beta,1(\infty)}$ Suppose $\underset{\sim}{h}_{reg} \varepsilon D^{reg\ c.n.}_{\beta,1(\infty)}$ and set

$$\underset{\sim}{g}_{reg} = \hat{\underset{\approx}{C}}(\hat{s}).\underset{\sim}{h}_{reg} \tag{3.5}$$

Then

$$\operatorname*{ess\ sup}_{z^n_{k,o}} \left| \frac{\left(\dfrac{v^n_1(s,z^n_{k,o})}{v_{th}}\right)^{p'} g^{(n)}_{reg_j}\left(z^n_i(s;z^n_{k,o});s\right)}{\prod_{k=1}^{n} \rho h(v^n_{k,o})} \right|$$

$$\leqslant \sup_{\left|\frac{v_1}{v_{th}}\right| \geqslant 1} \left( \frac{v^{-1}_{th} \int_{-\infty}^{+\infty} dv_{n+1} |v_{n+1}-v_1| h(v_{n+1})}{\left(\dfrac{v_1}{v_{th}}\right)} \right) . H^{p'+1}_j$$

$$+ \sup_{\left|\frac{v_1}{v_{th}}\right| \leqslant 1} \left( v^{-1}_{th} \int_{-\infty}^{+\infty} dv_{n+1} |v_{n+1}-v_1|\ h(v_{n+1}) \right) . H^{p'}_j$$

$$+ \sup_{\left|\frac{v_1}{v_{th}}\right| \geqslant 1} \left( \frac{v^{-1}_{th} \int_{v_1}^{+\infty} dv_{n+1} |v_{n+1}-v_1|\ h(v_{n+1})}{\left(\dfrac{v_1}{v_{th}}\right)} \right) . \left(H^{p'+1}_{j+1} + H^{p'+1}_{j-1}\right)$$

$$+ \sup_{\left|\frac{v_1}{v_{th}}\right| \leqslant 1} \left( v^{-1}_{th} \int_{v_1}^{+\infty} dv_{n+1} |v_{n+1}-v_1|\ h(v_{n+1}) \right) \left(H^{p'}_{j+1} + H^{p'}_{j-1}\right) \tag{3.6}$$

where $H_j^k$

$$= \underset{z_{k,o}^n}{\text{ess sup}} \left| \frac{\left(\frac{v_1^n(s,z_{k,o}^n)}{v_{th}}\right)^k h_{regj}^{(n+1)} \left(z_1^n(s,z_{k,o}^n), x_1^n(s,z_{k,o}^n)^-, v_{n+1};\ldots;s\right)}{\rho h(v_{n+1}) \prod_{i=1}^{n} \rho h(v_{i,o}^n)} \right| \tag{3.7}$$

We need the inequality

$$H_j^k \leqslant \underset{z_{k,o}^{n+1}}{\text{ess sup}} \left| \frac{\left(\frac{v_1^{n+1}(s,z_{k,o}^{n+1})}{v_{th}}\right)^k h_{regj}^{(n+1)} \left(z_i^{n+1}(s,z_{k,o}^{n+1}),s\right)}{\prod_{i=1}^{n+1} \rho h(v_{i,o}^{n+1})} \right| \tag{3.8}$$

where we have noted that $v_{k,o}^n$ and $v_{n+1}$ equal $v_{j,o}^{n+1}$ for some j if we set $\left(z_1^n(s,z_{k,o}^n);x_1^n(s,z_{k,o}^n)^-,v_{n+1};\ldots\right) = \left(z_1^{n+1}(s,z_{k,o}^{n+1});\ldots\right)$. From (3.8) it follows that

$$\| \underset{\sim}{g}_{reg} \|^{reg}_{\beta,1(\infty);p} \leqslant 2^\beta C(v_{th},h) \cdot \left( \| \underset{\sim}{h}_{reg} \|^{reg}_{\beta,1(\infty);p} + \| \underset{\sim}{h}_{reg} \|^{reg}_{\beta,1(\infty);p+1} \right) \tag{3.9}$$

where $C(v_{th},h) = v_{th}^{-1}\int_{-\infty}^{+\infty} dw|w-v_{th}|h(w) + 2v_{th}^{-1}\int_{-v_{th}}^{+\infty} dw|w-v_{th}|h(w)$

From (3.9), $\hat{\underset{\approx}{C}}(s)$ is bounded (or equivalently, continuous) in the topology of $D^{reg}_{\beta,1(\infty)}$ c.n.

To handle convergence considerations in the existence and uniqueness proof for solutions to the Cauchy problem for (3.4), we also need the following result : there is $K > o$ such that

$$\| \underset{\sim}{h}_{reg} \|^{reg}_{\beta,1(\infty);p+n} \leqslant K(n!)^{\frac{1}{\gamma}} \| \underset{\sim}{h}_{reg} \|^{reg}_{\beta,1(\infty);p} \tag{3.10}$$

for all n, where $\gamma$ is given in (3.3). The solution to the

Cauchy problem has the form given in (2.19)

$$\underset{\sim}{f}_{reg}(\hat{s}) = \wp\left[\sum_{m=o}^{\infty}\left[\int_o^{\hat{s}} d\hat{s}_m\, \hat{\underset{\approx}{C}}(\hat{s}_m)\int_o^{\hat{s}_m} d\hat{s}_{m-1}\, \hat{\underset{\approx}{C}}(\hat{s}_{m-1}) \cdots \int_o^{\hat{s}_2} d\hat{s}_1 \hat{\underset{\approx}{C}}(\hat{s}_1)\right] \cdot \underset{\sim}{f}_{reg}(\hat{s}=o)\right] \tag{3.11}$$

That (3.11) is Cauchy follows from the norm inequalities

$$\left\| \left[\int_o^{\hat{s}} d\hat{s}_m\, \hat{\underset{\approx}{C}}(\hat{s}_m) \int_o^{\hat{s}_m} d\hat{s}_{m-1}\, \underset{\approx}{C}(\hat{s}_{m-1}) \cdots \int_o^{\hat{s}_2} d\hat{s}_1\, \underset{\approx}{C}(\hat{s}_1)\right] \cdot \underset{\sim}{f}_{reg} \right\|^{reg}_{\beta,1(\infty);p}$$

$$\leq 2^{\beta}\, C(v_{th},h) \cdot \int_o^{\hat{s}} d\hat{s}_m \times$$

$$\left\{ \left\| \left(\int_o^{\hat{s}_m} d\hat{s}_{m-1} \hat{\underset{\approx}{C}}(\hat{s}_{m-1}) \cdots \int_o^{\hat{s}_2} d\hat{s}_1\, \hat{\underset{\approx}{C}}(\hat{s}_1)\right) \cdot \underset{\sim}{f}_{reg} \right\|^{reg}_{\beta,1(\infty);p} \right.$$

$$\left. + \left\| \left(\int_o^{\hat{s}_m} d\hat{s}_{m-1}\, \hat{\underset{\approx}{C}}(\hat{s}_{m-1}) \cdots \int_o^{\hat{s}_2} d\hat{s}_1\, \hat{\underset{\approx}{C}}(\hat{s}_1)\right) \cdot \underset{\sim}{f}_{reg} \right\|^{reg}_{\beta,1(\infty);p+1} \right\}$$

$$\leq \frac{\left(2^{\beta+1} C(v_{th},h)\hat{s}\right)^m}{m!} \cdot \max_{o\leq n\leq m} \left\| \underset{\sim}{f}_{reg} \right\|^{reg}_{\beta,1(\infty);p+n} \tag{3.12}$$

Since $D^{reg\ c.n.}_{\beta,1(\infty)}$ is complete, (3.11) is convergent in the countably normed topology to an element of this space. Next we must check that term-by-term differentiation of (3.11) is valid and that the result is equal to $\hat{\underset{\approx}{C}}(\hat{s}).\underset{\sim}{f}_{reg}(\hat{s})$. It can be easily checked that the term-by-term differentiated series is uniformly convergent with respect to time on any finite interval. The result then follows as a simple generalization of the proof for scalar function valued series. The jump conditions are easily checked separately.

Uniqueness comes from an analysis similar to that of section 3.2.,(2.21) for a solution of the Cauchy problem with zero initial conditions is used together with the norm inequality (3.12).

The above approach could be adapted to handle also the delta-function part of the r.d.f.'s. We would need to take account of the delta-function component in our choice of each of the countable number of norms.

## 3.4. ANALYSIS OF $f_j^{(1)\delta}$ FOR THE I.V.P. WITH A SINGLE SPECIFIED PARTICLE.

Exact closed equations for $f_j^{(1)\delta}$ are obtained for the i.v.p. where a single particle "o"has specified position $x = o$ and velocity $v'$ and the rest are in a suitable "factorizing" state at $t = o$. These states are constructed as follows. We start with the state where the background of particles is in equilibrium at $t = o$ (and thus homogeneous). Explicit initial conditions for this state are given in Chapter 2 (3.1-4). In this state certain factorization conditions are satisfied. The particle specified at the origin acts effectively as a hard wall. Since the particles confined to $x < o$ and $x > o$ do not interact, there are no correlations between these particles. So if $j\alpha > o$, $\alpha = 1,\ldots,m$ and $k_\beta < o, \beta = 1,\ldots n$, then

$$f^{(m+n)}_{j1\ldots jmk1\ldots kn}(z_1;\ldots;z_{m+n}) = f^{(m)}_{j1\ldots jm}(z_1;\ldots;z_m)\, f^{(n)}_{k1\ldots kn}(z_{m+1};\ldots;z_{m+n}) \tag{4.1}$$

From Chapter 2 (3.4) and support considerations, we also have the factorization condition

$$\sum_{\substack{j1\, j2\ldots jm \gtrless o \\ j\alpha\neq j\beta \text{ for } \alpha\neq\beta}} f^{(m)}_{j1\ldots jm}(z_1;\ldots;z_m) = \prod_{i=1}^{m} \sum_{j \gtrless o} f_j^{(1)}(z_i) \tag{4.2}$$

in terms of the symmetrized r.d.f.'s for $x \gtrless o$.

An inhomogeneous state is created by switching on an external potential for a certain period of time while specifying that particle "o" should remain at the origin. We examine the time evolution of the symmetrized r.d.f.'s $\sum_{j1 \ldots jm \gtrless o} f^{(m)}_{j1 \ldots jm}$ corresponding to the semi-infinite systems $x \gtrless o$ bounded by a hard wall at the origin. Since these distribution functions are symmetrized, they describe the behaviour of the corresponding systems of unlabelled particles. As observed by Jepsen[40] and Lebowitz & Percus[41] such a system is equivalent to a one-dimensional ideal gas of point particles (confined to $x \gtrless o$ by a hard wall). Consequently the symmetrized m-particle r.d.f.'s remain factorizable as a product of the symmetrized 1-particle r.d.f.'s. So (4.1) and (4.2) are still valid. If we choose for our initial conditions the value of the r.d.f.'s when the external potential is switched off, then

$$f_o^{(n)}(z_1;\ldots;z_n;o) = f_o^{(1)}(z_1;o) \prod_{i=2}^{n} \left( \sum_{k\neq o} f_k^{(1)}(z_i;o) \right) \tag{4.3}$$

using (4.1) and (4.2) for the initial state. If we consider the delta-function behaviour in $z_n$ at t=o, then it is clear that for $j\neq o$

$$f_j^{(n)}(z_1;\ldots;z_n;t) = f_j^{(n-1)}(z_1;\ldots;z_{n-1};o) \left( \sum_{k\neq o} f_k^{(1)}(z_n;o)+\delta(x_n)\delta(v_n-v') \right)$$

$$+ g_j^{(n)}(z_1;\ldots;z_n;o) \tag{4.4}$$

where $g_j^{(n)}(t=o)$ is regular in variables $z_1$ and $z_n$. A suitable limiting procedure must be adopted when considering points with delta-function or discontinuous behaviour (see Chapter 2). In fact (4.3) can also be expressed in the form (4.4) provided we adopt the above-mentioned limit interpretation. Consequently (4.4) may be used for all j.

The initial state has been prepared to satisfy this partial factorization result which shall be crucial for the following analysis. The factorization result is first extended to precollision regions of phase space for times $t > o$ and then used to truncate the hierarchy for the delta-function part of the r.d.f.'s.

The definition of $g_j^{(n)}$ is extended to times $t \geqslant o$ by writing, for $n \geqslant 2$, $f_j^{(n)}(z_1;\ldots;z_n;t)$

$$= f_j^{(n-1)}(z_1;\ldots;z_{n-1};t) \cdot \left[\sum_{k\neq o} f_k^{(1)}(x_n - v_n t, v_n; o) + \delta(x_n - v_n t)\delta(v_n - v')\right]$$

$$+ g_j^{(n)}(z_1;\ldots;z_n;t) \qquad (4.5)$$

with a suitable interpretation of points of discontinuity or delta-function behaviour. For our purposes $f_j^{(n-1)}$ in (4.5) could be replaced by $f_{j^\#}^{(n-1)}$ where $j^\#$ depends only on $v_\alpha - v_\alpha t$ and $j^\# = j$ when $x_1 - v_1 t = o$. We confine our attention from now on to the precollision regions of phase space $R_p^t$ defined in the last chapter. $g_j^{(n)}$ satisfy the same set of equations as $f_j^{(n)}$ here with $\left(\frac{\partial}{\partial t} + K_j^{(n)}\right)$ replaced by $\left(\frac{\partial}{\partial t} + \sum_{i=1}^{n} v_i \frac{\partial}{\partial x_i}\right)$. Since these equations are invariant on precollision regions, they may be integrated along the characteristics of $\left(\frac{\partial}{\partial t} + \sum_{i=1}^{n} v_i \frac{\partial}{\partial x_i}\right)$ in some region $\bigcup_{o\leqslant t\leqslant T} (R_p^t, t)$. Since $g_j^{(n)}$ is regular in $z_1$ and $z_n$ at $t = o$, it follows easily from the hierarchy equations that $g_j^{(n)}$ are regular in $z_1$ and $z_n$ throughout precollision regions. In particular $g_j^{(2)}(z_1;x_1^-,v_2;t)$ is regular for all $\epsilon > o$, $t \geqslant o$.

This is the main result used in the analysis of the first order hierarchy equations for $f_j^{(1)}$. Upon substitution of the factorized form for $f_j^{(2)}$, we obtain

$$\left(\frac{\partial}{\partial t} + v_1 \frac{\partial}{\partial x_1}\right) f_j^{(1)}(z_1;t) = \gamma_f(x_1 v_1;t)\left(f_{j-1}^{(1)}(z_1;t) - f_j^{(1)}(z_1;t)\right)$$

$$+ \beta_f(x_1,v_1;t)\left(f_{j+1}^{(1)}(z_1;t) - f_j^{(1)}(z_1;t)\right)$$

$$+ \lim_{\xi\to o} \delta(x_1^{=} - v't) \cdot \left[\begin{array}{c} H(v'-v_1)(v'-v_1)\left(f_{j+1}^{(1)}(z_1;t) - f_j^{(1)}(z_1;t)\right) \\ + \\ H(v_1-v')(v_1-v')\left(f_{j-1}^{(1)}(z_1;t) - f_j^{(1)}(z_1;t)\right)\end{array}\right]$$

$$+ \lim_{\epsilon\to o} \int_{-\infty}^{+\infty} dv_2 |v_2-v_1| \times \left(g_{(j)}^{(2)}(z_1;x_1^-,v_2;t) - g_j^{(2)}(z_1;x_1^-,v_2;t)\right) \qquad (4.6)$$

where $\gamma_f(x_1,v_1;t) = \int_{-\infty}^{v_1} dv_2 (v_1-v_2)\ f(x_1-v_2t,v_2;o)$

and $\beta_f(x_1,v_1;t) = \int_{v_1}^{+\infty} dv_2 (v_2-v_1)\ f(x_1-v_2t,v_2;o) \qquad (4.7)$

with $f = \sum_{k\neq o} f_k^{(1)}$ . Since the last term in (4.6) is regular, we conclude that the term exhibiting explicitly the delta-function may be replaced by the jump condition

$$\lim_{\xi\to o} f_j^{(1)}(v't-\xi,v_1;t) = \lim_{\xi\to o} f_{j+1}^{(1)}(v't+\xi,v_1;t) \qquad (4.8)$$

The resulting equation is satisfied everywhere except across the line $x_1=v't$ where $f_j^{(1)}$ have a simple discontinuity given by (4.8).

In the following we consider only the delta-function part of $f_j^{(1)}$. Consequently we make the decomposition

$$f_j^{(1)}(z_1;t) = f_j^{(1)\delta}(v',t)\,\delta(x_1-v_1t)\,\delta(v_1-v') + f_{reg_j}^{(1)}(z_1;t) \tag{4.9}$$

where $f_j^{(1)\delta}$ and $f_{reg_j}^{(1)}$ are regular. Substituting (4.9) into (4.6) gives uncoupled equations for $f_j^{(1)\delta}$ and $f_{reg_j}^{(1)}$.

In particular for $f_j^{(1)\delta}$, (4.9) yields the exact equations

$$\frac{d}{dt} f_j^{(1)\delta}(v',t) = \gamma_f(v',t) \cdot \left[f_{j-1}^{(1)\delta}(v',t) - f_j^{(1)\delta}(v',t)\right]$$

$$+ \beta_f(v',t) \cdot \left[f_{j+1}^{(1)\delta}(v',t) - f_j^{(1)\delta}(v',t)\right] \tag{4.10}$$

where $\gamma_f(v',t) = \gamma_f(v't,v';t)$, $\beta_f(v',t) = \beta_f(v't,v';t)$

These are the equations that we shall analyse throughout the remainder of this section.

The initial conditions associated with the problem described are simply

$$f_j^{(1)\delta}(v',o) = \delta_{j,o} \tag{4.11}$$

Consider now a class of i.v.p.'s, labelled by N, where the r.d.f.'s for particle "j" are given by $f_{j-N}^{(m)}(z_1;\ldots;z_m;o)$. If we take an arbitrary convex linear combination of these initial conditions, it follows that $f_j^{(1)\delta}$ will still satisfy (4.10), but now we have the more general initial conditions :

$$f_j^{(1)\delta}(v',o) \geqslant o \text{ for all } j \text{ and } \sum_{j=-\infty}^{+\infty} f_j^{(1)\delta}(v',o) = 1. \tag{4.12}$$

A conservation result is easily derived from (4.10) by summing over the index "j", namely

$$\sum_{j=-\infty}^{+\infty} f_j^{(1)\delta}(v',t) = \sum_{j=-\infty}^{+\infty} f_j^{(1)\delta}(v',o) = 1 \text{ for all } t \geqslant o \qquad (4.13)$$

i.e. there is a probability of one of finding a particle at $x_1 = v't$ given that this is the case at $t = o$.

The equations (4.10) can be solved by Fourier transform techniques described by Anstis et. al.[42]. However, the analysis developed below will exhibit more clearly the structure of these equations. First let us consider the case of an homogeneous background of particles with velocity distribution $h(v)$ (normalized to one). So $f(z;o) = \rho h(v)$. This includes the case of quasi-equilibrium initial conditions. From (4.7)

$$\gamma_{\rho h}(v',t) = \gamma_{\rho h}(v') = \rho\int_{-\infty}^{v'} dw(v'-w)\ h(w)$$

$$\beta_{\rho h}(v',t) = \beta_{\rho h}(v') = \rho\int_{v'}^{+\infty} dw(w-v')\ h(w) \qquad (4.14)$$

(4.10) may be written in vector form as

$$\frac{d}{dt} \underset{\sim}{f}^{(1)\delta} = \underset{\approx}{C}^{\delta} \cdot \underset{\sim}{f}^{(1)\delta} \qquad (4.15)$$

where $f^{(1)\delta}$ is regarded as a column vector in the sequence space $\iota^1$ with components $f_j^{(1)\delta}$. The $\iota^1$ norm is defined by

$$\left\| \underset{\sim}{f}^{(1)\delta} \right\|_1 = \sum_{j=-\infty}^{+\infty} \left| f_j^{(1)\delta} \right| .$$ $\underset{\approx}{C}^{\delta} : \iota^1 \to \iota^1$ is a bounded, non-compact, linear operator (see Taylor[59]). In the usual matrix representation $\underset{\approx}{C}^{\delta} = (C_{ij}^{\delta})$, we have

$$C_{ij}^{\delta} = \beta_{\rho h}(v')\delta_{j-1,i} + \gamma_{\rho h}(v')\delta_{j+1,i} - \left(\beta_{\rho h}(v')+\gamma_{\rho h}(v')\right)\delta_{j,i} \qquad (4.16)$$

We next determine the spectrum of $\underset{\approx}{C}^{\delta}$ as this will provide a qualitative understanding of the nature of the approach to equilibrium. Let $\sigma(\cdot)$ denote the spectrum of an operator so $\sigma(\cdot) = P\sigma(\cdot) \dot{\cup} R\sigma(\cdot) \dot{\cup} C\sigma(\cdot)$ where $P\sigma(\cdot)$, $R\sigma(\cdot)$ and $C\sigma(\cdot)$ denote the point, residue and continuous spectra (resp.) Define the bounded linear operator $\underset{\approx}{C}{}_o^\delta$ on $\iota^1$ by

$$\underset{\approx}{C}^\delta = \underset{\approx}{C}{}_o^\delta - (\gamma_{\rho h} + \beta_{\rho h})\, \underset{\approx}{I} \tag{4.17}$$

It will suffice to determine the spectrum of $\underset{\approx}{C}{}_o^\delta$.

First we prove that $P\sigma(\underset{\approx}{C}{}_o^\delta)$ is empty. The eigenvalue equation in component form for $\underset{\approx}{C}{}_o^\delta$ becomes

$$\lambda f_j = \gamma_{\rho h} f_{j-i} + \beta_{\rho h} f_{j+1} \quad \text{for all } j,\ \underset{\sim}{f}(\neq \underset{\sim}{o}) \in \iota^1 \tag{4.18}$$

Define the (continuous) function $\eta(\theta) = \sum_{j=-\infty}^{+\infty} e^{\hat{\imath}\theta j} f_j$.

$\eta(\theta)$ is not identically zero by Parseval's formula. Transforming (4.18) gives

$$\left[\lambda - (\gamma_{\rho h} e^{+\hat{\imath}\theta} + \beta_{\rho h} e^{-\hat{\imath}\theta})\right]\eta(\theta) = o \tag{4.19}$$

A contradiction is obtained from (4.19) by considering the range of "$\theta$" for which $\eta(\theta) \neq o$, since $\gamma_{\rho h}, \beta_{\rho h} > o$ and $\lambda$ must be independent of "$\theta$". Thus $P\sigma(\underset{\approx}{C}{}_o^\delta) = \emptyset$

To determine the other components of $\sigma(\underset{\approx}{C}{}_o^\delta)$, we consider $\underset{\approx}{C}{}_o^{\delta'}$, the Banach space adjoint of $\underset{\approx}{C}{}_o^\delta$. $\underset{\approx}{C}{}_o^{\delta'}$ is a bounded linear operator in the dual space $\iota^\infty$ of $\iota^1$ ($\iota^\infty$ is the space of bounded sequences). In the usual matrix representation $\underset{\approx}{C}{}_o^{\delta'} = (C_{o\,ij}^{\delta'})$, we have

$$C_{o\,ij}^{\delta'} = \gamma_{\rho h}\,\delta_{j-1,i} + \beta_{\rho h}\,\delta_{j+1,i} \tag{4.20}$$

To proceed further an alternative characterization of the spectrum is used. For a bounded linear operator $\underset{\approx}{G}$ on a sequence space $\ell$, define the compression spectrum to be

$$\Gamma(\underset{\approx}{G}) = \{\lambda \varepsilon C : R(\lambda \underset{\approx}{I} - \underset{\approx}{G}) \neq \ell\} \quad (R = \text{range}) \qquad (4.21)$$

Then $R\sigma = \Gamma \backslash P\sigma$ (see Halmos[60]). Consequently $\sigma(\underset{\approx}{C}_o^{\delta}) = C\sigma(\underset{\approx}{C}_o^{\delta}) \dot{\cup} \Gamma(\underset{\approx}{C}_o^{\delta})$. However since we also have $\Gamma(\underset{\approx}{C}_o^{\delta}) = P\sigma(\underset{\approx}{C}_o^{\delta'})$, $\sigma(\underset{\approx}{C}_o^{\delta}) = C\sigma(\underset{\approx}{C}_o^{\delta}) \dot{\cup} P\sigma(\underset{\approx}{C}_o^{\delta'})$.

We prove that $C\sigma(\underset{\approx}{C}_o^{\delta})$ is contained in the ellipse

$$E = \{\lambda \varepsilon C : \lambda = \gamma_{\rho h}\, e^{+\hat{i}\theta} + \beta_{\rho h} e^{-\hat{i}\theta} : \theta \varepsilon [o; 2\pi)\} \qquad (4.22)$$

From the corresponding analysis for $\underset{\approx}{C}_o^{\delta}$ on the Hilbert space $\ell^2 \geqslant \ell^1$ (Appendix D), $C\sigma(\underset{\approx}{C}_o^{\delta}) = E$ in $\ell^2$. Now suppose $\lambda \varepsilon C\sigma(\underset{\approx}{C}_o^{\delta})$ in $\ell^1$. Choose $\epsilon > o$ and $\underset{\sim}{y} \varepsilon \ell^2$. We may write $\underset{\sim}{y} = \underset{\sim}{y}_{\ell^1} + \delta \underset{\sim}{y}$ where $\underset{\sim}{y}_{\ell^1}$ has only a finite number of non-zero entries and $\|\delta \underset{\sim}{y}\|_2 < \epsilon/2$. Now since $\lambda \varepsilon C\sigma(\underset{\approx}{C}_o^{\delta})$ in $\ell^1$, there is $\underset{\sim}{x}_{\ell^1}$ in $\ell^1$ such that $\|(\lambda \underset{\approx}{I} - \underset{\approx}{C}_o^{\delta})\underset{\sim}{x}_{\ell^1} - \underset{\sim}{y}_{\ell^1}\|_1 < \epsilon/2$.

So $\|(\lambda \underset{\approx}{I} - \underset{\approx}{C}_o^{\delta})\underset{\sim}{x}_{\ell^1} - \underset{\sim}{y}\|_2 \leqslant \|(\lambda \underset{\approx}{I} - \underset{\approx}{C}_o^{\delta})\underset{\sim}{x}_{\ell^1} - \underset{\sim}{y}_{\ell^1}\|_1 + \|\delta \underset{\sim}{y}\|_2 < \epsilon$

Since $\|\cdot\|_2 \leqslant \|\cdot\|_1$ and consequently $\lambda \varepsilon C\sigma(\underset{\approx}{C}_o^{\delta})$ in $\ell^2$
Hence $C\sigma(\underset{\approx}{C}_o^{\delta}) \subseteq E$ in $\ell^1$.

To complete the analysis, we determine $P\sigma(C_o^{\delta'})$. Let $\underset{\sim}{x}(\neq \underset{\sim}{o}) \varepsilon \ell^{\infty}$ be an eigenvector of $\underset{\approx}{C}_o^{\delta'}$ corresponding to the eigenvalue $\lambda$. The $j^{th}$ component of the eigenvalue equation becomes $\lambda x_j = \gamma_{\rho h} x_{j+1} + \beta_{\rho h} x_{j-1}$. We transform this equation to one in a generalized function space $Q'$ (for a suitable class of test functions $Q$). Define

$$\zeta(\theta) = \sum_{j=-\infty}^{+\infty} e^{\hat{i}\theta j} x_j \;\varepsilon\; Q' \qquad (4.23)$$

For example, in the space of tempered distributions, the above series converges to a generalized function $\zeta$ if and only if $x_j = O(|j|^N)$ for some N as $|j|\to\infty$ (see Lighthill[61]). Furthermore $\underset{\sim}{x} \neq o$ in $\iota^\infty$ implies $\zeta \neq o$ in $Q'$. Transforming the eigenvalue equation gives

$$\left\{\lambda - (\gamma_{\rho h}e^{-\hat{i}\theta} + \beta_{\rho h}e^{+\hat{i}\theta})\right\}\zeta(\theta) = o \qquad (4.24)$$

If $\lambda \notin E$, this equation has no non-zero solutions $\zeta \in Q'$ (a contradiction). Therefore $P\sigma(\underset{\approx}{C}_o^{\delta'}) \subseteq E$. Suppose $\lambda = \gamma_{\rho h}\, e^{-\hat{i}\theta^*} + \beta_{\rho h}\, e^{+\hat{i}\theta^*}$ for some $\theta^* \in [o,2\pi]$ (so $\lambda \in E$). The corresponding $\iota^\infty$ eigenvector is given in component form by $x_j = \frac{1}{2\pi}\, e^{-\hat{i}\theta^* j}$ (j an integer). Consequently $P\sigma(\underset{\approx}{C}_o^{\delta'}) = E$.

In conclusion

$$\sigma(\underset{\approx}{C}^\delta) = R\sigma(\underset{\approx}{C}^\delta)$$

$$= \{\lambda \in C : \lambda = (\gamma_{\rho h} + \beta_{\rho h})(\cos\theta - 1) + (\gamma_{\rho h} - \beta_{\rho h})i \sin\theta : \theta\varepsilon[o,2\pi]\} \qquad (4.25)$$

Returning to the general case, we rewrite (4.10) as an $\iota^1$ equation

$$\frac{d}{dt}\, \underset{\sim}{f}^{(1)\delta} = \underset{\approx}{C}^\delta(t)\ .\ \underset{\sim}{f}^{(1)\delta} \qquad (4.26)$$

where in the usual matrix representation $\underset{\approx}{C}^\delta(t) = \{C_{ij}^\delta(t)\}$, we have

$$C_{ij}^\delta(t) = \beta_f(v',t)\delta_{j-1,i} + \gamma_f(v',t)\delta_{j+1,i} - \{\beta_f(v',t)+\gamma_f(v',t)\}\delta_{j,i} \qquad (4.27)$$

Using the commutation property (verified by direct calculation)

$$\left[\underset{\approx}{C}^\delta(t),\ \underset{\approx}{C}^\delta(t')\right]_- = o \text{ for all } t,t' \geqslant o. \qquad (4.28)$$

and the Baker-Campbell-Hausdorff theorem, it follows that the solution to (4.26) is given by

$$\underset{\sim}{f}^{(1)\delta}(v',t) = \exp\left(\left[\frac{1}{t}\int_o^t dt' \underset{\approx}{C}^{\delta}(t')\right].t\right) \cdot \underset{\sim}{f}^{(1)\delta}(v',o) \qquad (4.29)$$

The behaviour of $\underset{\sim}{f}^{(1)\delta}$ in time is determined by the spectrum of the operator $\frac{1}{t}\int_o^t dt' \underset{\approx}{C}^{\delta}(t')$. From (4.25), we may deduce that this is given by

$$\sigma\left(\frac{1}{t}\int_o^t dt' C^{\delta}(t')\right) = R\sigma\left(\frac{1}{t}\int_o^t dt' \underset{\approx}{C}^{\delta}(t')\right)$$

$$= \left\{\lambda\varepsilon C : \lambda = \left(\gamma_f^{av}(v',t)+\beta_f^{av}(v't)\right)(\cos\theta-1)+\left(\gamma_f^{av}(v',t)-\beta_f^{av}(v',t)\right) \times \hat{i}\sin\theta : \theta\varepsilon[o,2\pi]\right\} \qquad (4.30)$$

where $\gamma_f^{av}(v',t)=\frac{1}{t}\int_o^t dt'\gamma_f(v',t')$ and $\beta_f^{av}(v',t) = \frac{1}{t}\int_o^t dt'\beta_f(v',t')$

For such $\lambda$, Re $\lambda \leqslant o$, so the solutions of (4.26) decay towards equilibrium.

For a special choice of initial conditions, we consider the asymptotic behaviour of $\beta_f$, $\gamma_f$ as $t \to \infty$. Suppose for $j \neq o$, $f_j^{(1)}(z_1;o) = f_j^s(x_1;o)h(v_1)$ with $h(\ )$ as in (4.14) and with $f^s = \sum_{j\neq o} f_j^s$ (C-1) summable on $(o,\infty)$ and $(-\infty,o)$ to $\rho$. $f_j^s$ could for example be the spatial part of the equilibrium distributions $f_j^{(1)}$ under some external potential. In this case

$$\gamma_f(v',t) = \int_{-\infty}^{v'} dw\ (v'-w).f^s\left[(v'-w)t\right]\ h(w)$$

$$(4.31)$$

$$\beta_f(v',t) = \int_{v'}^{+\infty} dw\ (w-v').f^s\left[(v'-w)t\right]h(w)$$

$\beta_f(v',t)$ has the form

$$\beta_f(v',t) = \frac{1}{t}\int_o^{\infty} dy\ G\left(\frac{y}{t}\right)f^s(y) \qquad (4.32)$$

where $G(x) = xh(x+v') \ \varepsilon\ L^1(-\infty,+\infty)$ and $f^s$ is bounded and strongly measurable. Define a class of functions $G_1(\tau) \varepsilon W(o,\infty) \subseteq L^1(o,\infty)$ by the requirement that $\int_o^\infty d\tau\ \tau^{\lambda\hat{i}} G_1(\tau) \neq o$ for all real $\lambda$. In particular $G_1(\tau) = H(1-\tau) \varepsilon W(o,\infty)$. The asymptotic analysis of $\beta_f(v',t)$ shall be achieved using a Tauberian theorem proved by Wiener[62] (see also Hille[63]). If $G_1 \varepsilon W(o,\infty)$, $G \varepsilon L^1(o,\infty)$ and $f^s$ is bounded and strongly measurable, then

$$\lim_{t\to\infty} \frac{1}{t} \int_o^{+\infty} dy\ G_1\left(\frac{y}{t}\right) f^s(y) = a \int_o^{+\infty} dy\ G_1(y) \qquad (4.33)$$

implies $\lim_{t\to\infty} \frac{1}{t} \int_o^{+\infty} dy\ G\left(\frac{y}{t}\right) f^s(y) = a \int_o^{+\infty} dy\ G(y)$

The theorem may be proved by noting that the dilations about the origin of any $G_1 \varepsilon W(o,\infty)$ are dense in $L^1(o,\infty)$. Making the choice of functions indicated, it follows from (4.33) that $\lim_{t\to\infty} \beta_f(v',t) = \beta_{\rho h}(v')$. A similar analysis shows that

$\lim_{t\to\infty} \gamma_f(v',t) = \gamma_{\rho h}(v')$. So for this case, the form of the governing equations (4.10) in the $t\to\infty$ limit depends only on the details of $f^s$ through $\rho$ i.e. the details of the inhomogeneity of the initial distribution do not affect the asymptotic nature of the approach to equilibrium. Also since $\beta_f(v',t)$ $\left(\text{resp.}\,\gamma_f(v',t)\right)$ must be (C-1) summable to $\beta_{\rho h}(v')$ $\left(\text{resp.}\ \gamma_{\rho h}(v')\right)$, the set $\sigma\left[\frac{1}{t}\int_o^t dt' \underset{\approx}{C}^{\delta}(t')\right]$ approaches $\sigma\left(\underset{\approx}{C}^{\delta}\right)$ as $t\to\infty$.

A detailed analysis of the nature of the asymptotic approach to equilibrium may also be made. Specifically for the initial conditions $f_j^{(1)\delta}(t=o) = \delta_{j,o}$, the solution of (4.10) by Fourier analysis is

$$f_j^{(1)\delta}(v',t) = \frac{1}{2\pi}\int_{-\pi}^{+\pi} d\theta \, \exp\left\{\hat{i}[(\gamma_f^{av}-\beta_f^{av})(\sin\theta)t - j\theta]\right\}\exp\left\{(\gamma_f^{av}+\beta_f^{av})(\cos\theta-1)t\right\} \tag{4.34}$$

The asymptotic analysis of (4.34) as $t \to \infty$ is suited to Laplace's method (see Carrier et. al.[64]). We obtain

$$f_j^{(1)\delta}(v',t) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\theta \, \exp\left\{\hat{i}[(\gamma_f^{av}-\beta_f^{av})t-j]\theta\right\}\exp\left\{-\frac{1}{2}(\gamma_f^{av}+\beta_f^{av})\theta^2 t\right\}$$

$$\sim \frac{1}{(2\pi)^{\frac{1}{2}}}\exp\left[\frac{(\gamma_f^{av}-\beta_f^{av})}{(\gamma_f^{av}+\beta_f^{av})}\cdot j\right]\frac{1}{[(\gamma_f^{av}+\beta_f^{av})t]^{\frac{1}{2}}}\exp\left[-\frac{(\gamma_f^{av}-\beta_f^{av})^2 t}{2(\gamma_f^{av}+\beta_f^{av})}\right] \tag{4.35}$$

as $t \to \infty$

This decay is associated with a time scale "$t_{th}$", the mean free time. Correlation functions associated with the delta-function part of the r.d.f.'s are usually derived from expressions of the form

$$\int_{-\infty}^{+\infty} dv' C(v') \; f_j^{(1)\delta}(v',t) \tag{4.36}$$

for suitable $C(v')$. The asymptotic behaviour of (4.34) as $t \to \infty$ depends on the nature of $\gamma_f^{av} \pm \beta_f^{av}$ as functions of "$v'$" in this limit. For the above mentioned choice of initial conditions where $f(z;o) = f^s(x)h(v)$, we have

$$\gamma_f^{av}(v',t) - \beta_f^{av}(v',t) \sim \rho v' \qquad \text{as } t \to \infty \tag{4.37}$$

and $\gamma_f^{av}(v',t) + \beta_f^{av}(v',t) > \text{const.}(>o)$ for $t$ sufficiently large.

It follows that the major contribution to (4.33) for large "t" comes from the neighbourhood of $v' = o$. If $C(v') \sim c.v'^n$ as $v' \to o$, then

$$\int_{-\infty}^{+\infty} dv' C(v') \; f_j^{(1)\delta}(v',t) \sim k\left(\frac{t_{th}}{t}\right)^{\frac{n}{2}+1} \quad \text{as } t \to \infty \tag{4.38}$$

## 3.5. ANALYSIS OF $f_j^{(1)\delta p}$ FOR THE GENERAL I.V.P.

The specified particles at t = o are chosen as in section 2.8. The remaining particles in each cell $(X_i, X_{i+1})$ may be distributed inhomogeneously at t = o. We require that the higher order symmetrized r.d.f.'s for each cell should factorize as a product of symmetrized one-particle r.d.f.'s and that there be no correlations between particles in different cells at t = o. Such states may be prepared by the application of an external potential to the corresponding quasi-equilibrium state (c.f. section 3.4). There should also be appropriate (C-1) summability constraints on the initial conditions to ensure that the mean particle numbers $\rho_o$ (resp. $\rho_N$) exist for the cells $(-\infty, X_1)$ [resp. $(X_N, \infty)$].

If $m_K$ of the $x_i$ (i=1,2,...,n) lie in the cell $(X_K, X_{K+1})$, then because of the above factorization property

$$f_{n\alpha}^{(n)}(z_1;\dots;z_n;o) = f_{n\alpha}^{(1)}(z_1;o) \cdot \prod_{\substack{K=1\\ m_K\neq o}}^{N-1} \left( \prod_{j=1}^{m_K} \frac{P_K-j+1}{P_K} \right)$$

$$\times \prod_{j=2}^{n} \left[ \sum_{i=1}^{N} \delta(x_j - X_i)\delta(v_j - V_i) + f(z_j) \right]$$

$$= f_{n\alpha}^{(n-1)}(z_1,\dots,z_{n-1};o) \cdot C(x_2,\dots,x_n)$$

$$\times \left[ \sum_{i=1}^{N} \delta(x_n - X_i)\delta(v_n - V_i) + f(z_n) \right] \qquad (5.1)$$

where here $f(z) = \sum_{\substack{k\neq n\alpha\\ \alpha=1,\dots,N}} f_k^{(1)}(x,v;o)$

and $C(x_2;\ldots;x_n) = 1$ if $x_n = X_k$ for some k

$$= \frac{P_K - m_K + 1}{P_K} \quad \text{if } x_n \in (X_K, X_{K+1})$$

The numerical factor appears as a consequence of normalization. A suitable limit procedure must be adopted for the interpretation of (5.1) at points with delta-function or discontinuous behaviour. If we write

$$f_j^{(n)}(z_1;\ldots;z_n;t)$$
$$= f_j^{(n-1)}(z_1;\ldots;z_{n-1};t) \times \left[\sum_{i=1}^{N} \delta\left((x_n - v_n t) - X_i\right)\delta(v_n - V_i) + f(z_n;t)\right]$$
$$+ g_j^{(n)}(z_1;\ldots;z_n;t) \qquad (5.2)$$

again adopting a suitable limit interpretation where necessary. $g_j^{(n)}$ satisfies the same set of equations as $f_j^{(n)}$ with $\left(\frac{\partial}{\partial t} + K_j^{(n)}\right)$ replaced by $\left(\frac{\partial}{\partial t} + \sum_{i=1}^{n} v_i \frac{\partial}{\partial x_i}\right)$ on precollision regions of phase space and the equations may be integrated on such regions. It is clear from (5.2) and (5.1) that here $g_j^{(n)}(z_1;\ldots;z_n;o)$ is regular in $z_n$ and that the coefficient of the delta-function part of $g_j^{(n)}(t=o)$ with respect to $z_1$ (denoted $g_j^{(n)\delta p}$) has an order of magnitude

$$\delta_{j,np} \; f^{(n-2)}(z_2;\ldots;z_{n-1};o) \; f(z_n;o) \min\left[O(1), O\left((n-2)\epsilon\right)\right]$$
$$\text{where } \epsilon = \max_i \frac{1}{P_i} \qquad (5.3)$$

From the governing equations it therefore follows that, in precollision regions, $g_j^{(n)}$ will be regular in $z_n$ and $g_j^{(n)\delta p}$ will be bounded by exponential growth from the maximum initial value. Banach space techniques may again be employed here to provide a rigorous analysis. The above remarks apply, in particular, to $g_j^{(2)}(z_1;x_1^-,v_2;t)$.

If we make the decomposition

$$f_j^{(1)}(z_1;t) = \sum_{i=1}^{N} f_j^{(1)\delta i}(t)\,\delta\big((x_1-v_1t)-X_i\big)\,\delta(v_1-V_i)$$

$$+ f_{reg_j}^{(1)}(z_1;t)$$

$$g_j^{(2)}(z_1;x_1^-,v_2;t) = \sum_{i=1}^{N} g_j^{(2)\delta i}\big((X_i+V_it)^-,v_2;t\big)\,\delta\big((x_1-v_1t)-X_i\big)\,\delta(v_1-V_i)$$

$$+ g_{reg_j}^{(2)}(z_1;x_1^-,v_2;t) \qquad (5.4)$$

then (5.2) may be used to yield the following equation

$$\frac{d}{dt}\, f_j^{(1)\delta i}(t) = \gamma_f^i(t)\,.\,\left[f_{j-1}^{(1)\delta i}(t) - f_j^{(1)\delta i}(t)\right] \qquad (5.5)$$

$$+ \beta_f^i(t)\,.\,\left[f_{j+1}^{(1)\delta i}(t) - f_j^{(1)\delta i}(t)\right] + \varsigma_j^{\delta i}(t)$$

$$\text{with } \varsigma_j^{\delta i}(t) = \lim_{\epsilon\to o}\int_{-\infty}^{+\infty} dv_2\,|v_2-V_i|\,.\,\left[g_{(j)}^{(2)\delta i}\big((X_i+V_it)^-,v_2;t\big) - g_j^{(2)\delta i}\big((X_i+V_it)^-,v_2;t\big)\right] \qquad (5.6)$$

except for $t = t_{i,k}$ where $f_j^{(1)\delta i}$ are discontinuous and satisfy the jump conditions (8.12) of Chapter 2. We have set

$$\gamma_f^i\,(t) = \int_{-\infty}^{V_i} dw\,(w-V_i)\,.\,f(X_i+(V_i-w)t,w)$$

$$\beta_f^i\,(t) = \int_{V_i}^{+\infty} dw\,(V_i-w)\,.\,f(X_i+(V_i-w)t,w) \qquad (5.7)$$

Approximate kinetic equations for $f_j^{(1)\delta i}$ are obtained by neglecting the last term on the r.h.s. of (5.5). In the regime $P_i \geqq \frac{1}{\epsilon} >> 1$ they will be accurate for

$$o \leqslant \rho v_{th} t << \frac{\ell n P}{4\hat{\alpha}\left(\frac{V_i}{v_{th}}\right)} \tag{5.8}$$

For the case $f(x,v) = f^S(x)h(v)$, $N<\infty$, we have

$$\gamma_f^i\ (t) \sim \rho_N \int_{-\infty}^{V_i} dw(w-V_i)h(w),\ \beta_f^i\ (t) \sim \rho_{-1}\int_{V_i}^{+\infty} dw(V_i-w)h(w) \text{ as } t \to \infty \tag{5.9}$$

The periodic problem where the specified particles are at x = KL with velocity v´ at t = o may be treated as a subcase here. If $\bar{f}_j^{(1)\delta} = \sum_{j'\equiv j(\mathrm{mod}P+1)} f_{j'}^{(1)\delta}$ and

$\bar{\zeta}_j^{\delta} = \sum_{j'\equiv j(\mathrm{mod}P+1)} \zeta_{j'}^{\delta}$, we may sum (5.5) over equal j (mod P+1) to obtain

$$\frac{d}{dt}\ \underset{\sim}{\bar{f}}^{(1)\delta}(t) = \underset{\approx}{C}_f^P\ (v',t)\ .\ \bar{f}^{(1)\delta}(t) + \underset{\approx}{\bar{\zeta}}^{\delta}(t) \tag{5.10}$$

where $\underset{\sim}{\bar{f}}^{(1)\delta}$ (resp. $\underset{\approx}{\bar{\zeta}}^{\delta}$) is a (P+1) dimensional vector with components $\bar{f}_j^{(1)\delta}$ (resp. $\bar{\zeta}_j^{\delta}$) and

$$\underset{\approx}{C}_f^P\ (v',t) = \bar{\gamma}_f\ \underset{\approx}{\Delta}^- + \bar{\beta}_f\ \underset{\approx}{\Delta}^+ - (\bar{\gamma}_f + \bar{\beta}_f)\ \underset{\approx}{I}$$

$$\text{and } \bar{\gamma}_f\ (v',t) = \int_{-\infty}^{v'} dw(w-v')\ f\ \big((v'-w)\ t,\ w\big) \tag{5.11}$$

$$\bar{\beta}_f\ (v',t) = \int_{v'}^{+\infty} dw(v'-w)\ f\ \big((v'-w)\ t,\ w\big)$$

(5.10) has the same form as (5.14) of Chapter 2 and thus may be integrated in the same way. Note that the "P+1" eigenvalues of $\underset{\approx}{C}_f^P$ lie on a time dependent ellipse in the left half complex plane. In the t. l. P, L $\to \infty$, $\frac{P}{L} = \rho$, these eigenvalues coalesce to form the whole ellipse, thus recovering the result of section 4.

## 3.6. A SYSTEM WITH AN EXTERNAL POTENTIAL.

We reconsider the problem treated in section 4 with an external potential $V(x)$ included. Initial conditions on the r.d.f.'s are constructed exactly as in section 4, in particular (4.3) is valid. For example, we could choose $f_j^{(n)}(z_1;\ldots;z_n;o)$ to be the equilibrium distributions associated with the above potential (given that particle "o" is specified to be at $x = o$) provided such equilibrium r.d.f.'s exist.

First we describe the delta-function behaviour of the r.d.f.'s. Let $x(t|x',v';t')$ be the position at time $t$ of a single particle moving under the influence of an external potential $V(x)$ such that at time $t'$ its position is $x'$ and velocity $v'$ and $v(t|x',v';t')$ be the velocity at time $t$ of such a particle. Set $X(v',t) = x(t|o,v';o)$ and $V(v',t) = v(t|o,v';o)$. The delta-function dependence of the r.d.f.'s is then of the form

$$\delta\left(x_i - X(v',t)\right)\ \delta\left(v_i - V(v',t)\right) \tag{6.1}$$

$f_j^{(n)}$ here satisfy the hierarchy equations

$$\left[\frac{\partial}{\partial t} + K_j^{(n)} - \frac{1}{m}\sum_{i=1}^{n}\frac{\partial V(x_i)}{\partial x_i}\cdot\frac{\partial}{\partial v_i}\right] f_j^{(n)}\ (z_1;\ldots;z_n;t)$$

$$= \lim_{\epsilon\to o}\int_{-\infty}^{+\infty} dv_{n+1}|v_{n+1}-v_1| \cdot \left[f_{(j)}^{(n+1)}(z_1;x_1^-,v_{n+1};z_2;\ldots;z_n;t) - f_j^{(n+1)}(z_1;x_1^-,v_{n+1};z_2;\ldots;z_n;t)\right] \tag{6.2}$$

Define $f_j^{(n)}(z_1;\ldots;z_n;t)$

$$= f_j^{(n-1)}(z_1;\ldots;z_{n-1};t)\cdot\left[\delta\left(x_n - X(v',t)\right)\delta\left(v_n - V(v',t)\right) + f\left(x(o|x_n,v_n;t),v(o|x_n,v_n;t)\right)\right] + g_j^{(n)}(z_1;\ldots;z_n;t) \tag{6.3}$$

where $f(z) = \sum_{k\neq o} f_k^{(1)}(z;o)$. Since

$$\left[ \frac{\partial}{\partial t} + \sum_{i=1}^{n} v_i \frac{\partial}{\partial x_i} - \frac{1}{m} \sum_{i=1}^{n} \frac{\partial V(x_i)}{\partial x_i} \cdot \frac{\partial}{\partial v_i} \right] \tag{6.4}$$

$$\times \left[\delta\left(x_n - X(v',t)\right) \delta\left(v_n - V(v',t)\right) + f\left(x(o|x_n,v_n;t), v(o|x_n,v_n,t)\right)\right]$$

$$= o$$

it follows that $g_j^{(n)}$ satisfies the same set of equations (6.2) as $f_j^{(n)}$ on precollision regions of phase space with $K_j^{(n)}$ replaced by $\sum_{i=1}^{n} v_i \frac{\partial}{\partial x_i}$ (and the definition of precollision regions incorporates the effect of the external potential). For a certain range of $v_1$, given $x_1$ at time t, the equations for $g_j^{(n)}(\ ;t)$ are invariant on such regions and thus may be integrated there. For the invariance condition, we require that $(z_1;x_1^-,v_{n+1};z_2;\ldots;z_n;t)$ be in a precollision region if $(z_1;z_2;\ldots;z_n)$ is in one. A sufficient condition for this to be true is that

$$x\ (-\infty|x_1,v_1;t) = \text{sgn}\ (-v_1)\ \infty \tag{6.5}$$

i.e. a particle at $x_1$ with velocity $-v_1$ can escape to infinity $\left(x_1 = \text{sgn}(-v_1)\infty\right)$ so we are avoiding bound state phenomena. For such $v_1$, if two particles are at $z_1$ and $(x_1^-,v_{n+1})$ at time t, they will not have interacted in the time interval (o,t) under two body motion with an external potential. From the integration of the equations for $g_j^{(n)}$ on such precollision subregions, we see that since $g_j^{(n)}(z_1;\ldots;z_n;o)$ is regular in $z_1$ and $z_n$, the same will be true of $g_j^{(n)}(z_1;\ldots;z_n;t)$ provided $v_1 = V(v',t)$ lies in the prescribed range (6.5).

This will be true if

$$X(v',-\infty) = x\left(-\infty|X(v',t),V(v',t);t\right) = \text{sgn}(-v')\ \infty \qquad (6.6)$$

In particular, for such $v'$, $g_j^{(2)}(z_1;x_1^-,v_2;t)$ will be regular in all variables for all $\epsilon > o$ and $t \geq o$.

If $f_j^{(1)}$ is decomposed into regular and delta-function parts as $f_j^{(1)}(z_1;t) = f_j^{(1)\delta}(v',t)\,\delta\left(x_1-X(v',t)\right)\delta\left(v_1-V(v',t)\right)$ $+ f_{regj}^{(1)}(z_1;t)$, then from the first hierarchy equation we obtain, for $v'$ as specified above,

$$\begin{aligned}\frac{d}{dt} f_j^{(1)}(v',t) = &\int_{-\infty}^{V(v',t)} dw\left(V(v',t)-w\right) f\left[x\left(o|X(v',t),w;t\right),v\left(o|X(v',t),w;t\right)\right]\\ &\times\left[f_{j-1}^{(1)\delta}(v',t) - f_j^{(1)\delta}(v',t)\right]\\ + &\int_{V(v',t)}^{+\infty} dw\left(w-V(v',t)\right) f\left[x\left(o|X(v',t),w;t\right),v\left(o|X(v',t),w;t\right)\right]\\ &\times\left[f_{j+1}^{(1)\delta}(v',t) - f_j^{(1)\delta}(v',t)\right] \qquad (6.7)\end{aligned}$$

This equation may be solved in the usual way.

Finally we give a qualitative asymptotic analysis of the expressions appearing in (6.7) for $t \to \infty$ in the case where $\text{supp}V(x) \subseteq [-R,R]$ for some $R < \infty$. Suppose also that $f(z) = f^s(x)h(v)$ with $f^s(x)$ (C-1) summable to $\rho$ on $x \in (o,\infty)$ and $(-\infty,o)$. For large $t$,

$$\begin{aligned}v\left(o|X(v',t),w;t\right) &= w \text{ except for } w = V(v',t) + O(\tfrac{R}{t})\\ x\left(o|X(v',t),w;t\right) &= \left(V(v',t) - w\right)t + O(R) \qquad (6.8)\end{aligned}$$

We therefore expect that

$$\begin{aligned}&\int_{-\infty}^{V(v',t)} dw\left(V(v',t)-w\right)\ f^s\left[x\left(o|X(v',t),w,t\right)\right]\ h\left[v\left(o|X(v',t),w,t\right)\right]\\ &\sim\ \rho\int_{-\infty}^{V(v',\infty)} dw\left(V(v',\infty)-w\right)h(w) \qquad \text{as } t\to\infty \qquad (6.9)\end{aligned}$$

and that a similar result will hold for the other integral.

## 3.7 A POSITIVE PROPERTY FOR THE $f_j^{(1)\delta}$

Let us return again to the i.v.p. where there is a single specified particle (sections 3.4 and 3.6). If we make a (physical) choice of initial conditions $f_j^{(1)\delta}(t=o) \geqslant o$ then we show that the kinetic equations guarantee that $f_j^{(1)\delta}(t) \geqslant o$ for all $t > o$. It follows from a conservation result that the inequality is strict. The method used is a simple adaption of that discussed by Krasnoselski[65] for a finite autonomous system of ordinary differential equations.

The kinetic equations have the form

$$\frac{d}{dt}\,\underset{\sim}{f}^{(1)\delta}(t) = \underset{\approx}{C}^{\delta}(t)\,.\,\underset{\sim}{f}^{(1)\delta}(t) \qquad (7.1)$$

where $\underset{\sim}{f}^{(1)\delta}$ is an infinite dimensional vector with components $f_j^{(1)\delta}(t)$ (regarded as an element of $\iota^1$) and $\underset{\approx}{C}^{\delta}(t)$ is an infinite matrix which in the standard representation has components

$$C_{ij}^{\delta}(t) = \beta(t)\ \delta_{j-1,i} + \gamma(t)\ \delta_{j+1,i} - \big(\beta(t) + \gamma(t)\big)\ \delta_{j,i}$$

where $\beta(t),\ \gamma(t) > o$ for $t > o$. (7.2)

These equations are rewritten as

$$\frac{d}{dt}\, f_j^{(1)\delta}(t) = C\big(f_{j-1}^{(1)\delta},\ f_j^{(1)\delta},\ f_{j+1}^{(1)\delta};\ t\big) \qquad (7.3)$$

or in vector form $\frac{d}{dt}\,\underset{\sim}{f}^{(1)\delta}(t) = \underset{\sim}{C}(\underset{\sim}{f}^{(1)\delta};t)$

The property of C( ;t) which primarily guarantees the positive nature of the solutions is that

$$C(f,o,f';t) \geqslant o \quad \text{for all } t \text{ and } f,f' \geqslant o \qquad (7.4)$$

The linearity of $\underset{\sim}{C}(\ ;t)$ is not essential for the positivity result. In fact it is necessary only for $\underset{\sim}{C}(\ ;t)$ to satisfy a Lipschitz type condition of the form

$$\| \underset{\sim}{C}(\underset{\sim}{f};t) - \underset{\sim}{C}(\underset{\sim}{f}';t) \| \leq c(t) \; \| \underset{\sim}{f} - \underset{\sim}{f}' \| \tag{7.5}$$

where c(t) is a bounded, continuous function. $\|-\|$ is chosen to be the $\iota^p$ norm with $p = \infty$. (7.5) for $1 \leq p \leq \infty$ guarantees the existence and uniqueness of solutions to (7.3).

First we consider the solutions $f^{(1)\delta\epsilon}$ in $\iota^\infty$ of the related equations

$$\frac{d}{dt} \underset{\sim}{f}^{(1)\delta\epsilon}(t) = \underset{\sim}{C} \, (\underset{\sim}{f}^{(1)\delta\epsilon}(t);t) + \underset{\sim}{\epsilon} \tag{7.6}$$

with $\underset{\sim}{f}^{(1)\delta\epsilon}(o) = \underset{\sim}{f}^{(1)\delta}(o) + \underset{\sim}{\epsilon}$ and $\epsilon_j = \epsilon$ for all j.

From (7.5)

$$\begin{aligned} \| \underset{\sim}{f}^{(1)\delta\epsilon}(t_1) - \underset{\sim}{f}^{(1)\delta\epsilon}(t_2) \|_\infty &\leq \left| \int_{t_2}^{t_1} dt \; c(t) \, \| \underset{\sim}{f}^{(1)\delta\epsilon}(t) \|_\infty \right| + \\ &\qquad \| \underset{\sim}{\epsilon} \|_\infty \cdot |t_1 - t_2| \\ &= O(|t_1 - t_2|) \text{ as } t_1 - t_2 \to o \end{aligned} \tag{7.7}$$

From (7.7) with $t_2 = o$ and $t_1 = t$, it follows that there exists $\tau > o$ (independent of j) such that

$$f_j^{(1)\delta\epsilon}(t) > o \text{ for } t \in [o,\tau). \tag{7.8}$$

Suppose that $f_j^{(1)\delta\epsilon}(t) > o$ for $t \in [o,\tau_j)$ (if such a $\tau_j$ exists) and set $\tau' = \inf_j \tau_j$. If $\tau' < \infty$ and $\tau'$ is attained by some $\tau_j$ (for $j = j^*$ say), then we must have

$$\frac{d}{dt} f_{j^*}^{(1)\delta\epsilon}(t) \Big|_{t=\tau'} \leq o \tag{7.9}$$

but using (7.4) and (7.6),

$$\frac{d}{dt} f_{j^*}^{(1)\delta\epsilon}(t) \Big|_{t=\tau'} = C\left( f_{j^*-1}^{(1)\delta\epsilon}(\tau'), o, f_{j^*+1}^{(1)\delta\epsilon}(\tau'); \tau' \right) + \epsilon > o \tag{7.10}$$

So a contradiction is obtained. Next suppose that $\tau' < \infty$ but $\tau' \neq \tau_j$ for any j. Now for any $\eta > o$ there is a $j'$ such that $\tau' < \tau_{j'} < \tau' + \eta$. For any $t \in (\tau,\tau+\eta)$ the

$f_j^{(1)\delta\epsilon}$ are either positive or negative and small (of the order of magnitude $O(\eta)$ from (7.7)). The equation for $f_{j'}^{(1)\delta\epsilon}(t)$ at $t = \tau_{j'}$ is written

$$\frac{d}{dt} f_{j'}^{(1)\delta\epsilon}(t)\Big|_{t=\tau_{j'}}$$

$$= C\Big[H\big(f_{j'-1}^{(1)\delta\epsilon}(\tau_{j'})\big)\cdot f_{j'-1}^{(1)\delta\epsilon}(\tau_{j'}),\ o,\ H\big(f_{j'+1}^{(1)\delta\epsilon}(\tau_{j'})\big)\cdot f_{j'+1}^{(1)\delta\epsilon}(\tau_{j'})\ ;\ \tau_{j'}\Big]$$

$$+\ C\Big[H\big(-f_{j'-1}^{(1)\delta\epsilon}(\tau_{j'})\big)\cdot f_{j'-1}^{(1)\delta\epsilon}(\tau_{j'}),\ o,\ H\big(-f_{j'+1}^{(1)\delta\epsilon}(\tau_{j'})\big)\cdot f_{j'+1}^{(1)\delta\epsilon}(\tau_{j'})\ ;\ \tau_{j'}\Big]$$

$$+\ \epsilon \tag{7.11}$$

The l.h.s. of (7.11) is non-positive. The first term on the r.h.s. is non-negative from (7.4) and the third is strictly positive (independent of j). The second can be made as small as we like by a suitable choice of $\eta$ (and hence $j'$). For such a choice a contradiction is obtained. Consequently

$$f_j^{(1)\delta\epsilon}(t)\ >\ o \text{ for } t \geq 0 \text{ and all } j. \tag{7.12}$$

Finally we show that $f_j^{(1)\delta\epsilon}(t) \to f_j^{(1)\delta}(t)$ as $t \to o$.

Again the linearity of $\underset{\sim}{C}$ is not essential. In fact from (7.4)

$$\Big\|\ \underset{\sim}{f}^{(1)\delta\epsilon}(t) - \underset{\sim}{f}^{(1)\delta}(t)\Big\|_\infty \tag{7.13}$$

$$\leq \exp\Big(\int_o^t dt' C(t')\Big)\,\|\ \underset{\sim}{f}^{(1)\delta\epsilon}(o) - \underset{\sim}{f}^{(1)\delta}(o)\ \|_\infty + \int_o^t dt' \exp\Big(\int_t^t dt'' C(t'')\Big)\epsilon\,.$$

and $\|\ \underset{\sim}{f}^{(1)\delta\epsilon}(o) - \underset{\sim}{f}^{(1)\delta}(o)\ \|_\infty = \epsilon$. The result is immediate using the definition of $\|-\|_\infty$ and may be used to show that

$$f_j^{(1)\delta}(t) \geq o \text{ for } t \geq o \text{ and all } j. \tag{7.14}$$

The strict inequality may be proved noting the conservation result $\sum_{j=-\infty}^{+\infty} f_j^{(1)\delta}(t) = \sum_{j=-\infty}^{+\infty} f_j^{(1)\delta}(o) > o$. If for example

$f_{j*}^{(1)\delta}(t^*) = o$, then

$$o = \frac{d}{dt} f_{j*}^{(1)\delta}(t) \Bigg|_{t=t^*} = \gamma(t^*)\, f_{j*-1}^{(1)\delta}(t^*) + \beta(t^*)\, f_{j*+1}^{(1)\delta}(t^*) \qquad (7.15)$$

so $f_{j*\pm1}^{(1)\delta}(t^*) = o$. Repeating this analysis for $f_{j*\pm1}^{(1)\delta}$ and so on, we find that $f_j^{(1)\delta}(t^*) = o$ for all j. This is a contradiction.

For the general i.v.p. a similar positive property for the $f_j^{(1)\delta p}$ follows from the approximate closed kinetic equations.

# CHAPTER 4

## REVERSIBILITY AND ENTROPY CONSIDERATIONS

### 4.1 INTRODUCTION

The reversibility of the hierarchy equations for the one-dimensional hard "sphere" gas is demonstrated here. Our aim is to elucidate the nature of the introduction of irreversibility (i.e. the restriction to entropy increasing solutions) and to compare it with other approaches. For the case where we have exact closed equations for the delta-function part of the one-particle reduced distribution functions (r.d.f.) $f_j^{(1)\delta}$, we show that the entropy associated with this part of the r.d.f.'s is a monotonically increasing function of time. Furthermore the entropy associated with the regular part of the one-particle r.d.f.'s $f_{\text{reg } j}^{(1)}$ may be shown independent of the delta-function part.

Various techniques have been used to obtain irreversible (entropy increasing) time evolution equations from the reversible Liouville equation or B.B.G.K.Y. hierarchy. An approach originated by Bogoliubov [3], Born & Green [4] and Kirkwood [2] involves truncating the hierarchy using a factorization approximation justified by physical arguments. Prigogine [13] obtained irreversible behaviour by taking a suitable long time limit for the formal solutions of the Liouville equation. Balescu [14] has shown that there exists an invariant subdynamics associated with the Liouville equation. Time evolution in this subdynamics exhibits irreversible behaviour. However it is unclear in this work at which point irreversibility is introduced. This type of analysis has also been carried out by Gibberd and Hoffman [66]. In their derivation of the Choh-Uhlenbeck equation, irreversibility enters through the choice of a causal (rather than anticausal) solution to a matrix equation. The concept of a subdynamics also plays an important role in the introduction of irreversibility to the Liouville equation via a non-canonical (star unitary) transformation (see Prigogine and Mayne [67]).

In the following we recast our previous derivation of the evolution equations for the $f_j^{(1)\delta}$ for the case of a single specified particle. This shall be done in a way that emphasizes the existence of a certain subdynamics associated with the governing hierarchy equations. This subdynamics is different in nature from that implemented by Balescu and others (see above). However it is related to irreversible behaviour and the reformulation serves to emphasize the point at which we restrict our attention to irreversible (entropy increasing) solutions.

Since we essentially obtain entropy increasing solutions by restricting our attention to a suitable class of initial conditions, it is instructive to compare our work with the discussion given by Biel [68]. Biel rewrites the Liouville equation, under certain restrictions, as a hierarchy of non-Markovian integral equations for the velocity distribution functions involving the initial conditions on these functions. Suppose there is an entropy increasing solution of these equations $\{h^{(n)}(P_i;t)\}_{n=1}^{\infty}$ for $t \geqslant 0$ with initial conditions

$\{h^{(n)}(P_i)\}_{n=1}^{\infty}$ and that it may be extended to a range of times $t \in [-\tau, 0)$ retaining the entropy increasing behaviour. Then there is an entropy decreasing solution of the equations given by $\{h^{(n)}(-P_i;\tau-t)\}_{n=1}^{\infty}$ for $t \in [0,\tau]$ with initial conditions $\{h^{(n)}(-P_i)\}_{n=1}^{\infty}$. For the initial value problems (i.v.p.) that we consider, the solutions may not be extended to range of negative times and still retain entropy increasing behaviour. This may be regarded as a consequence of the special nature of these i.v.p.'s where a certain number of particles have specified positions and velocities at $t = 0$. Since these i.v.p.'s arise naturally in association with the correlation functions used to calculate transport coefficients, we expect that the corresponding solutions should decay to equilibrium and thus be entropy increasing.

## 4.2 REVERSIBILITY OF THE HIERARCHY EQUATIONS

Reversibility may, of course, be proved in general but we give an explicit proof here for the case of the one-dimensional hard "sphere" gas. To prove reversibility, we use the hierarchy equations (2.19) of Chapter 2 together with the asymptotic Liouville property and the impenetrability property ((2.17) and (2.18) of Chapter 2) for the $f_j^{(n)}$. Let us suppose that we have a solution $f_j^{(n)}(z_1;\ldots;z_n;t)$ for $t \geqslant 0$ satisfying the hierarchy equations and the above constraints. We show that

$$\hat{f}_j^{(n)}(z_1;\ldots;z_n;t) = f_j^{(n)}(x_1,-v_1;\ldots;x_n,-v_n;\tau-t) \quad t \in [0,\tau] \tag{2.1}$$

also satisfies the hierarchy equations and the above constraints. The latter is true by inspection. Since

$$K_j^{(n)}(x_i,v_i) = - K_j^{(n)}(x_i,-v_i) \quad , \tag{2.2}$$

it follows that

$$\begin{aligned}
&(\frac{\partial}{\partial t} + K_j^{(n)}(x_i,v_i))\ \hat{f}_j^{(n)}(z_1;\ldots;z_n;t) \\
&- \lim_{\epsilon\to 0} \int_{-\infty}^{+\infty} dv_{n+1}|v_{n+1}-v_1| \times (\hat{f}_{(j)}^{(n+1)}(z_1;x_1^-,v_{n+1};z_2;\ldots;z_n;t) \\
&\qquad\qquad - \hat{f}_j^{(n+1)}(z_1;x_1^-,v_{n+1};\ldots;z_n;t)) \\
&= - (\frac{\partial}{\partial t'} + K_j^{(n)}(x_i',v_i'))f_j^{(n)}(z_1';\ldots;z_n';t') \\
&+ \lim_{\epsilon\to 0} \int_{-\infty}^{+\infty} dv_{n+1}'|v_{n+1}'-v_1'| \times (f_j^{(n+1)}(z_1';x_1'^+,v_{n+1}';z_2';\ldots;z_n';t) \\
&\qquad\qquad - f_{(j)}^{(n+1)}(z_1';x_1'^+,v_{n+1}';z_2';\ldots;z_n';t))
\end{aligned} \tag{2.3}$$

where $x_i' = x_i$, $v_i' = -v_i$, $z_i' = (x_i',v_i')$, $x_1'^{\pm} = x_1' \pm \epsilon\ \text{sgn}(v_{n+1}' - v_1') = x_1^{\mp}$ and $t' = \tau - t$. Implementing (2.17) and (2.18) of Chapter 2 and writing $(j)' = j + \text{sgn}(v_{n+1}' - v_1')$ so $((j))' = j$, the r.h.s. of (2.3) becomes

$$\begin{aligned}
&- (\frac{\partial}{\partial t'} + K_j^{(n)}(x_i',v_i'))f_j^{(n)}(z_1';\ldots;z_n';t') \\
&+ \lim_{\epsilon\to 0} \int_{-\infty}^{+\infty} dv_{n+1}'|v_{n+1}' - v_1'| \times (f_{(j)'}^{(n+1)}(z_1';x_1'^-,v_{n+1}';z_2';\ldots;z_n';t') \\
&\qquad\qquad - f_j^{(n+1)}(z_1';x_1'^-,v_{n+1}';z_2';\ldots;z_n';t'))
\end{aligned} \tag{2.4}$$

(2.4) is identically zero since $f_j^{(n)}$ satisfy the hierarchy equations, consequently $\hat{f}_j^{(n)}$ also satisfies the hierarchy equations over a time interval $t \in [0,\tau]$. If $f_j^{(n)}$ exhibits entropy increasing behaviour on $t \in [0,\tau]$, then $\hat{f}_j^{(n)}$ must exhibit entropy decreasing behaviour on $t \in [0,\tau]$ and vice versa. This proves the reversibility of the hierarchy equations.

## 4.3 THE INTRODUCTION OF IRREVERSIBILITY

In this section we restrict our attention to precollision regions of phase space. So $K_j^{(n)} = \sum_{i=1}^{n} v_i \frac{\partial}{\partial x_i}$ and the equations may be integrated along the characteristics of $(\frac{\partial}{\partial t} + K_j^{(n)})$. This restriction in itself does not introduce irreversibility.

The subdynamics which we construct incorporates the time dependence of the r.d.f.'s unlike that of Balescu[14]. By so doing we introduce irreversible characteristics in the allowed solutions. In the treatment of Balescu, the Liouville equation in hierarchy form is used:

$$\frac{\partial}{\partial t} \underset{\sim}{f}(t) = \mathcal{L} \; \underset{\sim}{f}(t) \tag{3.1}$$

where $\underset{\sim}{f}(t)$ has components $f^{(n)}(z_i;t)\ldots$ the n-particle r.d.f.'s. This equation has the formal solution

$$\underset{\sim}{f}(t) = \mathcal{U}(t)\underset{\sim}{f}(o) \quad \text{where} \quad \mathcal{U}(t) = \exp(t\,\mathcal{L}) \tag{3.2}$$

Then the subdynamics is associated with a non-trivial projection operator $\Pi$ such that $\mathcal{U}(t)\Pi = \Pi\,\mathcal{U}(t)$ for all $t \geqslant 0$. $\Pi$ must also satisfy certain other conditions. We shall construct a projection operator with similar properties for our problem.

For such purposes, it is convenient to first integrate the appropriate hierarchy equations. In precollision regions, the integrated equations have the form

$$f_j^{(n)}(x_1,v_1;\ldots;x_n,v_n;t) - f_j^{(n)}(x_1-v_1t,v_1;\ldots;x_n-v_nt,v_n;0)$$

$$= \lim_{\epsilon\to 0} \int_0^t ds \int_{-\infty}^{+\infty} dv_{n+1}|v_{n+1}-v_1| \times$$

$$(f_{(j)}^{(n+1)}(x_1-v_1(t-s),v_1;\bar{x_1}-v_1(t-s),v_{n+1};x_2-v_2(t-s),v_2;\ldots$$

$$\ldots,x_n-v_n(t-s),v_n;s)$$

$$- f_j^{(n+1)}(x_1-v_1(t-s),v_1;\ldots \qquad \ldots;x_n-v_n(t-s),v_n;s))$$

$$\text{for} \quad t \geqslant 0 \tag{3.3}$$

where $\lim\limits_{\epsilon\to 0}$ has been interpreted as a weak limit since it refers to a generalized function limit. Let us now define a subspace of the function space D in which solutions of (3.3) are found. This function space could for example be chosen as $D^{reg\ c.n.}_{\beta,1(\infty)}$ restricted to precollision regions for the regular part of the r.d.f.'s and a corresponding choice made for the delta-function part. We choose $F(x,v) \geqslant 0$ to be locally integrable and (c-1) summable to $\rho > 0$ on $x \in (0,\infty)$ and $x \in (-\infty,0)$. Also $F(x,v)$ may have delta-function behaviour of the form

$$\delta(x-X_i)\delta(v-V_i) \quad i = 1,2,\ldots,N \quad .$$

Then for any $\underset{\sim}{f}$ in the function space (with components $f_j^{(n)}$), we make the decomposition

$$f_j^{(n)}(z_1;z_2;\ldots;z_n;t) = f_j^{(n-1)}(z_1;z_2;\ldots;z_{n-1};t)F(x_n-v_n(t-c),v_n)$$

$$+ g_j^{(n)}(z_1;z_2;\ldots;z_n;t) \tag{3.4}$$

for some constant $c \in R$, where a suitable limit interpretation is required for evaluation at points with delta-function or discontinuous behaviour (c.f. Chapter 2). $P$ shall denote the projection operator for the subspace where

$$(P\underset{\sim}{f})_j^{(n)} = P_n \; f_j^{(n)} \tag{3.5}$$

and the $P_n$ are defined iteratively through the relations

$$P_1 \; f_j^{(1)} = f_j^{(1)} \tag{3.6}$$

$$P_n \; f_j^{(n)}(z_1;\ldots;z_n;t) = P_{n-1} \; f_j^{(n-1)}(z_1;\ldots;z_{n-1};t)F(x_n-v_n(t-c),v_n)$$
$$+ \; g_{reg(1,n)j}^{(n)}(z_1;\ldots;z_n;t) \quad n \geq 2 \tag{3.7}$$

for some $c \in R$ where $h_{reg(1,n)j}^{(n)}$ is the part of $h_j^{(n)}$ which is regular with respect to the variables $z_1$ and $z_n$. To prove that the subspace is a subdynamics, we must show that $P$ commutes with the integral operator appearing in (3.3). Because of (3.6) it is only necessary to examine the hierarchy equations (3.3) for $n \geq 2$. For such $n$, (3.3) is rewritten using (3.4) as

$$f_j^{(n)}(x_1,v_1;\ldots;x_n,v_n;t) - f_j^{(n)}(x_1-v_1t,v_1;\ldots;x_n-v_nt,v_n;0)$$
$$= (f_j^{(n-1)}(x_1,v_1;\ldots;x_n,v_n;t) - f_j^{(n-1)}(x_1-v_1t,v_1;\ldots$$
$$\ldots;x_{n-1}-v_{n-1}t,v_{n-1};0))F(x_n-v_n(t-c),v_n)$$
$$+ \; G_j^{(n)}(x_1,v_1;\ldots;x_n,v_n;t) \tag{3.8}$$

where $G_j^{(n)}(x_1,v_1;\ldots;x_n,v_n;t)$

$$= \lim_{\epsilon\to 0} \int_0^t ds \int_{-\infty}^{+\infty} dv_{n+1} |v_{n+1}-v_n| \times$$

$$(g_{(j)}^{(n+1)}(x_1-v_1(t-s),v_1;\bar{x_1}-v_1(t-s),v_{n+1};x_2-v_2(t-s),v_2;\ldots$$
$$\ldots;x_n-v_n(t-s),v_n;s)$$

$$- g_j^{(n+1)}(x_1-v_1(t-s),v_1;\ldots \quad \ldots;x_n-v_n(t-s),v_n;s)) . \quad (3.9)$$

The action of $P$ is now easily calculated using (3.7) as

$$P_n f_j^{(n)}(x_1,v_1;\ldots;x_n,v_n;t) - P_n f_j^{(n)}(x_1-v_1t,v_1;\ldots;x_n-v_nt,v_n;0)$$

$$= (P_{n-1} f_j^{(n-1)}(x_1,v_1;\ldots;x_{n-1},v_{n-1};t) - P_{n-1} f_j^{(n-1)}(x_1-v_1t,v_1;\ldots$$
$$\ldots;x_{n-1}-v_{n-1}t,v_{n-1};0))F(x_n-v_n(t-c),v_n)$$

$$+ G_{reg(1,n)j}^{(n)}(x_1,v_1;\ldots;x_n,v_n;t) . \quad (3.10)$$

To complete the proof of the commutation result we must show that

$$G_{reg(1,n)j}^{(n)}(x_1,v_1;\ldots;x_n,v_n;t)$$

$$= \lim_{\epsilon\to 0} \int_0^t ds \int_{-\infty}^{+\infty} dv_{n+1} |v_{n+1}-v_1| \times \quad (3.11)$$

$$(g_{reg(1,n)(j)}^{(n+1)}(x_1-v_1(t-s),v_1;\bar{x_1}-v_1(t-s),v_{n+1};x_2-v_2(t-s),v_2;\ldots$$
$$\ldots;x_n-v_n(t-s),v_n;s)$$

$$- g_{reg(1,n)j}^{(n+1)}(x_1-v_1(t-s),v_1;\ldots \quad \ldots;x_n-v_n(t-s),v_n;s)) .$$

This simply amounts to proving that the delta-function dependence of $g_{j'}^{(n+1)}(z_1;z_1^*;z_2;\ldots;z_n;t)$ in the variable $z_1^*$

does not contribute to the delta-function dependence of $G_j^{(n)}$. This may be easily checked by direct calculation.

It is possible to show that time evolution in the subdynamics PD possesses some irreversible characteristics. Note that elements of PD are defined for all $t \geqslant 0$. Given a solution $f_j^{(n)}$ in PD, the time reversed solution $\hat{f}_j^{(n)}(z_1;\ldots;z_n;t) = f_j^{(n)}(x_1,-v_1;\ldots;x_n,-v_n;\tau-t)$ will not be in PD since it is not defined for the appropriate range of precollision variables or time. Certainly if the solutions we consider have delta-function components, then the subclass of solutions in PD exhibit entropy increasing behaviour at least in the delta-function part for $t \in [0,\infty)$. This shall be shown later.

Another subdynamics may be constructed on precollision regions of phase space. The subdynamics will be non-trivial provided the $f_j^{(n)}$ have delta-function dependence in the first variable. For any $\underset{\sim}{f}$ in D, we assume the delta-function dependence is of the form

$$\delta(x_j-v_jt-X_i)\,\delta(v_j-V_i) \quad i = 1,2,\ldots,N \tag{3.12}$$

and make the unique decomposition

$$\begin{aligned} &f_j^{(n)}(z_1;\ldots;z_n;t) \\ &= \sum_{i=1}^{N} f_j^{(n)\delta(1)i}(z_2;\ldots;z_n;t)\,\delta(x_1-v_1t-X_i)\,\delta(v_1-V_i) \\ &\quad + f_{reg(1)}^{(n)}(z_1;\ldots;z_n;t) \end{aligned} \tag{3.13}$$

The projection operator $P^{\delta}$ with components $P_n^{\delta}$ such that

$$(P^{\delta}\underset{\sim}{f})_j^{(n)} = P_n^{\delta} f_j^{(n)} \tag{3.14}$$

is defined by

$$P_n^{\delta}\ f_j^{(n)}(z_1;\ldots;z_n;t)$$

$$= \sum_{i=1}^{N} f_j^{(n)\delta(1)i}(z_2;\ldots;z_n;t)\,\delta(x_1-v_1t-X_i)\,\delta(v_1-V_i)\ . \tag{3.15}$$

We now show that $P^{\delta}$ commutes with the integral operator, in (3.3) for $n \geqslant 1$. All we need do is to show that

$$P_n^{\delta} \lim_{\epsilon\to 0} \int_0^t ds \int_{-\infty}^{+\infty} dv_{n+1} |v_{n+1}-v_1| \times$$

$$(f_{(j)}^{(n+1)}(x_1-v_1(t-s),v_1;x_1^{-}-v_1(t-s),v_{n+1}; \quad \ldots \qquad \ldots;s)$$

$$- f_j^{(n+1)}(x_1-v_1(t-s),v_1;x_1^{-}-v_1(t-s),v_{n+1}; \quad \ldots \qquad \ldots;s))$$

$$= \lim_{\epsilon\to 0} \int_0^t ds \int_{-\infty}^{+\infty} dv_{n+1} |v_{n+1}-v_1| \times$$

$$(P_{n+1}^{\delta} f_{(j)}^{(n+1)}(x_1-v_1(t-s),v_1;x_1^{-}-v_1(t-s),v_{n+1};\ldots \qquad \ldots;s)$$

$$- P_{n+1}^{\delta} f_j^{(n+1)}(x_1-v_1(t-s),v_1;x_1^{-}-v_1(t-s),v_{n+1},\ldots \qquad \ldots;s))\ . \tag{3.16}$$

This simply amounts to proving that the delta-function dependence of $f_j^{(n+1)}(z_1;z_1^*;z_2;\ldots;t)$ in the variable $z_1^*$ does not contribute to the delta-function dependence of the r.h.s. of (3.16). The calculation is analogous to that performed for $G_j^{(n)}$ . So this proves the existence of a subdynamics $P^{\delta}D$ corresponding to the projection operator $P^{\delta}$.

We now consider the nature of the time evolution in the subdynamics $P^{\delta}(PD)$ for the case where the delta-function dependence of $F(x,v)$ is chosen to be of the form $\delta(x)\delta(v-v')$, where $c = 0$ and the delta-function dependence of the r.d.f.'s is of the form $\delta(x-vt)\delta(v-v')$. The i.v.p. where a single particle has specified position $x = 0$ and velocity $v'$ at $t = 0$ is covered by this case. In particular, we shall examine the equations for $f_j^{(1)\delta}$. For $f_j^{(n)}$ in PD, the equations for $f_j^{(1)}$ may be written in the form

$$f_j^{(1)}(z_1;t) - f_j^{(1)}(x_1-v_1t,v_1;0)$$

$$= \lim_{\epsilon\to 0}\int_0^t ds \left(\int_{v_1}^{+\infty} dv_2 (v_2-v_1) F(x_1-v_1t+(v_1-v_2)s-\epsilon,v_2)\right)$$

$$\times \left(f_{j+1}^{(1)}(x_1-v_1(t-s),v_1;s) - f_j^{(1)}(x_1-v_1(t-s),v_1;s)\right)$$

$$+ \lim_{\epsilon\to 0}\int_0^t ds \left(\int_{-\infty}^{v_1} dv_2 (v_1-v_2) F(x_1-v_1t+(v_1-v_2)s+\epsilon,v_2)\right)$$

$$\times \left(f_{j-1}^{(1)}(x_1-v_1(t-s),v_1;s) - f_j^{(1)}(x_1-v_1(t-s),v_1;s)\right)$$

$$+ \lim_{\epsilon\to 0}\int_0^t ds \int_{-\infty}^{+\infty} dv_2 |v_2-v_1| \times$$

$$\left(g_{reg(j)}^{(2)}(x_1-v_1(t-s),v_1;\bar{x_1}-v_1(t-s),v_2;s)\right.$$

$$\left. - g_{reg\ j}^{(2)}(x_1-v_1(t-s),v_1;\bar{x_1}-v_1(t-s),v_2;s)\right) \qquad (3.17)$$

Applying $P^{\delta}$ to (3.17) and examining the coefficient of the delta-function part gives

$$f_j^{(1)\delta}(v',t) - f_j^{(1)\delta}(v',0) =$$

$$\lim_{\in\to 0} \int_0^t ds \left( \int_{v'}^{+\infty} dv_2 (v_2-v') F((v'-v_2)s-\in, v_2) \right) \cdot (f_{j+1}^{(1)\delta}(v',s) - f_j^{(1)\delta}(v',s))$$

$$+ \lim_{\in\to 0} \int_0^t ds \left( \int_{-\infty}^{v'} dv_2 (v'-v_2) F((v'-v_2)s-\in, v_2) \right) \cdot (f_{j-1}^{(1)\delta}(v',s) - f_j^{(1)\delta}(v',s) \tag{3.18}$$

We have specified that here $F$ should have the form

$$F(x,v) = F_{reg}(x,v) + k\ \delta(x) \cdot \delta(v-v') \tag{3.19}$$

where $F_{reg}$ is a regular function satisfying previously specified conditions of local integrability and (c-1) summability. If we consider the integrals over $v_2$ appearing in (3.19) then, because of the factor $v_2-v'$ present in the integrands, it is clear that the delta-function component of $F$ will not contribute. (3.18) may be expressed in differential form as

$$\frac{d}{dt} f_j^{(1)\delta}(v',t) = \left( \int_{v'}^{+\infty} dw (w-v') \cdot F_{reg}((v'-w)s, w) \right) \cdot (f_{j+1}^{(1)\delta}(v',t) - f_j^{(1)\delta}(v',t))$$

$$+ \left( \int_{-\infty}^{v'} dw (v'-w) \cdot F_{reg}((v'-w)s, w) \right) \cdot (f_{j-1}^{(1)\delta}(v',t) - f_j^{(1)\delta}(v',t)) \ . \tag{3.20}$$

By choosing $F_{reg}(x,v) = \sum_{k\neq 0} f_k^{(1)}(x,v;0)$ for the i.v.p. with a single specified particle "0" at $t = 0$, we recover the equations derived in the last chapter.

## 4.4 ENTROPY CONSIDERATIONS FOR $f_j^{(1)\delta}$

First we consider the definition of an entropy functional associated with the $P^{\delta}$(PD) subdynamics. Only the case is considered where the delta-function dependence of $F(x,v)$ and the r.d.f.'s has the special form considered the the last part of section 4.3. This has been shown to correspond to a physical initial value problem. The entropy functional is defined in terms of $f_j^{(1)\delta}$ . A natural choice is to define a "Shannon type" entropy functional of the form

$$S^{\delta}(t) = S^{\delta}(\underset{\sim}{f}^{(1)\delta}(v',t)) = -\sum_{j=-\infty}^{+\infty} |f_j^{(1)\delta}(v',t)|\ \ell n(|f_j^{(1)\delta}(v',t)|) \tag{4.1}$$

where we adopt the convention that $0.\ell n\ 0 = 0$. The following properties shall be proved for $S^{\delta}(t)$. Firstly we shall show that if $|S^{\delta}(0)| < +\infty$, then $|S^{\delta}(t)| < +\infty$ for all $t < \infty$ . Secondly we shall show that $S^{\delta}(t)$ is monotonically increasing in time.

With regard to the first property, we note that $\underset{\sim}{f}^{(1)\delta}(v',t)$ is naturally regarded as an element of $l^1$ and under time evolution governed by (3.20) will satisfy

$$\| \underset{\sim}{f}^{(1)\delta}(v',t)\|_1 = \| \underset{\sim}{f}^{(1)\delta}(v',0)\|_1 < +\infty \tag{4.2}$$

provided $f_j^{(1)\delta}(v',0) \geq 0$ for all $j$. However (4.2) is not sufficient to guarantee that $|S^{\delta}(t)| < +\infty$ . Consider the vector with components

$$f_j = \begin{cases} \dfrac{K}{j(\ell n\ j)^{\alpha}} & \text{for } j \geq 2 \\ 0 & \text{otherwise} \end{cases} \tag{4.3}$$

Then $\underset{\sim}{f} \in \ell^1$ only for $\alpha > 1$ (see Ferrar[69]) and for $1 < \alpha < 2$ it is easy to show that the series $S^\delta(\underset{\sim}{f})$ is divergent. So in order that the entropy (4.1) be well defined, we must restrict our attention to sequences in

$$\ell^s = \ell^1 \cap \{\underset{\sim}{f}:S^\delta(\underset{\sim}{f}) < +\infty\} \tag{4.4}$$

Our aim is to show that given $\underset{\sim}{f}^{(1)\delta}(v',t)$ satisfying (3.20) and $\underset{\sim}{f}^{(1)\delta}(v',0) \in \ell^s$, then $\underset{\sim}{f}^{(1)\delta}(v',t) \in \ell^s$ for all $t > 0$. This will in part justify our choice of (4.1) as the entropy functional.

As a preliminary, we show that $\ell^s$ is a vector space and in fact a complete metric space for a suitable choice of metric. Consider any $\underset{\sim}{f} \in \ell^1$ so $f_j \to 0$ as $|j| \to \infty$. Thus whether or not $\underset{\sim}{f} \in \ell^s$ can only depend on the nature of the function

$$\psi(f) = |f \,\ell n(|f|)| \tag{4.5}$$

in a neighbourhood of $f = 0$ rather than on the global properties of $\psi(\ )$. With this in mind, we shall give an equivalent definition of $\ell^s$.

An even function $\psi_\epsilon(x)$ is defined by

$$\psi_\epsilon(x) = \begin{cases} \psi(x) & \text{for } x \in [0,\epsilon] \\ \psi(\epsilon) + \psi'(\epsilon)(x-\epsilon) & \text{for } x \in (\epsilon,\infty) \end{cases} \tag{4.6}$$

and where $\epsilon \in (0,e^{-1})$. By construction $\psi_\epsilon(x)$ is convex and strictly monotonically increasing on $x \geqslant 0$. Modified versions of the functional (4.1) are defined by

$$S_\infty^\delta(t) = S_\infty^\delta(\underset{\sim}{f}^{(1)\delta}(v',t)) = \sum_{j=-\infty}^{+\infty} \psi(f_j^{(1)\delta}(v',t))$$

and

$$S_\epsilon^\delta(t) = S_\epsilon^\delta(\underset{\sim}{f}^{(1)\delta}(v',t)) = \sum_{j=-\infty}^{+\infty} \psi_\epsilon(f_j^{(1)\delta}(v',t)) \tag{4.7}$$

for $0 < \in < e^{-1}$. Since $\psi_\in$ and $\psi$ agree in a neighbourhood of the origin, $\iota^s$ may be equivalently defined by

$$\begin{aligned} \iota^s &= \iota^1 \cap \{\underset{\sim}{f} : S_\in^\delta(\underset{\sim}{f}) < +\infty\} \\ &= \iota^1 \cap \{\underset{\sim}{f} : S_\infty^\delta(\underset{\sim}{f}) < +\infty\} . \end{aligned} \tag{4.8}$$

Using the convexity and monotonity of $\psi_\in$, it is possible to show that $\iota^s$ becomes a metric space under the translationally invariant metric given by

$$d_\in(\underset{\sim}{f},\underset{\sim}{f}') = \sum_{j=-\infty}^{+\infty} \psi_\in(f_j - f_j') \tag{4.9}$$

for $\underset{\sim}{f}, \underset{\sim}{f}' \in \iota^s$. Furthermore $\iota^s$ is complete under this metric. The proof is similar to that showing $\iota^1$ is Banach under the norm $\| - \|_1$ (see Taylor[59]).

In addition to being a metric space, $\iota^s$ is also a vector space (and thus a subspace of $\iota^1$) since

(i) if $\underset{\sim}{f} \in \iota^s$, then $\lambda f \in \iota^s$ for all $\lambda \in R$. Since $\underset{\sim}{f} \in \iota^1$, there is a finite subset of the integers denoted $S(\eta)$ such that

$$| f_j | \geqslant \eta \quad \text{for} \quad j \in S(\eta) \tag{4.10}$$

Then $\sum_{j=-M}^{N} \psi_\in(\lambda f_j) \leqslant$

$$\sum_{j \in S(\in/|\lambda|)} \psi_\in(\lambda f_j) + |\lambda| \, S_\in^\delta(\underset{\sim}{f}) + |\lambda \log(|\lambda|)| \, \|\underset{\sim}{f}\|_1 \tag{4.11}$$

$< +\infty$ as required.

(ii) if $\underset{\sim}{f}, \underset{\sim}{f}' \in \iota^s$, then $\underset{\sim}{f} + \underset{\sim}{f}' \in \iota^s$. Since $\iota^s$ is a metric space under the translationally invariant metric, the result is immediate. Furthermore since $d_\in(\underset{\sim}{f} + \underset{\sim}{f}',0) \leqslant d_\in(\underset{\sim}{f},0) + d_\in(\underset{\sim}{f}',0)$, $S_\in^\delta(\underset{\sim}{f} + \underset{\sim}{f}') \leqslant S_\in^\delta(\underset{\sim}{f}) + S_\in^\delta(\underset{\sim}{f}')$.

The proof of the finite entropy property shall be based on the following observation. It is well known that a convolution algebra may be defined on $\ell^1$ (c.f. Simmons[70]). If $\underset{\sim}{f},\underset{\sim}{g} \in \ell^1$, then the convolution of $\underset{\sim}{f}$ and $\underset{\sim}{g}$, $\underset{\sim}{f} * \underset{\sim}{g} \in \ell^1$ is defined by

$$\underset{\sim}{f}*\underset{\sim}{g} = \sum_{k=-\infty}^{+\infty} f_{j-k}\, g_k = \sum_{k=-\infty}^{+\infty} f_k\, g_{j-k} \quad . \tag{4.12}$$

In fact this convolution algebra is a Banach algebra since $\|\underset{\sim}{f}*\underset{\sim}{g}\|_1 = \|\underset{\sim}{f}\|_1 \|\underset{\sim}{g}\|_1$. We now show that under convolution defined by (4.12), $\ell^s$ becomes a convolution subalgebra of $\ell^1$. The following result from (4.6) is needed. For $f,g \in R$ such that $|fg| < \epsilon$,

$$\psi_\epsilon(fg) = \psi(fg) = |f|\psi(g) + |g|\psi(f). \tag{4.13}$$

For $\underset{\sim}{f},\underset{\sim}{g} \in \ell^s$, let $S'(\epsilon)$ be the set of $(k,j')$ such that $|f_k g_{j'}| \geq \epsilon$. Then $S'(\epsilon)$ is finite. Now

$$\sum_{j=-M}^{N} \psi_\epsilon((\underset{\sim}{f}*\underset{\sim}{g})_j)$$

$$\leq \overline{\sum_{(k,j')\in S'(\epsilon)}} \psi_\epsilon(f_k g_{j'}) + \sum_{k=-\infty}^{+\infty} \Big(|f_k| \sum_{j=-M}^{N} \psi(g_{j-k}) + \psi(f_k) \sum_{j=-M}^{N} |g_{j-k}|\Big)$$

using the convexity and monotonicity of $\psi_\epsilon$ together with (4.13)

$$\leq \overline{\sum_{(k,j')\in S'(\epsilon)}} \psi_\epsilon(f_k g_{j'}) + \|\underset{\sim}{f}\|_1 \cdot S_\infty^\delta(\underset{\sim}{g}) + S_\infty^\delta(\underset{\sim}{f}) \cdot \|\underset{\sim}{g}\|_1 \tag{4.14}$$

(4.14) provides a finite upper bound for $S_\epsilon^\delta(\underset{\sim}{f}*\underset{\sim}{g})$ so $\underset{\sim}{f}*\underset{\sim}{g} \in \ell^s$.

Returning to entropy considerations, we wish to show that if $\underset{\sim}{f}^{(1)\delta}(v',0) \in \ell^s$, then from (3.20) $\underset{\sim}{f}^{(1)\delta}(v',t) \in \ell^s$ for all $t > 0$. This result is proved by showing that $\underset{\sim}{f}^{(1)\delta}(v',t)$ can be obtained from $\underset{\sim}{f}^{(1)\delta}(v',0)$ by convolution with a time dependent element of $\iota^s$. (3.20) may be solved by Fourier transform techniques and the solution written in the form

$$\underset{\sim}{f}^{(1)\delta}(v',t) = \underset{\sim}{C}(v',t) * \underset{\sim}{f}^{(1)\delta}(v',0) \tag{4.15}$$

where $C_j(v',t) =$

$$\frac{1}{2\pi}\int_0^{2\pi} d\theta\; e^{-\hat{i}\theta j} \exp\left(\int_0^t ds[\gamma_{F_{reg}}(v',s)(e^{\hat{i}\theta}-1)+\beta_{F_{reg}}(v',s)(e^{-\hat{i}\theta}-1)]\right) \tag{4.16}$$

with

$$\gamma_{F_{reg}}(v',s) = \int_{-\infty}^{v'} dw(v'-w)F_{reg}((v'-w)s,w)$$

and

$$\beta_{F_{reg}}(v',s) = \int_{v'}^{+\infty} dw(w-v')F_{reg}((v'-w)s,w) .$$

It remains to show that $\underset{\sim}{C}(v',t) \varepsilon\, \iota^s$ for $t \geqslant 0$. Now $C_j(v',t)$ is of the form

$$C_j(v',t) = \frac{1}{2\pi}\int_0^{2\pi} d\theta\; e^{-\hat{i}\theta j}\phi(\theta,v';t) \tag{4.17}$$

where, for each $t$, $\phi(\theta,v';t)$ is periodic in "$\theta$" of period $2\pi$. Furthermore $\phi(\theta,v';t)$ and all of its derivatives with respect to $\theta$ are absolutely continuous. Consequently

$$C_j(v',t) = o\left(\frac{1}{|j|^M}\right) \quad \text{as} \quad |j| \to \infty \quad \text{for any} \quad M = 1,2,\ldots , \tag{4.18}$$

so $\underset{\sim}{C}(v',t) \varepsilon\, \iota^s$ as required. The convolution structure (4.15) is also easily derived from the matrix form of the solution to (3.20)

$$\underset{\sim}{f}^{(1)\delta}(v',t) = \exp\left(\int_0^t ds\; \underset{\approx}{C}(v',s)\right)\cdot \underset{\sim}{f}^{(1)\delta}(v',0) . \tag{4.19}$$

where

$$C_{ij}(v',s) = \beta_{Freg}\delta_{i-j,-1} + \gamma_{Freg}\delta_{i-j,+1} - (\beta_{Freg}+\gamma_{Freg})\delta_{i-j,0}$$

depends only on $i - j$.

Finally we note a special case where the finiteness of entropy may be proved easily without introducing the above apparatus. This is the case where $f_k^{(1)\delta}(v',0) \neq 0$ only for a finite number of values of "k". From (4.15) and (4.16)

$$f_j^{(1)\delta}(v',t) = \frac{1}{2\pi}\int_0^{2\pi} d\theta\ e^{-\hat{i}\theta j}\cdot\xi(\theta,v';t) \qquad (4.20)$$

where

$$\xi(\theta,v';t) = \exp\left(\int_0^t ds[\gamma_{Freg}(v',s)(e^{\hat{i}\theta}-1)+\beta_{Freg}(v',s) \times (e^{-\hat{i}\theta}-1)]\right)\eta(\theta,v')$$

with

$$\eta(\theta,v') = \sum_{k=-\infty}^{+\infty} f_k^{(1)\delta}(v',0)\,e^{\hat{i}\theta k}$$

and the sum $\sum_k$ is in fact finite. So $\xi(\theta,v';t)$ is a periodic function of "$\theta$" (period $2\pi$) and, together with all of its derivatives with respect to "$\theta$", is absolutely continuous in "$\theta$". Consequently $f_j^{(1)\delta}(v',t) = o(\frac{1}{|j|^M})$ as $|j| \to \infty$ for each $M = 1,2,\ldots$ and each $t \geq 0$. So $\underset{\sim}{f}^{(1)\delta}(v',t) \in l^s$ for each $t \geq 0$.

If we now restrict our attention to non-negative, normalized solutions of (3.20) in $l^s$, $S^\delta(t) = S^\delta(\underset{\sim}{f}^{(1)\delta}(v',t))$ is shown to be monotonically increasing. From (4.1) and (3.20)

$$\frac{d}{dt} S^{\delta}(t) = \gamma_{Freg}(v',t) \cdot \sum_{j=-\infty}^{+\infty} (f_j^{(1)\delta}(v',t) - f_{j-1}^{(1)\delta}(v',t)) \ln f_j^{(1)\delta}(v',t)$$

$$+ \beta_{Freg}(v',t) \cdot \sum_{j=-\infty}^{+\infty} (f_j^{(1)\delta}(v',t) - f_{j+1}^{(1)\delta}(v',t)) \times \ln f_j^{(1)\delta}(v',t) \qquad (4.21)$$

Since

$$\sum_{j=-\infty}^{+\infty} f_j^{(1)\delta}(v',t) = 1,$$

an infinite version of Shannon's Inequality (see Aczel [71]) may be applied to show that each of $\sum_j (f_j^{(1)\delta} - f_{j-1}^{(1)\delta}) \ln f_j^{(1)\delta}$ and $\sum_j (f_j^{(1)\delta} - f_{j+1}^{(1)\delta}) \ln f_j^{(1)\delta}$ are non-negative. Consequently, since $\gamma_{Freg}(v',t)$, $\beta_{Freg}(v',t) > 0$ for $t > 0$,

$$\frac{d}{dt} S^{\delta}(t) \geqslant 0 \quad \text{for} \quad t \geqslant 0 . \qquad (4.22)$$

Alternatively (4.22) may be derived more directly by employing the inequality

$$x \ln x - x \ln y - x + y \geqslant 0 \text{ for all } x,y > 0 . \qquad (4.23)$$

Another application of this inequality is in finding an upper bound for the H-function of Boltzmann's H-theorem (see Thompson [50]).

Unlike the proof of Boltzmann's H-theorem (see Green [5] or Balescu [14]) or generalizations of this theorem (see Green [72]), we did not have to implement microscopic reversibility explicitly to prove that $\frac{d}{dt} S^{\delta}(t) \geqslant 0$. Since (3.20) is exact, it must contain all the necessary information about time evolution in the subdynamics $P^{\delta}(PD)$. Microscopic reversibility has been used in its derivation (in the form of the asymptotic

Liouville property (2.17) of Chapter 2). Similar comments apply for example to the analysis by Balescu[14] of the homogeneous Landau equation. The approximate closed kinetic equations for the $f_j^{(1)\delta i}$ of the general i.v.p. also produce entropy increasing behaviour.

For the special i.v.p. discussed above, a natural definition of the entropy associated with the regular part of the one-particle r.d.f.'s is as a functional of

$$\sum_{j=-\infty}^{+\infty} f^{(1)}_{\text{reg } j} \ \ln f^{(1)}_{\text{reg } j} \ . \tag{4.24}$$

As $f^{(1)}_{\text{reg } j}$ depend on $v'$ only through the jump conditions which interchange $f^{(1)}_{\text{reg } j}$ with $f^{(1)}_{\text{reg } j\pm 1}$, (4.24) is left invariant and is thus independent of the behaviour of the $f_j^{(1)\delta}$ .

In closing this section we give a brief outline of the application of discrete variational techniques to the proof of the inequalities $\sum_{j=-\infty}^{+\infty} (f_j - f_{j\pm 1}) \ln f_j \geqslant 0$ where $f_j \geqslant 0$ and $\sum_{j=-\infty}^{+\infty} f_j = 1$. This method resembles that used for certain problems in equilibrium statistical mechanics (see Sears[73]). The above result may be obtained from an analysis of the corresponding cyclic system. We prove that

$$\sum_{j=0}^{p-1} (f_j - f_{j+1}) \ln \ f_j \geqslant 0 \quad \text{where} \quad f_j \geqslant 0, \ f_0 = f_p \quad \text{and} \sum_{j=0}^{p-1} f_j = 1. \tag{4.25}$$

A Lagrange multiplier method is used to find the extrema of $\sum_{j=0}^{p-1} (f_j - f_{j+1}) \ln f_j$ . We must solve the non-linear difference equations

$$\frac{f_{j+1}}{f_j} = \Psi\left(\frac{f_j}{f_{j-1}}\right) \text{ with } \ f_0 = f_p \tag{4.26}$$

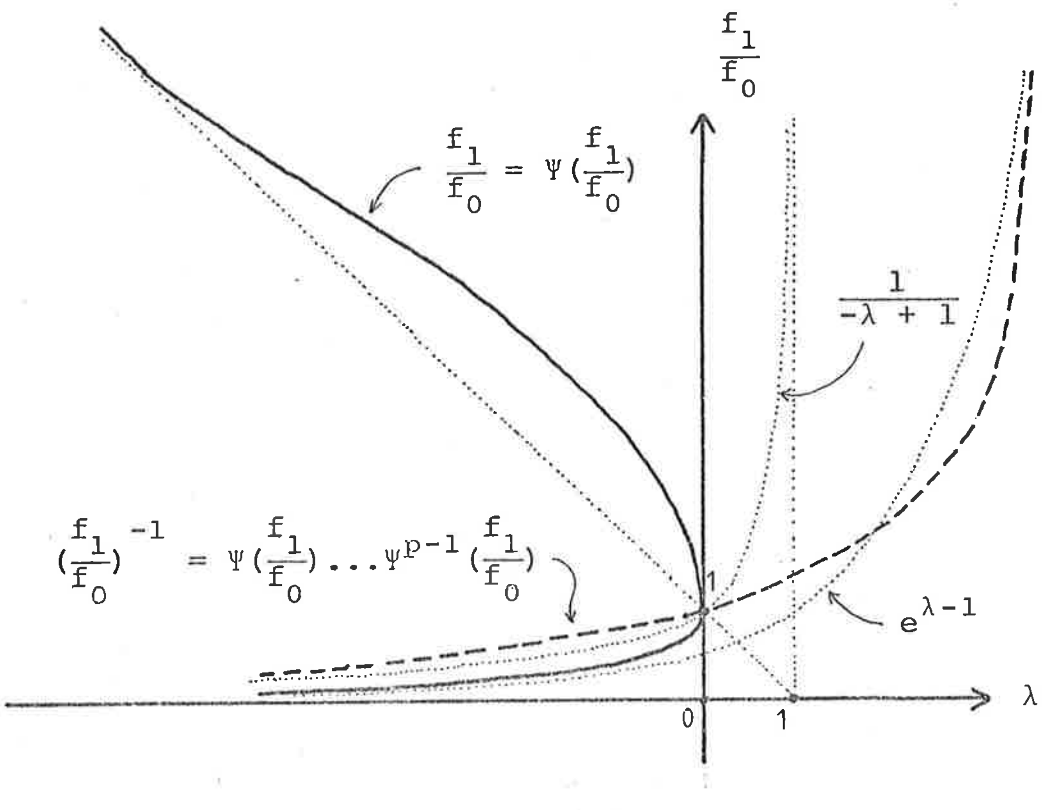
where $\Psi$ is the convex monotonic function $\Psi(y) = \ell n\, y + (1-\lambda)$ and $\lambda$ is the Lagrange multiplier. It is clear that once we know $\frac{f_1}{f_0}$, the complete solution for the extrema can be calculated using (4.26) recursively together with the constraint $\sum_{j=0}^{p-1} f_j = 1$. Solving (4.26) amounts to finding the simultaneous solutions for $(\frac{f_1}{f_0}, \lambda)$ of the equations

$$\frac{f_1}{f_0} = \Psi^p\left(\frac{f_1}{f_0}\right)$$

and

$$\left(\frac{f_1}{f_0}\right)^{-1} = \Psi\left(\frac{f_1}{f_0}\right)\Psi^2\left(\frac{f_1}{f_0}\right) \ldots \Psi^{p-1}\left(\frac{f_1}{f_0}\right) \qquad (4.27)$$

The first equation is the $p^{th}$ iteration of (4.26) and the second comes from the identity $\left(\frac{f_1}{f_0}\right)^{-1} = \frac{f_2}{f_1}\frac{f_3}{f_2} \ldots \frac{f_0}{f_{p-1}}$. It is possible to show that the fixed points of $\Psi^p$ are just those of $\Psi$ so the first equation of (4.27) may be replaced by $\frac{f_1}{f_0} = \Psi(\frac{f_1}{f_0})$. By inspection $(\frac{f_1}{f_0}, \lambda) = (1,0)$ is a solution. We may easily show that this solution, $f_j = \frac{1}{p}$, corresponds to a stationary minimum of $\sum_{j=0}^{p-1} (f_j - f_{j+1}) \ell n\, f_j$. The diagram shows that this solution is unique.



A similar analysis applies to prove that

$$\sum_{j=1}^{p} (f_j - f_{j-1}) \ln f_j \geq 0 \text{ where } f_j \geq 0,\ f_0 = f_p \text{ and } \sum_{j=1}^{p} f_j = 1. \tag{4.28}$$

# CHAPTER 5

# VELOCITY CORRELATION FUNCTIONS FOR FINITE ONE-DIMENSIONAL HARD "SPHERE" SYSTEMS

## 5.1 INTRODUCTION

Certain finite systems consisting of one-dimensional hard "spheres" are considered. Because of the well known relationships between correlation functions and transport coefficients, there is considerable interest in calculating the former for various infinite many body systems. The long time behaviour is of particular interest. For such calculations to be tractible, it is usually necessary to examine the infinite systems directly rather than performing calculations for the finite system and then taking the thermodynamic limit (t.l.). However, for the special types of finite systems mentioned above, it is possible to calculate exactly certain correlation functions and to examine their long time behaviour. Most of the results of this chapter are given by Evans[74].

The case where the particles are on a ring was considered by Frisch[75] who defined the concept of a "weak" approach to equilibrium and demonstrated the decay to an equilibrium limit of certain correlation functions. The technique that we use to examine the ring system was developed by Jepsen[40]. It is used to provide exact expressions for the velocity correlation functions (v.c.f.) which are then analyzed in the long time limit. We discover that after a slow (inverse power) decay for times of the order of the relaxation time, there is a "fast" decay to the equilibrium value on a time scale associated with the finite size of the system. The asymptotic "fast" decay property of the v.c.f.'s exhibited here has also appeared in the work of Hobson and Loomis[76] on an ideal gas in a finite box. Their expressions for the asymptotic behaviour of the v.c.f.'s have the same structure as those obtained for the ring system (adopting in both cases Maxwellian velocity distributions), namely

$$\sim K\, t^k\, e^{-c\left(\frac{v_{th}t}{L}\right)^2} \quad \text{as } t \to \infty$$

where L is the length of the ring or size of the box.

The case where the particles are in a hard walled box has been briefly considered by Lebowitz and Sykes[77]. We adapt Jepsen's technique to handle this problem and show that the v.c.f.'s have the same type of asymptotic behaviour as for the ring system. The dependence of the v.c.f.'s on the initial position of the specified particle when near the boundary of the box is analyzed. These considerations are generalized to systems of higher spatial dimension and more general interparticle interaction.

Similar techniques are appropriate to an analysis of the corresponding infinite systems. Jepsen takes the t.l. for the ring system. The convergence in this limit is examined here. Gervois and Pomeau[78] have considered the corresponding semi-infinite system. The effect of the inclusion of a perturbing interparticle potential on this infinite system has also been treated by Gervois and Pomeau[79]. Another modification is the treatment of an infinite one-dimensional mixture of hard "spheres" of different diameters by Aizenman et al.[80]

The final section of the chapter deals with the stochastic version of the ring system. A non-zero probability of transmission is associated with each collision so that the system is no longer deterministic.

## 5.2 THE RING SYSTEM

We describe briefly the formulation developed by Jepsen. The particles are labelled in order around the ring by an integer index $j \in \{1,2,...,N\}$. We call trajectory $j$ the path that particle $j$ would follow if it did not interact with other particles. Let $A_{jk}(t)$ be equal to one if particle $j$ is on trajectory $k$ at time $t$ and zero otherwise. Define $r_n(h,k,t)$ to be equal to one if trajectory $h$ crosses trajectory $k$ exactly $n$ times in the time interval $(0,t)$ and zero otherwise. A crossing from the right counts as "+1" and from the left as "-1".

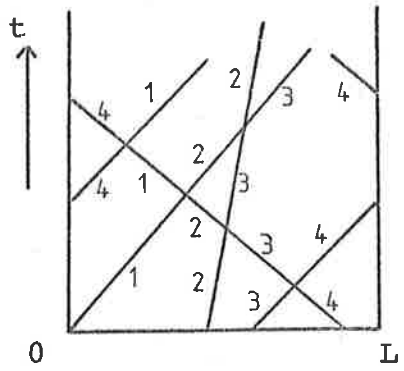



Fig. 5.1: Diagram showing the nature of the dynamics of the system.

Now

$$A_{jk}(t) = \sum_{n1=-\infty}^{+\infty} \sum_{n2=-\infty}^{+\infty} \cdots \sum_{nN=-\infty}^{+\infty} \delta^{N}_{n1+n2+\ldots nN+j-k,0}$$

$$\times\, r_{n1}(1,k,t)\, r_{n2}(2,k,t) \;\ldots\; r_{nN}(N,k,t). \qquad (2.1)$$

If we define

$$s(u,h,k,t) = \sum_{n=-\infty}^{+\infty} r_n(h,k,t)\, e^{\hat{\imath} n u} \;, \qquad (2.2)$$

then $s(u,h,k,t)$ is given by

$$s(u,h,k,t) = S[u,w_{kh}] \quad , \; k < h$$

$$s(u,h,k,t) = e^{-\hat{\imath} u}\, S[u,w_{kh}], k > h \qquad (2.3)$$

with

$$w_{kh} = (x_k + v_k\, t) - (x_h + v_h\, t)$$

and

$$S[u,w] = e^{\hat{\imath} n u} \quad \text{when} \quad (n-1)L < w \leqslant nL \quad \text{for each } n. \qquad (2.4)$$

Using a Fourier-type representation of the Kronecker-delta in (2.1), we obtain

$$A_{jk}(t) = \frac{1}{N} \sum_u e^{-\hat{\imath}(j-1)u} \prod_{h=1}^{N} S[u, w_{kh}]$$

and (2.5)

$$u = \frac{2\pi l}{N} \quad \text{and} \quad \sum_u = \sum_{l=0}^{N-1} .$$

We wish to calculate ensemble averages of the form

$$F_{N,L} = \langle f(v_1(o);\ x_j(t),\ v_j(t)) \rangle_{N,L} \tag{2.6}$$

where particle 1 is specified to be at the origin at $t=0$ and the remaining particles are distributed around the ring uniformly with velocity distributions $h(v)$ (taken to be Maxwellian in this section). i.e. a quasi-equilibrium initial distribution. From Jepsen's work:

$$\begin{aligned} F_{N,L} &= \sum_{k=1}^{N} \langle f(v_1; x_k + v_k t,\ v_k)\ A_{jk}(t) \rangle_{N,L} \\ &= \frac{1}{N} \sum_u \frac{N-1}{L} \quad e^{-\hat{\imath}(j-1)u} \int_o^L dx_k \int_{-\infty}^{+\infty} dv_k h(v_k) \\ &\times \ Q[u,\ x_k + v_k t,\ v_k, t] \\ &\times \left[\frac{1}{L} \int_o^L dx_n \ R[u,\ x_k + v_k t - x_n, t]\right]^{N-2} \\ &+ \frac{1}{N} \sum_u e^{-\hat{\imath}(j-1)u} \int_{-\infty}^{+\infty} dv_1 h(v_1)\ f(v_1;\ v_1 t,\ v_1) \\ &\times \left[\frac{1}{L} \int_o^L dx_n \ R[u,\ v_1 t - x_n,\ t]\right]^{N-1} \end{aligned} \tag{2.7}$$

where

$$h(v) = \frac{1}{(2\pi)^{\frac{1}{2}}} \frac{1}{v_{th}} \exp\left(-\tfrac{1}{2}\left(\frac{v}{v_{th}}\right)^2\right)$$

$$Q[u,x,v,t] = \int_{-\infty}^{+\infty} dv_1\ h(v_1)\ f(v_1;x,v)\ S[u,x-v_1t]$$

and

$$R[u,x,t] = \int_{-\infty}^{+\infty} dv_n\ h(v_n)\ S[u,\ x-v_nt]\ . \qquad (2.8)$$

For the v.c.f.'s, $f(\ \ )$ has the form $f(v_1;x,v) = v_1v$. So from (2.7)

$$F_{N,L} = \langle v_1(o)\ v_j(t)\rangle_{N,L}$$

$$= \frac{1}{N}\sum_u \frac{N-1}{L}\, e^{-\hat{\imath}(j-1)u} \int_{-\infty}^{+\infty} dv_k\ v_k\ h(v_k)$$

$$\times \int_o^L dx_k\ \hat{Q}[u,x_k + v_kt,\ t] \times \left[\frac{1}{L}\int_o^L dx_n R[u,x_k+v_kt-x_n,t]\right]^{N-2}$$

$$+ \frac{1}{N}\sum_u e^{-\hat{\imath}(j-1)u} \int_{-\infty}^{+\infty} dv_1\ v_1^2\ h(v_1)$$

$$\times \left[\frac{1}{L}\int_o^L dx_n\ R[u,v_1t - x_n,t]\right]^{N-1} \qquad (2.9)$$

where

$$\hat{Q}[u,x,t] = \int_{-\infty}^{+\infty} dv_1\ v_1\ h(v_1)\ S[u,x - v_1t]\ . \qquad (2.10)$$

It is instructive to examine the contribution to (2.9) from the $u = 0$ term in the sum. We note that $S[o,x] = 1$, hence $R[o,x,t] = 1$ and $\hat{Q}[o,x,t] = 0$. So the total contribution to (2.9) from this term is

$$\frac{1}{N}\int_{-\infty}^{+\infty} dv_1\ v_1^2\ h(v_1) = \frac{1}{N}\langle v_1(o)^2\rangle \qquad (2.11)$$

which we shall show to be the asymptotic value of $F_{N,L}$ as $t \to \infty$. This comes from the $k = 1$ term in the sum

$$\sum_{k=1}^{N} \langle v_1(o)\ v_k\ A_{jk}(t)\rangle_{N,L}$$

i.e. the contribution to the v.c.f. from particle $j$ being on trajectory 1 (1 being the particle with specified position and velocity). We may also check the initial conditions on the v.c.f.'s from (2.9). Clearly $\hat{Q}[u,x,o] = 0$ and $R[u,x,o] = S[u,x]$ so from (2.4)

$$\frac{1}{L}\int_{o}^{L} dx_n\ R[u,v_1 t - x_n,t]\Big|_{t=0} = 1. \qquad (2.12)$$

So

$$\langle v_1(o)v_j(t)\rangle_{N,L} = \frac{1}{N}\sum_u e^{-\hat{\imath}(j-1)u}\int_{-\infty}^{+\infty} dv_1\ v_1{}^2h(v_1)$$

$$= \delta^N_{j,1}\ \langle v_1(o)^2\rangle \text{ as required.} \qquad (2.13)$$

Next we consider the asymptotic analysis of $\langle v_1(o)v_j(t)\rangle_{N,L}$ in the $t \to \infty$ limit. The following results are needed:

$$\frac{1}{L}\int_{o}^{L} dx_n R[u,w + L - x_n,t] = e^{+\hat{\imath}u}\frac{1}{L}\int_{o}^{L} dx_n R[u,w - x_n,t]$$

and $$\hat{Q}[u,w + L,t] = e^{+\hat{\imath}u}\ \hat{Q}[u,w,t]. \qquad (2.14)$$

The $x_k$- integration in (2.9) may be performed explicitly (c.f. Jepsen [40]) and the integrals in (2.9) over an infinite velocity range may be transformed using (2.14) to a sum of integrals over a finite range. So

$$<v_1(o)v_j(t)>_{N,L} = v_{th}^2\ t\ \frac{1}{N} \sum_{u\neq o} \frac{N-1}{L}\ e^{-\hat{i}(j-1)u}$$

$$\times \sum_{m=-\infty}^{+\infty} \int_o^{L/t} dv_k h(v_k+\frac{mL}{t})\, e^{-\hat{i}mu}$$

$$\times\ (e^{-\hat{i}u}-1)\ \hat{Q}[u,v_kt,t]\ \left[\frac{1}{L}\int_o^L dx_n R[u,v_kt-x_n,t]\right]^{N-2}$$

$$+\ \frac{1}{N}\sum_{u\neq o} e^{-\hat{i}(j-1)u} \sum_{m=-\infty}^{+\infty} \int_o^{L/t} dv_1 (v_1+\frac{mL}{t})^2 h(v_1+\frac{mL}{t})\, e^{-\hat{i}mu}$$

$$\times\ \left[\frac{1}{L}\int_o^L dx_n\ R[u,v_1t - x_n,t]\right]^{N-1}$$

$$+\ \frac{1}{N} <v_1(o)^2>\ . \qquad (2.15)$$

In (2.15) $\sum_{m=-\infty}^{+\infty}$ and $\int_o^{L/t} dv_k$ or $\int_o^{L/t} dv_1$ may be interchanged using Lebesgue's dominated convergence theorem. So it is necessary to examine sums of the form

$$\sum_{m=-\infty}^{+\infty} h(v+\frac{mL}{t})\, e^{-\hat{i}mu} \quad \text{and} \quad \sum_{m=-\infty}^{+\infty} (v+\frac{mL}{t})^2 h(v+\frac{mL}{t})\, e^{-\hat{i}mu} \qquad (2.16)$$

(2.16) may be expressed in a more convenient form using a Poisson sum formula (see Carrier et al[64]). Let $g(\ )$ be a piecewise continuous, integrable function which can be represented in terms of its Fourier transform (in the usual way) and such that

$$\sum_{m=-\infty}^{+\infty} (g(m+) + g(m-))$$

is convergent. Then

$$\sum_{m=-\infty}^{+\infty} \tfrac{1}{2}(g(m+) + g(m-)) = \sum_{m=-\infty}^{+\infty} G(2\pi n)$$

where

$$G(\lambda) = \int_{-\infty}^{+\infty} dx\ e^{\hat{\imath}\lambda x} g(x) \quad . \qquad (2.17)$$

Performing the Fourier transforms indicated in (2.17), (2.16) becomes

$$\sum_{m=-\infty}^{+\infty} h(v+\frac{mL}{t})\ e^{-\hat{\imath}mu} = \sum_{m=-\infty}^{+\infty} \frac{t}{L}\ e^{-\hat{\imath}(2\pi m-u)\frac{vt}{L}}\ e^{-\frac{1}{2}\left(\frac{v_{th}t}{L}\right)^2 (2\pi m-u)^2} \qquad (2.18)$$

$$\sum_{m=-\infty}^{+\infty} (v + \frac{mL}{t})^2\ h(v + \frac{mL}{t})\ e^{-\hat{\imath}mu}$$

$$= \sum_{m=-\infty}^{+\infty} v_{th}^{\ 2}\ \frac{t}{L}\{1 - (2\pi m - u)^2 . \left(\frac{v_{th}t}{L}\right)^2\}$$

$$\times\ e^{-\hat{\imath}(2\pi m-u)\cdot\frac{vt}{L}}\ e^{-\frac{1}{2}\left(\frac{v_{th}t}{L}\right)^2 (2\pi m-u)^2} \qquad (2.19)$$

A similar analysis shows that

$$Q[u,vt,t] = \int_{v}^{v+\frac{L}{t}} dv_1\ \left(\sum_{n=-\infty}^{+\infty} (v_1 + \frac{nL}{t}) h(v_1 + \frac{nL}{t}) e^{-\hat{\imath}nu}\right)$$

$$= \sum_{n=-\infty}^{+\infty}\ - \frac{t}{L}v_{th}^{\ 2}(e^{\hat{\imath}u}-1)\ e^{-\hat{\imath}(2\pi n-u)\frac{vt}{L}}\ e^{-\frac{1}{2}\left(\frac{v_{th}t}{L}\right)^2 (2\pi n-u)^2} \qquad (2.20)$$

Finally, we note that

$$F[u,w] = \frac{1}{L}\int_{o}^{L} dx_n S[u,w - x_n]$$

$$= n\ e^{\hat{\imath}(n-1)u} - (n-1)\ e^{\hat{\imath}nu} + \frac{w}{L}(1-e^{\hat{\imath}u})\ e^{\hat{\imath}nu}$$

$$\text{for } (n-1)L < w \leqslant nL, \qquad (2.21)$$

so

$$\frac{1}{L}\int_{o}^{L} dx_n\ R[u,vt - x_n,t]$$

$$= \int_{-\infty}^{+\infty} dv_n h(v_n) F[u,(v - v_n)t]$$

$$= \sum_{p=-\infty}^{+\infty} 2\frac{(1 - \cos u)}{(2\pi p - u)^2} e^{-\hat{\imath}(2\pi p-u)\frac{vt}{L}} e^{-\frac{1}{2}\left(\frac{v_{th}t}{L}\right)^2 (2\pi p-u)^2} . \quad (2.22)$$

We may now substitute (2.18/19/20/22) into (2.15) to obtain the following asymptotic result (see Appendix E).

$$\langle v_1(o)v_j(t)\rangle_{N,L} \overset{t\to\infty}{\sim} \frac{1}{N}\langle v_1(o)^2\rangle$$

$$- v_{th}{}^2\frac{N-1}{N}\left(\frac{v_{th}t}{L}\right) 4(1-\cos\frac{2\pi}{N}) \left(\frac{2(1 - \cos\frac{2\pi}{N})}{(\frac{2\pi}{N})^2}\right)^{N-2}$$

$$\times(2 + \frac{N-2}{(N-1)^2}) \cos(\frac{2\pi}{N}(j-1))e^{-\frac{1}{2}(2\pi)^2\left(\frac{v_{th}t}{L}\right)^2(1-\frac{2}{N})}$$

$$+ v_{th}{}^2\frac{1}{N}\{(1 + \frac{1}{N-1}) - (1 + \frac{1}{(N-1)^2})(\frac{N-1}{N})^2(2\pi)^2\left(\frac{v_{th}t}{L}\right)^2\}$$

$$\times\left(\frac{2(1-\cos\frac{2\pi}{N})}{(\frac{2\pi}{N})^2}\right)^{N-1}\cos(\frac{2\pi}{N}(j-1))e^{-\frac{1}{2}(2\pi)^2\left(\frac{v_{th}t}{L}\right)^2(1-\frac{1}{N})^2(1+\frac{1}{N-1})} \quad (2.23)$$

The terms retained in (2.23) give an accurate description of $\langle v_1(o)v_j(t)\rangle_{N,L}$ for $t >> t_{th}$ where $t_{th} = \frac{L}{v_{th}}$ is the time required for a particle travelling at the thermal velocity to traverse the ring of length L. As a consequence of the symmetry of the system, (2.23) is invariant under the transformation $(j-1) \to -(j-1)$.

Systems of most physical interest will be those for which N,L are large and $\rho = \frac{N-1}{L}$ is held fixed (the regime of the thermodynamic limit). We shall show that the v.c.f. (2.9) converges pointwise for all t to the v.c.f. written down by Jepsen in the thermodynamic limit. For a finite ring system, from (2.9) we have

$$<v_1(o)v_j(t)>_{N,L} = \frac{2\pi}{N}\sum_u f_{N,L}(u,t) + \frac{2\pi}{N}\sum_u \tilde{f}_{N,L}(u,t) \qquad (2.24)$$

and for an infinite system

$$<v_1(o)v_j(t)> = \int_o^{2\pi} du\ f_\rho(u,t) + \int_o^{2\pi} du\ \tilde{f}_\rho(u,t) \qquad (2.25)$$

where

$$\begin{pmatrix} f_{N,L}(u,t) \\ f_\rho\ (u,t) \end{pmatrix} =$$

$$\frac{1}{2\pi} v_{th}{}^2\ \rho t\ e^{-\hat{\imath}(j-1)u} \int_{-\infty}^{+\infty} dv_k h(v_k)(e^{-\hat{\imath}u}-1)\hat{Q}[u,v_k t,t]$$

$$\times \begin{pmatrix} [\frac{1}{L}\int_o^L dx_n\ R[u,v_k t-x_n,t]]^{N-2} \\ \exp(\rho(1-e^{-\hat{\imath}u})T[u,v_k t]) \end{pmatrix} \qquad (2.26)$$

and

$$\begin{pmatrix} \tilde{f}_{N,L}(u,t) \\ \tilde{f}_\rho\ (u,t) \end{pmatrix} =$$

$$\frac{1}{2\pi} e^{-\hat{\imath}(j-1)u} \int_{-\infty}^{+\infty} dv_1 v_1{}^2 h(v_1)$$

$$\times \begin{pmatrix} [\frac{1}{L}\int_o^L dx_n\ R[u,v_1 t - x_n,t]]^{N-1} \\ \exp(\rho(1-e^{-\hat{\imath}u})T[u,v_k t]) \end{pmatrix} \qquad (2.27)$$

with

$$T[u,w] = \int_{-\infty}^{+\infty} dv_n (w - v_n t)\ S[u,w - v_n t]\ h(v_n). \quad (2.28)$$

It can be shown that $f_{N,L}(u,t) \overset{t.l.}{\to} f_\rho(u,t)$ uniformly in $u$ and that $f_\rho(u,t)$ is Riemann- integrable (more specifically continuous) in $u$ (similarly for $\tilde{f}$).

Now

$$\left|\frac{2\pi}{N} \sum_u f_{N,L}(u,t) - \int_0^{2\pi} du\ f_\rho(u,t)\right|$$

$$\leqslant \left|\frac{2\pi}{N} \sum_u f_\rho(u,t) - \int_0^{2\pi} du\ f_\rho(u,t)\right|$$

$$+ \left|\frac{2\pi}{N} \sum_u (f_{N,L}(u,t) - f_\rho(u,t))\right|. \quad (2.29)$$

The first term on the right hand side of (2.29) approaches zero in the t.l. because $f_\rho(u,t)$ is Riemann- integrable (see Olmsted [81]) and the second approaches zero because of the above mentioned uniform convergence.

To prove the continuity (in $u$) of $f_\rho(u,t)$ is easy.

For the uniform convergence, we write

$$|f_{N,L}(u,t) - f_\rho(u,t)|$$

$$\leqslant \left|\frac{1}{2\pi} v_{th}^2\ \rho t\ e^{-\hat{\imath}(j-1)u} (e^{-\hat{\imath}u} - 1)\right| \times \left\{ \left| \int_{|v_k| < \lambda \frac{L^\alpha}{t}} dv_k h(v_k) \hat{Q}[u, v_k t, t] \right.\right.$$

$$\left. \times \left( \left(\frac{1}{L}\int_0^L R[u, v_k t - x_n, t] dx_n\right)^{N-2} - \exp(\rho(1-e^{-\hat{\imath}u}) T[u, v_k t]) \right) \right|$$

$$+ \left| \int_{|v_k| > \lambda \frac{L^\alpha}{t}} dv_k h(v_k) \hat{Q}[u, v_k, t, t]\ \exp\ (\rho(1-e^{-\hat{\imath}u}) T[u, v_k t]) \right|$$

$$+ \left| \int_{|v_k|>\lambda\frac{L^\alpha}{t}} dv_k h(v_k)\hat{Q}[u,v_k t,t] \left[\frac{1}{L}\int_o^L R[u,v_k t-x_n,t]dx_n\right]^{N-2} \right| \Bigg\} \quad (2.30)$$

Choosing $0 < \alpha < \frac{1}{2}$, we may show that the first term is $0(\frac{1}{N^{1-2\alpha}})$ as $N,L \to \infty$ uniformly in $u$. Suitable upper bounds (uniform in $u$) which approach zero in the t.l. may be found for the last two terms. Similar remarks apply again to $\tilde{f}$. Thus pointwise convergence of the v.c.f.'s is proved.

A qualitative description of the v.c.f. for N,L large and $\rho = \frac{N-1}{L}$ fixed is now possible by comparison with t.l. results. From the analysis of Lebowitz and Percus[41], for $t \lesssim \frac{\sqrt{\pi}}{N} t_{th}$

$$<v_1(o)v_1(t)>_{N,L} - \frac{1}{N} <v_1(o)>^2 \approx <v_1(o)^2> \exp\left(-\frac{4}{\sqrt{\pi}}\left(\frac{t}{t_{th}/N}\right)\right) \quad (2.31)$$

for $t = 0(\frac{1}{N}t_{th}) << t_{th}$,

$$<v_1(o)v_1(t)>_{N,L} - \frac{1}{N}<v_1(o)^2> \approx \frac{v_{th}^2}{(2\pi)^{\frac{1}{2}}}(-1 + \frac{5}{2\pi}) \left(\frac{t}{t_{th}/N}\right)^{-3} \quad (2.32)$$

for $t >> t_{th}$, the behaviour of $<v_1(o)v_1(t)>_{N,L} - \frac{1}{N}<v_1(o)^2>$ is dominated by a decay of the form

$$e^{-\frac{1}{2}(2\pi)^2\left(\frac{t}{t_{th}}\right)^2 (1 + 0(\frac{1}{N}))} .$$

Finally we make some remarks on the relationship between $<v_1(o)v_1(t)>_{N,L}$ and the coefficient of self diffusion $D$. For an infinite system it is usual to assume the Einstein relation

$$D = \frac{1}{3}\int_o^\infty dt\langle v_1(o)v_1(t)\rangle \ . \qquad (2.33)$$

That (2.33) is inappropriate for a finite system contained by walls may be demonstrated using the techniques of ergodic theory (see Lebowitz[82]). This fact may also be demonstrated using the relation

$$\int_o^t ds\langle v_1(o)v_1(s)\rangle = \tfrac{1}{2}\frac{\partial}{\partial t}\langle(x_1(t) - x_1(o))^2\rangle \qquad (2.34)$$

(see Lebowitz and Sykes[77]). However these arguments are not applicable to a finite periodic system. For such a system, it appears from the work of Green[18] and Anstis[44], that a more appropriate expression for D is given by (at least for the dilute case $\rho << 1$)

$$D = \frac{1}{3}\int_o^\infty dt(\langle v_1(o)v_1(t)\rangle - \frac{1}{N}\langle v_1(o)^2\rangle) \ . \qquad (2.35)$$

For the periodic system considered above, we have shown that the integral is strongly convergent.

## 5.3 THE HARD-WALLED BOX

For this system the N-particles, labelled as in section 5.2, are situated in a hard-walled box of length "L". On collision with the walls, they are reflected elastically. Lebowitz and Sykes[77] have extended Jepsen's[40] work to this case and have written down a formula for the v.c.f.'s. The only essential difference is that the straight line trajectories of section 5.2 (representing collisionless motion) must now be replaced by trajectories which are reflected at the walls of the box. In this treatment, however, we shall use a different technique. One must realize that the properties of the above system may be determined by examining a system of $2N$ particles labelled $\{1^{\pm}, 2^{\pm}, \ldots, N^{\pm}\}$ on a ring of length $2L$ if we impose an antisymmetry condition of the form

$$\begin{aligned} x_{j^-}(t) &= -x_{j^+}(t) \\ v_{j^-}(t) &= -v_{j^+}(t) \quad \text{for} \quad t = 0 \;. \end{aligned} \tag{3.1}$$

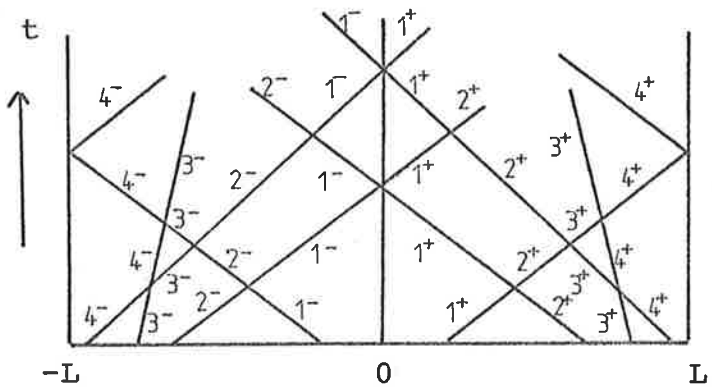



Fig. 5.2: Diagram showing the nature of the dynamics of the system.

This technique has been used by Gervois and Pomeau [78] for the corresponding semi-infinite case.

The notation of section 5.2 is applicable to this case if we write $j^+ = j$ for $j \in \{1,2,\ldots,N\}$ and $j^- = -j+1$ for $j \in \{1,2,\ldots,N\}$. Because (3.1) will be true for all $t \geqslant 0$, the following relations hold:

$$r_n(h^{\pm},k^{\pm},t) = r_{-n}(h^{\mp},k^{\mp},t)$$

$$s(u,h^{\pm},k^{\pm},t) = s(-u,h^{\mp},k^{\mp},t)$$

$$A_{j^{\pm}k^{\pm}}(t) = A_{j^{\mp}k^{\mp}}(t)$$

and
$$w_{k^{\pm}h^{\pm}} = - w_{k^{\mp}h^{\mp}} \tag{3.2}$$

where any choice of the signs $(\pm,\mp)$ is possible. In this case $s(u,h^{\pm},k^{\pm},t)$ is given by

$$s(u,h^{\pm},k^{\pm},t) = \underset{\sim}{S}[u,w_{k^{\pm}h^{\pm}}] \quad k^{\pm} < h^{\pm}$$

$$= e^{-\hat{\imath}u}\,\underset{\sim}{S}[u,w_{k^{\pm}h^{\pm}}] \quad k^{\pm} > h^{\pm}$$

and
$$\underset{\sim}{S}[u,w] = e^{\hat{\imath}nu} \quad \text{for} \quad (n-1)2L < w \leqslant n.2L$$

$$\text{for each } n. \tag{3.3}$$

Then

$$A_{j^{\pm}k^{\pm}}(t) = \frac{1}{2N} \sum_{\iota\varepsilon\{1^{\pm}2^{\pm}\ldots N^{\pm}\}} (-1)^{\iota} e^{+\hat{\imath}u} e^{-\hat{\imath}j^{\pm}u} \prod_{h\varepsilon\{1^{\pm}2^{\pm}\ldots N^{\pm}\}} \underset{\sim}{S}[u,w_{k^{\pm}h}] \tag{3.4}$$

where $u = \frac{2\pi\iota}{2N}$ here.

We wish to calculate ensemble averages of the form

$$F_{N,L} = \langle f(x_{k^+}(o),v_{k^+}(o) \; ; \; x_{j^+}(t),v_{j^+}(t))\rangle_{N,L} \tag{3.5}$$

where particle $k^+$ is assumed to be at a position $x_{k^+} = x_{k^+}(o)\ \varepsilon\ (0,L)$ at the initial time. Particles $1^+, 2^+,\ldots,k^+ - 1$ are assumed to be distributed uniformly in $(0,x_{k^+}(o))$ and particles $k^+ + 1$, $k^+ + 2, \ldots, N^+$ distributed uniformly in $(x_{k^+}(o),L)$ at the initial time. These particles have an initial velocity distribution $h(\ )$ assumed to be Maxwellian here. So again we have a quasi-equilibrium initial distribution and

$$F_{N,L} = \sum_{m\varepsilon\{1^\pm,2^\pm,\ldots,N^\pm\}} \langle f(x_{k^+},v_{k^+}\ ;\ x_m+v_m t,v_m)A_{j^+m}\rangle_{N,L}$$

$$= \int_{-\infty}^{+\infty} dv_{k^+}h(v_{k^+}) \prod_{\substack{\ell=1\\ \neq k^+}}^{N} \int_{-\infty}^{+\infty} dv_\ell\, h(v_\ell)$$

$$\times \left[\frac{(k^+-1)!}{x_{k^+}(o)^{k^+-1}} \int_o^{x_{k^+}(o)} dx_{k^+-1} \int_o^{x_{k^+-1}} dx_{k^+-2}\cdots \int_o^{x_2} dx_1\right]$$

$$\times \left[\frac{(N-k^+)!}{(L-x_{k^+}(o))^{N-k^+}} \int_{x_{k^+}(o)}^{L} dx_N \int_{x_{k^+}(o)}^{x_N} dx_{N-1}\cdots \int_{x_{k^+}(o)}^{x_{k^++2}} dx_{k^++1}\right]$$

$$\times \sum_{m\varepsilon\{1^\pm,2^\pm,\ldots,N^\pm\}} f(x_{k^+},v_{k^+}\ ;\ x_m+v_m t,v_m)A_{j^+m}(t) \quad (3.6)$$

From (3.4) $A_{j^+m}(t)$ may be written completely in terms of the variables $(x_m,v_m)$, $m\ \varepsilon\ \{1^+,2^+,\ldots,N^+\}$. Upon substitution into (3.6), we see that after integration over velocities, the integrand is totally symmetric with respect to the variables $(x_1,x_2,\ldots,x_N)$. Consequently the spatial integrations may be rewritten as

$$\left[\prod_{i=1}^{k^+-1} \frac{1}{x_{k^+}(o)} \int_o^{x_{k^+}(o)} dx_i\right]\left[\prod_{i=k^++1}^{N} \frac{1}{L-x_{k^+}(o)} \int_{x_{k^+}(o)}^{L} dx_i\right]. \quad (3.7)$$

Using (3.4) and (3.7), (3.6) becomes after some manipulation

$$F_{N,L} = \frac{1}{2N} \sum_u (-1)^l \, e^{\hat{i}u} \, e^{-\hat{i}ju}$$

$$\times \Big\{ (k^+ - 1) \cdot \int_{-\infty}^{+\infty} dv_m h(v_m) \; \Big(\frac{1}{x_{k^+}(o)} \int_o^{x_{k^+}(o)} dx_m\Big)$$

$$\times \left[ \Big|{}^{1,k^+-2,N-k^+}_{[u,x_m+v_mt,v_m,x_{k^+},t]} + \Big|{}^{1,k^+-2,N-k^+}_{[u,-x_m-v_mt,-v_m,x_{k^+},t]} \right]$$

$$+ (N-k^+) \cdot \int_{-\infty}^{+\infty} dv_m h(v_m) \cdot \Big(\frac{1}{L-x_{k^+}(o)} \int_{x_{k^+}(o)}^{L} dx_m\Big)$$

$$\times \left[ \Big|{}^{1,k^+-1,N-k^+-1}_{[u,x_m+v_mt,v_m,x_{k^+},t]} + \Big|{}^{1,k^+-1,N-k^+-1}_{[u,-x_m-v_mt,-v_m,x_{k^+},t]} \right]$$

$$+ \int_{-\infty}^{+\infty} dv_{k^+} h(v_{k^+}) f(x_{k^+},v_{k^+};x_{k^+}+v_{k^+}t,v_{k^+}) \Big|{}^{0,k^+-1,N-k^+}_{[u,x_{k^+}+v_{k^+}t,v_{k^+},t]}$$

$$+ \int_{-\infty}^{+\infty} dv_{k^+} h(v_{k^+}) f(x_{k^+},v_{k^+};-x_{k^+}-v_{k^+}t,-v_{k^+}) \Big|{}^{0,k^+-1,N-k^+}_{[u,-x_{k^+}-v_{k^+}t,-v_{k^+},x_{k^+},t]} \tag{3.8}$$

with

$$\Big|{}^{j_0,j_1,j_2}_{[u,w,v,x_{k^+}\;,t]}$$

$$= \underset{\sim}{S}[u,2w] \; \underset{\sim}{Q}[u,w,v,x_{k^+}\;,t]^{j_0}$$

$$\times \Big(\frac{1}{x_{k^+}} \int_o^{x_{k^+}} dx_n \underset{\sim}{R}[u,w,x_n,t]\Big)^{j_1} \Big(\frac{1}{L-x_{k^+}} \int_{x_{k^+}}^{L} dx_n \underset{\sim}{R}[u,w,x_n,t]\Big)^{j_2} \tag{3.9}$$

where

$$\underset{\sim}{Q}[u,w,v,x_{k^+},t]$$

$$= \int_{-\infty}^{+\infty} dv_{k^+} h(v_{k^+}) f[x_{k^+},v_{k^+};w,v] \prod_{\pm} \underset{\sim}{S}[u,w\pm(x_{k^+}+v_{k^+}t)] \tag{3.10}$$

and

$$R[u,w,x_n,t] = \int_{-\infty}^{+\infty} dv_n h(v_n) \prod_{\pm} \underset{\sim}{S}[u,w\pm(x_n+v_nt)]. \tag{3.11}$$

For the v.c.f.'s f( ) has the form $f(x_{k^+},v_{k^+};x,v) = v_{k^+}v$. So from (3.8)

$$F_{N,L} = \langle v_{k^+}(o)v_{j^+}(t)\rangle_{N,L}$$

$$= \frac{1}{2N} \sum_u (-1)^l \, e^{+\hat{\imath}u} \, e^{-\hat{\imath}ju} \times$$

$$\Big\{(k^+-1) \int_{-\infty}^{+\infty} dv_m v_m h(v_m) \cdot \Big(\frac{1}{x_{k^+}(o)} \int_o^{x_{k^+}(o)} dx_m\Big)$$

$$\times \Big[\hat{\prod}_{(-\infty,+\infty)}^{1,k^+-2,N-k^+}[u,x_m+v_mt,x_{k^+},t] - \hat{\prod}_{(-\infty,+\infty)}^{1,k^+-2,N-k^+}[u,-x_m-v_mt,x_{k^+},t]\Big]$$

$$+ (N-k^+) \int_{-\infty}^{+\infty} dv_m v_m h(v_m) \cdot \Big(\frac{1}{L-x_{k^+}(o)} \int_{x_{k^+}(o)}^{L} dx_m\Big)$$

$$\times \Big[\hat{\prod}_{(-\infty,+\infty)}^{1,k^+-1,N-k^+-1}[u,x_m+v_mt,x_{k^+},t] - \hat{\prod}_{(-\infty,+\infty)}^{1,k^+-1,N-k^+-1}[u,-x_m-v_mt,x_{k^+},t]\Big]$$

$$+ \int_{-\infty}^{+\infty} dv_{k^+} h(v_{k^+}) v_{k^+}^2$$

$$\times \Big[\hat{\prod}_{(-\infty,+\infty)}^{0,k^+-1,N-k^+}[u,x_{k^+}+v_{k^+}t,x_{k^+},t] - \hat{\prod}_{(-\infty,+\infty)}^{0,k^+-1,N-k^+}[u,-x_{k^+}-v_{k^+}t,x_{k^+},t]\Big]\Big\} \tag{3.12}$$

where $\hat{\int}^{j_0,j_1,j_2}_{(\alpha,\beta)}$ is obtained from $\int^{j_0,j_1,j_2}$ by replacing $\underset{\sim}{Q}(\ )$ with

$$\hat{\underset{\sim}{Q}}_{(\alpha,\beta)}[u,w,x_{k^+},t] = \int_\alpha^\beta dv_{k^+}h(v_{k^+})v_{k^+}\prod_{\pm}S[u,w\pm(x_{k^+}+v_{k^+}t)]. \quad (3.13)$$

The following property is easily verified from (3.3):

$$\hat{\int}^{j_0,j_1,j_2}_{(\alpha,\beta)}[u,w+2L,x_{k^+},t] = e^{2\hat{\imath}u(j_0+j_1+j_2+1)}\hat{\int}^{j_0,j_1,j_2}_{(\alpha,\beta)}[u,w,x_{k^+},t] \quad (3.14)$$

and $e^{2\hat{\imath}u(1+j_0+j_1+j_2)} = 1$ if $1 + j_0 + j_1 + j_2 \equiv 0 \pmod N$.

We examine the contribution to (3.12) from the $u(l) = 0$ term. Note that $\underset{\sim}{S}[o,x] = 1$ so $\underset{\sim}{R}[o,x,x',t] = 1$ and hence

$$\frac{1}{|A|}\int_A dx\ \underset{\sim}{R}[o,x,x',t] = 1. \quad (3.15)$$

By inspection, contributions from the first four terms of (3.12) are identically zero. The fifth gives a contribution $\frac{1}{2N}\langle v_{k^+}(o)^2\rangle$ and the sixth gives a contribution $-\frac{1}{2N}\langle v_{k^+}(o)^2\rangle$. So there is a complete cancelation (of contributions where particle $j^+$ is on trajectories $k^+$ and $k^-$ respectively). The initial conditions on the v.c.f.'s may also be checked. From (3.3),

$$\underset{\sim}{S}[u,\pm 2x_{k^+}] = \begin{pmatrix} e^{\hat{\imath}u} \\ 1 \end{pmatrix}, \quad \frac{1}{x_{k^+}(o)}\int_o^{x_{k^+}(o)} dx_n \underset{\sim}{R}[u,\pm x_{k^+},x_n,o] = \begin{pmatrix} e^{2\hat{\imath}u} \\ 1 \end{pmatrix} \quad (3.16)$$

and

$$\frac{1}{L-x_{k^+}(o)} \int_{x_{k^+}(o)}^{L} dx_{\underset{\sim}{n}} R[u,\pm x_{k^+},x_n,o] = 1$$

So (3.12) gives

$$\langle v_{k^+}(o)v_{j^+}(t)\rangle_{N,L} = \frac{1}{2N}\sum_u e^{-\hat{\imath}(j^+-k^+)u} \langle v_{k^+}(o)^2\rangle$$

$$- \frac{1}{2N}\sum_u e^{-\hat{\imath}(j^++k^+)u}\langle v_{k^+}(o)^2\rangle$$

$$= \delta^{2N}_{j^+,k^+} \langle v_{k^+}(o)^2\rangle \qquad (3.17)$$

as required.

Using (3.14), we may rewrite (3.12) as follows (cf. section 5.2)

$$F_{N,L} = \langle v_{k^+}(o)v_{j^+}(t)\rangle_{N,L} = \frac{1}{2N}\sum_{u\neq o} (-1)^l e^{-\hat{\imath}(j-l)u}$$

$$\times \Big\{ v_{th}{}^2 \frac{t}{x_{k^+}} (k^+-1) \int_o^{\frac{2L}{t}} dv_m \sum_{m=-\infty}^{+\infty} h(v_m + \frac{2Lm}{t})$$

$$\times \Big[ \hat{\prod}^{1,k^+-2,N-k^+}_{(-\infty,+\infty)} [u,x_{k^+}+v_m t,x_{k^+},t] - \hat{\prod}^{1,k^+-2,N-k^+}_{(-\infty,+\infty)} [u,-x_{k^+}-v_m t,x_{k^+},t] \Big]$$

$$+ v_{th}{}^2 \frac{t}{L-x_{k^+}} (N-k^+) \int_o^{\frac{2L}{t}} dv_m \sum_{m=-\infty}^{+\infty} h(v_m + \frac{2Lm}{t})$$

$$\times \Big[ \hat{\prod}^{1,k^+-1,N-k^+-1}_{(-\infty,+\infty)} [u,-x_{k^+}-v_m t,x_{k^+},t] - \hat{\prod}^{1,k^+-1,N-k^+-1}_{(-\infty,+\infty)} [u,x_{k^+}+v_m t,x_{k^+},t] \Big]$$

$$+ \int_0^{\frac{2L}{t}} dv_{k^+} \sum_{m=-\infty}^{+\infty} h(v_{k^+} + \frac{2Lm}{t}) (v_{k^+} + \frac{2Lm}{t})^2$$

$$\times \left[ \hat{\int}^{0,k^+-1,N-k^+}_{(-\infty,+\infty)} [u, x_{k^+}+v_{k^+}t, x_{k^+}, t] - \hat{\int}^{0,k^+-1,N-k^+}_{(-\infty,+\infty)} [u, -x_{k^+}-v_{k^+}t, x_{k^+}, t] \right] \quad (3.18)$$

The sums $\sum_{m=-\infty}^{+\infty}$ in (3.18) may be expressed in a more convenient form using relations of the type (2.18) and (2.19). The $m=0$ terms in the rearranged sums cancel. Physically this represents a partial cancellation of contributions to $\langle v_{k^+}(o)v_{j^+}(t)\rangle_{N,L}$ from a particle $j^+$ on trajectories $(1^+, 2^+, \ldots, k^+-1, k^++1, \ldots, N^+)$ and $(1^-, 2^-, \ldots k^--1, k^-+1, \ldots, N^-)$ and also on trajectories $k^+$ and $k^-$. The remaining terms are characterized by the usual "fast" decrease. To complete the analysis, we must consider the long time behaviour of

$$\hat{\int}^{j_0,j_1,j_2}_{(-\infty,+\infty)} [u, w, x_{k^+}, t].$$

The behaviour of

$$\left(\frac{1}{x_{k^+}} \int_0^{x_{k^+}} dx_n \underset{\sim}{R}[u,w,x_n,t]\right) \quad \text{and} \quad \left(\frac{1}{L-x_{k^+}} \int_{x_{k^+}}^{L} dx_n \underset{\sim}{R}[u,w,x_n,t]\right)$$

is considered in Appendix F. These expressions have a non-zero component as $t \to \infty$. Using the appropriate Poisson summation formula we obtain

$$\hat{\underset{\sim}{Q}}[u,w,x_{k^+},t] \underset{\sim}{\overset{t\to\infty}{}} - v_{th}\left(\frac{v_{th}t}{2L}\right)^2 . 2\pi . e^{-\frac{1}{2}(2\pi)^2\left(\frac{v_{th}t}{2L}\right)^2}$$

$$\times \int_o^1 dw_{k^+} \sin(2\pi w_{k^+}) \prod_{\pm} \underset{\sim}{S}[u, w\pm(x_{k^+}+2Lw_{k^+})] \quad (3.19)$$

So the last two terms in (3.18) (the contributions from particle $j^-$ on trajectories $k^+$ and $k^-$) will dominate the others as $t \to \infty$ and we may write

$$\langle v_{k^+}(o) v_{j^+}(t) \rangle_{N,L} \overset{t\to\infty}{\sim} 2\, v_{th} \left(1-(2\pi)^2\left(\frac{v_{th}t}{L}\right)^2\right) e^{-\frac{1}{2}(2\pi)^2\left(\frac{v_{th}t}{2L}\right)^2}$$

$$\times \int_o^1 dw_{k^+} \cos(2\pi w_{k^+}) \cdot \left(\frac{1}{2N} \sum_u (-1)^l e^{-\hat{i}(j-1)u}\right)$$

$$\times \left[ \underset{\sim}{S}[u, 2(x_{k^+}+2Lw_{k^+})] \left(\frac{1}{x_{k^+}} \int_o^{x_{k^+}} dx_n \underset{\sim}{R}[u, x_{k^+}+2Lw_{k^+}, x_n, t]\right)^{k^+-1}\right.$$

$$\times \left(\frac{1}{L-x_{k^+}} \int_{x_{k^+}}^{L} dx_n \underset{\sim}{R}[u, x_{k^+}+2Lw_{k^+}, x_n, t]\right)^{N-k^+}$$

$$- \underset{\sim}{S}[u, -2(x_{k^+}+2Lw_{k^+})] \cdot \left(\frac{1}{x_{k^+}} \int_o^{x_{k^+}} dx_n \underset{\sim}{R}[u, -(x_{k^+}+2Lw_{k^+}), x_n, t]\right)^{k^+-1}$$

$$\left. \times \left(\frac{1}{L-x_{k^+}} \int_{x_{k^+}}^{L} dx_n \underset{\sim}{R}[u, -(x_{k^+}+2Lw_{k^+}), x_n, t]\right)^{N-k^+}\right] \qquad (3.20)$$

Behaviour of the type (3.20) is associated with a time scale $0(t_{th})$ just as for the ring system. The behaviour of the v.c.f.'s for large times $t \gg t_{th}$ is dominated by a decay of the form

$$e^{-\frac{1}{2}(2\pi)^2\left(\frac{v_{th}t}{2L}\right)^2} .$$

## 5.4 BOUNDARY EFFECTS ON VELOCITY CORRELATION FUNCTIONS

Firstly let us consider the problem where the physical system is the same as in section 5.3. We evaluate the v.c.f.'s where we specify that $k^+ = 1^+$ and that this particle is situated on the wall at $t = 0$ (i.e. $x_{1^+}(o) = 0$). Furthermore, in calculating the ensemble average $\langle - \rangle_{N,L}$ the integration over $v_{1^+}(o) = v_{1^+}$ becomes $2\int_o^{+\infty} dv_{1^+} h(v_{1^+})$. where $h(\ )$ is again assumed to be Maxwellian (i.e. the specified particle on the wall must initially have a velocity toward the interior of the container). With this modification, the formulation of section 5.3 is applicable and we obtain for the v.c.f.'s

$$\langle v_{1^+}(o) v_{j^+}(t) \rangle_{N,L} = \frac{1}{2N} \sum_u (-1)^{l} e^{-\hat{\imath}(j-1)u}$$

$$\times \Bigg( 4\, v_{th}{}^2 t \left(\frac{N-1}{L}\right) \int_o^{\frac{2L}{t}} dv_m \sum_{m=-\infty}^{+\infty} h\left(v_m + \frac{2Lm}{t}\right) \hat{\Big[}^{1,0,N-2}_{(o,\infty)} [u, L+v_m t, o, t]$$

$$- 4\, v_{th}{}^2 t \left(\frac{N-1}{L}\right) \int_o^{\frac{2L}{t}} dv_m \sum_{m=-\infty}^{+\infty} h\left(v_m + \frac{2Lm}{t}\right) \hat{\Big[}^{1,0,N-2}_{(o,\infty)} [u, +v_m t, o, t]$$

$$+ 2\int_0^{\frac{2L}{t}} dv_{1^+} \sum_{n=0}^{+\infty} \left(v_{1^+} + \frac{2Ln}{t}\right)^2 h\left(v_{1^+} + \frac{2Ln}{t}\right) \Bigg[ \hat{\Big[}^{0,0,N-1}_{(o,\infty)} [u, v_{1^+} t, o, t]$$

$$- \hat{\Big[}^{0,0,N-1}_{(o,\infty)} [u, -v_{1^+} t, o, t] \Bigg] \Bigg)$$

$$\text{where} \quad u = 2\pi \cdot \frac{l}{2N} \,. \qquad (4.1)$$

The first two terms may be analyzed using the standard Poisson sum formula. In the rearranged sums, the m=0 terms cancel leaving the usual fast decreasing terms. For the remaining terms, we must use the most general form of (2.17) for the piecewise continuous function

$$g(x) = H(x)\ (v_1 + \frac{2Lx}{t})^2\ h(v_1 + \frac{2Lx}{t})$$

with H( ) the Heaviside step function. We obtain

$$\sum_{n=0}^{+\infty} (v_1+\frac{2Ln}{t})^2 h(v_1+\frac{2Ln}{t}) = \tfrac{1}{2}v_1{}^2 h(v_1)+2(\tfrac{1}{2}H_c(o)+\sum_{n=1}^{+\infty} H_c(2\pi n)) \quad (4.2)$$

$$H_c(\lambda) = \int_o^{+\infty} dx\ \cos(\lambda x)(v_1+\frac{2Lx}{t})^2 h(v_1+\frac{2Lx}{t})$$

$$= \frac{v_{th}}{\lambda^2}\ (\frac{2L}{t})\ \left(2\left(\frac{v_1}{v_{th}}\right)h(v_1) - \left(\frac{v_1}{v_{th}}\right)^3 h(v_1)\right)$$

$$- \frac{1}{\lambda^2}\ (\frac{2L}{t})^2 \int_o^{+\infty} dx\ \cos(\lambda x)\left(2-5\left(\frac{v_1+\frac{2Lx}{t}}{v_{th}}\right)^2 + \left(\frac{v_1+\frac{2Lx}{t}}{v_{th}}\right)^4\right)h(v_1+\frac{2Lx}{t}). \quad (4.3)$$

The first term in (4.2) produces a contribution

$$2^4\ v_{th}{}^2\ (\frac{t_{th}}{t})^3 \int_o^1 dw_1\ \tfrac{1}{2}\cdot w_1{}^2\ v_{th} h(\frac{2L}{t}\ w_1)$$

$$\times \left[\hat{\int}_{(o,\infty)}^{0,0,N-1} [u,2Lw_1,o,t] - \hat{\int}_{(o,\infty)}^{0,0,N-1} (u,2L(1-w_1),o,t]\right]$$

$$= O((\frac{t_{th}}{t})^3) \quad \text{as} \quad t \to \infty. \quad (4.4)$$

The second gives

$$- 2^4 v_{TH}^2\left(\frac{t_{th}}{t}\right)^3 \int_o^1 dw_1 \int_o^{w_1} dw' w'^2 v_{th} h(\frac{2L}{t} w')$$

$$\times \left[\hat{\prod}^{0,0,N-1}_{(o,\infty)} [u, 2Lw_1, o, t] - \hat{\prod}^{0,0,N-1}_{(o,\infty)} [u, 2L(1-w_1) o, t]\right]$$

$$= 0((\frac{t_{th}}{t})^3) \quad \text{as} \quad t \to \infty. \qquad (4.5)$$

It may also be easily shown that the remaining terms produce a contribution

$0((\frac{t_{th}}{t})^3)$ as $t \to \infty$, so in conclusion

$$\langle v_{1+}(o) v_{j+}(t) \rangle_{N,L} = 0((\frac{t_{th}}{t})^3) \quad \text{as} \quad t \to \infty \qquad (4.6)$$

Let us now reconsider the behaviour of the v.c.f.'s with emphasis on the $x_{k+}(o)$ dependence. (3.12) may be written as the sum of two contributions; one where the velocity of the specified particle $v_{k+} < 0$ and the other where $v_{k+} > 0$, that is

$$\langle v_{k+}(o) v_{j+}(t) \rangle_{N,L} = \int_o^{+\infty} dv_{k+} \ldots + \int_{-\infty}^{o} dv_{k+} \ldots . \qquad (4.7)$$

By comparison with the analysis above, the contributions to both $\int_o^{+\infty} dv_{k+} \ldots$ and $\int_{-\infty}^{o} dv_{k+} \ldots$ in (4.7) from the first four terms in (3.12) have a "fast" decreasing asymptotic time behaviour. The contributions from the last two, however, exhibit a behaviour dominated by a decay of the form

$$0((\frac{t_{th}}{t})^3) \quad \text{as} \quad t \to \infty$$

Consequently there must be a complete cancellation of the "slow" decreasing parts of $\int_o^{+\infty} dv_{k^+} \ldots$ and $\int_{-\infty}^{o} dv_{k^+} \ldots$ leaving just a fast decreasing part. This is valid for all $x_{k^+}(o)$. Furthermore, we shall show now that as $x_{k^+}(o)$ approaches the boundary, there is a complete cancellation of "fast" and "slow" decreasing parts of $\int_o^{+\infty} dv_{k^+} \ldots$ and $\int_{-\infty}^{o} dv_{k^+} \ldots$ .

For definiteness consider the case where $x_{k^+} \to 0$. For any specific set of initial conditions on $v_{j^+}$, define $v^{j^+}$, $j^+ \in \{1,2,\ldots,k\}$ as follows. Let $(v^{1^+}, v^{2^+}, \ldots v^{k^+})$ be a rearrangement of $(|v_{1^+}|, |v_{2^+}|, \ldots, |v_{k^+}|)$ so that $v^{1^+} \leqslant v^{2^+} \leqslant \ldots \leqslant v^{k^+}$. Then as $x_{k^+}(o) \to 0$, it becomes increasingly probable (excluding a neighbourhood $0(x_{k^+}(o))$ of the initial time) that the particles $(1^+ \ 2^+ \ \ldots \ k^+)$ will be travelling with velocities $(v^{1^+}, v^{2^+}, \ldots v^{k^+})$ respectively before interacting with any other particles. Their trajectories before collision will approach $(v^{1^+}t, v^{2^+}t, \ldots, v^{k^+}t)$ respectively. Because only moduli of velocities are involved, it follows that $\int_o^{+\infty} dv_{k^+} \ldots$ and $\int_{-\infty}^{o} dv_{k^+} \ldots$ will give opposite contributions to $\langle v_{k^+}(o) v_{j^+}(t) \rangle_{N,L}$

in this limit. Note that the special case $k^+ = 1$ is more physical.

We shall now give a mathematical verification of the above statements. We must evaluate (3.12) in the limit $x_{k^+}(o) \to 0$. From the definition of

$$\hat{\int}^{j_0,j_1,j_2}_{(\alpha,\beta)} [u,w,x_{k^+},t]$$

and the analysis of Appendix F, it follows that these functions are uniformly continuous in $(w,x_{k^+})$ on $(-\infty,+\infty) \times [0,L]$. It then follows that $\lim_{x_{k^+}\to 0}$ may be taken under the velocity integrals appearing explicitly in (3.12). Also from the above mentioned continuity property

$$\lim_{x_{k^+}\to 0} \left(\frac{1}{x_{k^+}} \int_o^{x_{k^+}} dx_m\right) \cdot = \cdot \left|x_m=0\right| x_{k^+}=0$$

$$\lim_{x_{k^+}\to 0} \left(\frac{1}{L-x_{k^+}} \int_{x_{k^+}}^{L} dx_m\right) \cdot = \frac{1}{L}\int_o^L dx_m \cdot \Big|_{x_{k^+}=0}. \tag{4.8}$$

Now the expression $\hat{\int}^{1,j_0,j_1}_{(-\infty,+\infty)}[u,w,o,t]$ contains a factor

$$\hat{\underset{\sim}{Q}}_{(-\infty,+\infty)}[u,w,o,t] = \int_{-\infty}^{+\infty} dv_{k^+} h(v_{k^+}) v_{k^+} \Pi \underset{\pm}{\underset{\sim}{S}}[u,w\pm v_{k^+}t]$$

which is identically zero since the integrand is odd. So (3.12) becomes

$$\lim_{x_{k^+}\to 0} \langle v_{k^+}(o)v_{j^+}(t)\rangle_{N,L}$$

$$= \frac{1}{2N}\sum_u (-1)^l e^{-\hat{i}(j-1)u} \times \int_{-\infty}^{+\infty} dv_{k^+} h(v_{k^+})v_{k^+}^2 \tag{4.9}$$

$$\times \left[ \hat{\int}_{(-\infty,+\infty)}^{0,k^+-1,N-k^+} [u,v_{k^+}t,o,t] - \hat{\int}_{(-\infty,+\infty)}^{0,k^+-1,N-k^+} [u,-v_{k^+}t,o,t] \right]$$

Employing a trivial change of variable $v_{k^+} \to -v_{k^+}$ in the last term, we conclude that

$$\lim_{x_{k^+}\to 0} \langle v_{k^+}(o)v_{j^+}(t)\rangle_{N,L} = 0. \tag{4.10}$$

We expect that there will be a partial generalization of this property to higher dimensional systems of particles which interact with the walls elasticity. We suppose interaction potentials associated with particles are spherically symmetric and $\underline{x}$ denotes the centre of the particle. The arguments given here apply to a hard sphere potential but may be easily adapted to handle more general cases. For (finite) two or three dimensional systems, we define a class of v.c.f.'s as follows:

$$\langle \underline{v}_k(o)\cdot\underline{v}_j(t)\rangle = \int_V d\underline{x} \int_{R^n} d\underline{v} \int_{R^n} d\underline{v}_k(o) h^n(\underline{v}_k(o))\underline{v}_k(o)\cdot\underline{v} \tag{4.11}$$

$$\times f_j(\underline{x},\underline{v},t \mid \underline{x}_k(o),\underline{v}_k(o),k) \qquad n=2,3$$

where the particle centres are confined to a region $V$

in $R^n$. $f_j(\underline{x},\underline{v},t \mid \underline{x}_k(o),\underline{v}_k(o),k)$ gives the probability that particle $j$ will have a position $\underline{x}$, velocity $\underline{v}$ at time $t$ given that particle $k$ has position $\underline{x}_k(o)$, velocity $\underline{v}_k(o)$ at the initial time and the remaining particles are in equilibrium at this time. $h^n(\ )$ is the n-dimensional Maxwellian distribution.

Now suppose $\underline{x}^P$ is on a smooth part of the boundary $\partial V$ of $V$. Let $\underline{e}^\perp$ be the inward normal to $\partial V$ at $\underline{x}^P$. Then every vector can be uniquely decomposed in the form

$$\underline{v} = v^\perp \underline{e}^\perp + \underline{v}'' \quad \text{where} \quad \underline{e}^\perp . \underline{v}'' = 0. \tag{4.12}$$

Then

$$<\underline{v}_k(o).\underline{v}_j(t)>$$

$$= \int_V d\underline{x} \int_{R^n} d\underline{v} \int_{R^{n-1}} d\underline{v}_k''(o) h^{n-1}(\underline{v}_k''(o)) \int_R dv_k^\perp(o) h^1(v_k^\perp(o)) v_k^\perp(o) v^\perp$$

$$\times f_j(\underline{x},\underline{v},t \mid \underline{x}_k(o),\underline{v}_k(o),k)$$

$$+ \int_V d\underline{x} \int_{R^n} d\underline{v} \int_{R^n} d\underline{v}_k(o) h^n(\underline{v}_k(o)) \underline{v}_k''(o).\underline{v}_k'' f_j(\underline{x},\underline{v},t \mid \underline{x}_k(o),\underline{v}_k(o),k). \tag{4.13}$$

We now consider the behaviour of the first term of (4.13) as $\underline{x}_k(o) \to \underline{x}^P$. In this limit it becomes increasingly probable (excluding a neighbourhood $O\left(\frac{|\underline{x}_k(o)-\underline{x}^P|}{|v_k^\perp(o)|}\right)$ of the initial time) that particle $k$ will have a velocity $|v_k^{\perp}(o)|\underline{e}^{\perp} + \underline{v}_k''(o)$ before interaction with other particles. The trajectory of particle $k$ before collision will approach

$$\underline{x}_k(t) = \underline{x}^P + (|v_k^{\perp}(o)|\underline{e}^{\perp} + \underline{v}_k''(o))t.$$

Since this only depends on $v_k^{\perp}(o)$ through its modulus, we conclude that $\int_o^{+\infty} dv_k^{\perp}(o)\ldots$ and $\int_{-\infty}^{o} dv_k^{\perp}(o)$ give opposite contributions to the first term of (4.13) as $\underline{x}_k(o) \to \underline{x}^P$. So

$$\lim_{\underline{x}_k(o)\to\underline{x}^P} \langle \underline{v}_k(o) \cdot \underline{v}_j(t)\rangle$$

$$= \int_V d\underline{x}\int_{R^n} d\underline{v}\int_{R^n} d\underline{v}_k(o)h^n(\underline{v}_k(o))\underline{v}_k''(o)\cdot\underline{v}''f_j(\underline{x},\underline{v},\underline{t}|\underline{x}_k(o),\underline{v}_k(o),k). \tag{4.14}$$

The behaviour of the v.c.f. as $\underline{x}_k(o)$ approaches the corners and edges of $V$ may also be considered. Consider first the case of a two dimensional rectangular region and suppose $\underline{x}^P$ is a corner point. Before $k$ interacts with other particles, we have the following pictures:

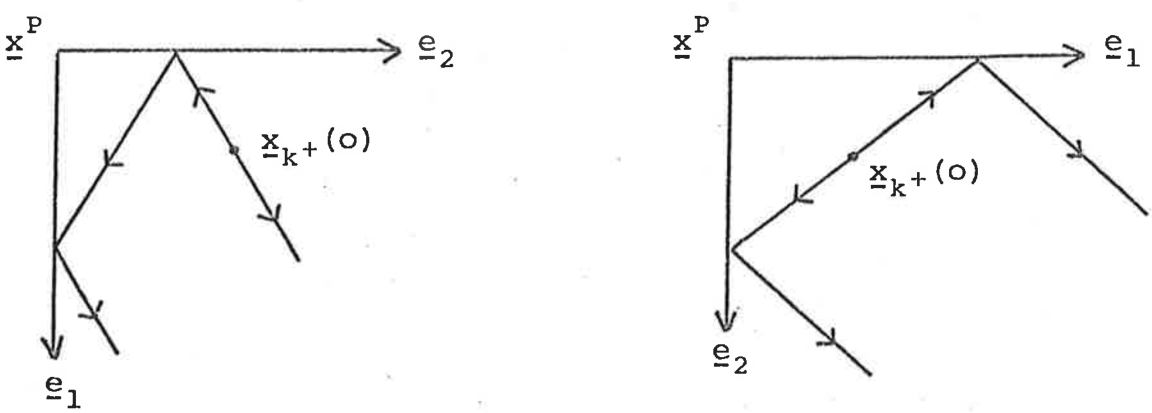



Fig. 5.3: Reflection from a corner.

Let us write $\underline{v}_k(o) = v_k^1(o)\,\underline{e}_1 + v_k^2(o)\,\underline{e}_2$. Then as $\underline{x}_k(o) \to \underline{x}^P$, the trajectory of particle k before collision approaches

$$\underline{x}_k(t) = \underline{x}^P + (|v_k^1(o)|\underline{e}_1 + |v_k^2(o)|\underline{e}_2)t\,. \tag{4.15}$$

By comparison with the previous analysis, we expect that contributions to $<\underline{v}_k(o)\,.\,\underline{v}_j(t)>$ from $\underline{v}_k(o) = -\underline{v}$ and $+\underline{v}$ will cancel in the limit $\underline{x}_k(o) \to \underline{x}^P$. Therefore

$$\lim_{\underline{x}_k(o)\to\underline{x}^P} <\underline{v}_k(o)\,.\,\underline{v}_j(t)> = 0. \tag{4.16}$$

Finally we consider the situation in three dimensions where V is a rectangular box. If $\underline{x}^P$ is an edge point (excluding corners), we set up a coordinate system through orthogonal basis vectors $(\underline{e}_1,\underline{e}_2,\underline{e}_3)$ with $\underline{e}_3$ along the edge and $\underline{e}_1,\underline{e}_2$ along the walls. The v.c.f.'s may be expressed as

$$<\underline{v}_k(o)\,.\,\underline{v}_j(t)> = \int_V d\underline{x}\int_{R^3} d\underline{v}\int_{R^3} d\underline{v}_k(o)\,h^3(\underline{v}_k(o))$$

$$\times\ (v_k^1(o)v^1+v_k^2(o)v^2+v_k^3(o)v^3)$$

$$\times\ f_j(\underline{x},\underline{v}t\,|\,\underline{x}_k(o),\underline{v}_k(o),k)$$

$$\text{where}\quad \underline{v} = v^1\,\underline{e}_1 + v^2\,\underline{e}_2 + v^3\,\underline{e}_3. \tag{4.17}$$

Contributions to the first two terms from $\underline{v}_k(o)=w^1\underline{e}_1+w^2\underline{e}_2+w^3\underline{e}_3$

and $\underline{v}_j(o) = -w^1\underline{e}_1 - w^2\underline{e}_2 + w^3\underline{e}_3$ cancel in the limit $\underline{x}_k(o) \to \underline{x}^P$. We conclude that

$$\lim_{\underline{x}_k(o)\to\underline{x}^P} \langle \underline{v}_k(o).\underline{v}_j(t)\rangle = \int_V d\underline{x} \int_{R^3} d\underline{v} \int_{R^3} d\underline{v}_k(o) h(\underline{v}_k(o)) v_k^3(o) v^3$$

$$\times\ f_j(\underline{x},\underline{v},t)\,|\,\underline{x}_k(o),\underline{v}_k(o),k). \qquad (4.18)$$

For the case where $\underline{x}^P$ is a corner point, $(\underline{e}_1,\underline{e}_2,\underline{e}_3)$ are set up along the edges. As $\underline{x}_k(o) \to \underline{x}^P$, the trajectory of particle $k$ before collision approaches

$$\underline{x}_k(t) = \underline{x}^P + (|v_k^1(o)|\underline{e}_1 + |v_k^2(o)|\underline{e}_2 + |v_k^3(o)|\underline{e}_3)t. \qquad (4.19)$$

So contributions from $\underline{v}_k(o) = +\underline{v}$ and $-\underline{v}$ cancel in this limit. Thus

$$\lim_{\underline{x}_k(o)\to\underline{x}^P} \langle \underline{v}_k(o)\ .\ \underline{v}_j(t)\rangle = 0. \qquad (4.20)$$

For semi-infinite systems, we expect analogous results to hold. To prove this, we would only have to take the thermodynamic limit of a suitable sequence of finite volumes.

## 5.5 THE LONG TIME BEHAVIOUR FOR A GENERAL VELOCITY DISTRIBUTION

In the preceding sections, we have exclusively considered a velocity distribution function which is Maxwellian. It is of some interest to examine the dependence of the long-time behaviour of the v.c.f. on the choice of distribution function. A natural generalization is to choose $h(v) \geqslant 0$ to be an arbitrary member of the Schwarz class. Such functions are $C^{\infty}$ and satisfy

$$|P(x)h(x)| \to 0 \quad \text{as} \quad |x| \to \infty \quad \text{for any polynomial} \quad P(\ ). \qquad (5.1)$$

The Fourier transforms of such functions are also in the Schwarz class with respect to the transform variable (see Challifour[83]). For the analysis of the long time behaviour of v.c.f.'s, Poisson summation techniques are again appropriate. For both a ring system and a hard walled box and for times much greater than $t_{th}$, it is clear that the v.c.f.'s will decrease faster than any inverse power of time. An example of weaker constraints which may be imposed on $h(\ )$ would be to choose the $k^{th}$ derivative $h^{(k)}$ absolutely continuous and integrable for $k=1,2,\ldots,q \geqslant 2$. If $H(\lambda)$ is the Fourier transform, then

$$H(\lambda) = o\left(\frac{1}{|\lambda|^{q}}\right) \quad \text{as} \quad |\lambda| \to \infty$$

Poisson summation techniques are again applicable for the analysis of the v.c.f.'s and we conclude they have a long-time behaviour of the form

$$O\left(\left(\frac{t}{t_{th}}\right)^{2-q}\right). \qquad (5.2)$$

This first decrease behaviour will disappear if we take the t.l. so $t_{th} \to \infty$ leaving a residual slow decay. The results of section 5.4 are also valid for a general class of velocity distributions provided they are even i.e. $h(\underset{\sim}{v}) = h(-\underset{\sim}{v})$.

For more general finite systems, one would expect there may also be a cuttoff to the slow decay to equilibrium on a time scale $t_{th} = \frac{L}{v_{th}}$ where now L is a characteristic length for the size of the system.

## 5.6 A STOCHASTIC VERSION OF THE RING SYSTEM

The only difference between the system considered here and that section 5.2 is that for any collision we specify that the particles have a probability $P'$ of transmission (a non-interacting collision) and a probability $P = 1-P'$ of reflection (a hard "sphere" interaction involving interchange of velocities).

We define a class of functions $C^n(j,k|x_i(o),v_i(o))$ for each $j,k \in \{1,2,...,N\}$ and depending on the initial conditions $(x_i(o),v_i(o))$ on the N particles. $C^n(j,k|...)$ gives the probability that particle j is on trajectory k after trajectory k has been crossed n times by other trajectories (counting crossings from both the left and right as positive). We shall prove that

$$C^n(j,k|...) \to \frac{1}{N} \quad \text{as} \quad n \to \infty \tag{6.1}$$

except for possibly a finite number of $v_{k}^{*}(o)$ (where $k^*$ is chosen from $\{1,2,...,N\}$). We choose an initial velocity $v_k^*(o)$ so that trajectory $k^*$ intersects all other trajectories. It is sufficient to choose $v_k^*(o) \neq v_i(o)$ $i \neq k^*$. The $C^n(j,k|\ldots)$ have the initial conditions

$$C^0(j,k|\ldots) = \delta^N_{j,k} \tag{6.2}$$

and since some particle must always be on trajectory $k$, we have the conservation result

$$\sum_{j=1}^{N} C^n(j,k|\ldots) = 1 \tag{6.3}$$

It is convenient to define a class of functions $C^n(j,k|x_i(o),v_i(o))$ which give the probability that particle $j$ is on trajectory $k$ after a total of $n$ collisions between trajectories. It is clear that $C^n(j,k|\ldots)$ is equal to $C^m(j,k|\ldots)$ for some $m \leqslant n$. The $C^n(j,k|\ldots)$ have the initial conditions

$$C^0(j,k|\ldots) = \delta^N_{j,k} \tag{6.4}$$

They satisfy the following recurrence relations. If the $n^{th}$ collision involves trajectories $k'$ and $k''$ then

$$C^n(j,k|\ldots) = C^{n-1}(j,k|\ldots) \quad \text{for} \quad k \neq k',k''$$

$$C^n(j,k'|\ldots) = PC^{n-1}(j,k''|\ldots) + P'C^{n-1}(j,k'|\ldots) \tag{6.5}$$

$$C^n(j,k''|\ldots) = PC^{n-1}(j,k'|\ldots) + P'C^{n-1}(j,k''|\ldots)$$

Since particle j must always be on some trajectory, the $C^n(j,k|\ldots)$ satisfy the conservation result

$$\sum_{k=1}^{N} C^n(j,k|\ldots) = 1 \tag{6.6}$$

Let us consider the set

$$S^n(j|x_i(o),v_i(o)) = \{C^n(j,k|x_i(o),v_i(o)):k=1,2,\ldots,N\} \tag{6.7}$$

It is useful to examine the diameter of the set $S^n(j|\ldots)$ (in the sense of the usual metric on R) as a function of n. From (6.5) we see that $S^n(j|\ldots)$ is obtained from $S^{n-1}(j|\ldots)$ by replacing one pair of points $(c', c'')$ with the pair of convex linear combinations $(Pc' + P'c'', P'c' + Pc'')$ and leaving the rest invariant. Consequently

$$\text{diam } S^n(j|\ldots) \leqslant \text{diam } S^{n-1}(j|\ldots) \tag{6.8}$$

Our aim is to find an integer $M > 0$ and number $\alpha \varepsilon (0,1)$ such that

$$\text{diam } S^{n+M}(j|\ldots) < \alpha \text{ diam } S^n(j|\ldots) \tag{6.9}$$

Now trajectory $k^*$ crosses any other trajectory k periodically in time with a period $\tau_k^* < \infty$ since $v_k(o) \neq v_k^*(o)$. Let $\tau^* = \max_{k \neq k^*} \tau_k^*$. Then in any time interval of length $\tau^*$, trajectory $k^*$ crosses every other trajectory. It is possible to find an upper bound

$N_\tau = N_\tau(x_i(o), v_i(o))$ for the total number of collisions between trajectories in any time interval of length $\tau$. Thus during any $N_{\tau*}$ collisions, trajectory $k*$ must have crossed with every other trajectory. We show that $N_{\tau*}$ is a suitable candidate for $M$ in (5.9).

In the determination of the diameter, it is useful to define the following quantities. Let

$$d_n^+ \; S^m(j|\ldots) = \max_{k=1}^{N} C^m(j,k|\ldots) - C^n(j,k*|\ldots)$$

$$\text{for} \quad m \geqslant n . \qquad (6.10)$$

Define $C_+^n(j,k*|\ldots) = C^n(j,k*|\ldots)$ and

$$C_+^n(j,k|\ldots) = \max_{k'=1}^{N} C^n(j,k'|\ldots) \quad \text{for} \quad k \neq k* \qquad (6.11)$$

and suppose that $C_+^m(j,k|\ldots)$ for $m > n$ are determined recursively by relations of the form (6.5). Then

$$C_+^m(j,k|\ldots) \geqslant C^m(j,k|\ldots) \quad k=1,2,\ldots,N \qquad (6.12)$$

If $S_+^m(j|\ldots) = \{C_+^m(j,k|\ldots): \; k=1,2,\ldots,N\}$ , $m \geqslant n$

then from (6.12)

$$d_n^+ \; S_+^m(j|\ldots) \geqslant d_n^+ \; S^m(j|\ldots), \quad m \geqslant n. \qquad (6.13)$$

From the choice of $N_{\tau*}$, it is clear that for each $k$ there exists $m_k : 1 \leqslant m_k \leqslant N_{\tau*}$ such that

$$C_{+}^{n+m}(j,k|\ldots) < \max_{k'=1}^{N} C_{+}^{n}(j,k'|\ldots) \qquad (6.14)$$

for $m_k \leqslant m \leqslant N_{\tau^*}$. Furthermore the following upper estimate on the $C_{+}^{n+N_{\tau^*}}(j,k|\ldots)$ holds:

$$\max_{k'=1}^{N} C_{+}^{n}(j,k'|\ldots) - \max_{k'=1}^{N} C^{n+N_{\tau^*}}(j,k'|\ldots)$$

$$\geqslant (P^{-})^{N_{\tau^*}} d_n^{+} S^{n}(j|\ldots) \qquad (6.15)$$

where $P^{-} = \min(P,P')$. Consequently

$$d_n^{+} S^{n+N_{\tau^*}}(j|\ldots) \leqslant (1-(P^{-})^{N_{\tau^*}}) d_n^{+} S^{n}(j|\ldots) \qquad (6.16)$$

Similarly we let

$$d_n^{-} S^{m}(j|\ldots) = -\min_{k=1}^{N} C^{m}(j,k|\ldots) + C^{m}(j,k^*|\ldots)$$

$$\text{for } m \geqslant n \qquad (6.17)$$

Define $C_{-}^{n}(j,k^*|\ldots) = C^{n}(j,k^*|\ldots)$ and

$$C_{-}^{n}(j,k|\ldots) = \min_{k'=1}^{N} C^{n}(j,k'|\ldots) \quad \text{for } k \neq k^* \qquad (6.18)$$

and suppose that $C_{+}^{m}(j,k|\ldots)$ for $m > n$ are determined recursively by relations of the form (6.5). Then if $S_{-}^{m}(j|\ldots) = \{C_{-}^{m}(j,k|\ldots) : k=1,2,\ldots,N\}$ $m \geqslant n$, it follows that

$$d_n^{-} S_{-}^{m}(j|\ldots) \geqslant d_n^{-} S^{m}(j|\ldots) \qquad (6.19)$$

and $d_n^- S_-^{n+N_{\tau^*}}(j|\ldots) \leq (1-(P^-)^{N_{\tau^*}})\; d_n^- S^n(j|\ldots)$ (6.20)

Combining (6.16) and (6.20),

$$\begin{aligned}\text{diam } S^{n+N_{\tau^*}}(j|\ldots) &= d_n^- S^{n+N_{\tau^*}}(j|\ldots) + d_n^+ S^{n+N_{\tau^*}}(j|\ldots) \\ &\leq d_n^- S_-^{n+N_{\tau^*}}(j|\ldots) + d_n^+ S_+^{n+N_{\tau^*}}(j|\ldots) \\ &\leq (1-(P^-)^{N_{\tau^*}})\; (d_n^- S^n(j|\ldots) + d_n^+ S^n(j|\ldots)) \\ &= (1-(P^-)^{N_{\tau^*}})\; \text{diam } S^n(j|\ldots) \qquad (6.21)\end{aligned}$$

which has the form (6.8) as required. So

$$\text{diam } S^n(j|\ldots) \to 0 \quad \text{as} \quad n \to \infty$$

monotonically. It also follows as a simple consequence of (6.6) that for $k=1,2,\ldots,N$

$$|C^n(j,k|\ldots) - \tfrac{1}{N}| \to 0 \quad \text{as } n \to \infty \qquad (6.22)$$

so $$C^n(j,k|\ldots) \to \frac{1}{N} \quad \text{as} \quad n \to \infty \qquad (6.23)$$

and thus $$C^n(j,k|\ldots) \to \frac{1}{N} \quad \text{as} \quad n \to \infty\,. \qquad (6.24)$$

The analysis of a special case will help elucidate some of the above concepts. We consider the rate of convergence of (5.22) in the regime where $|v_k^*(o)| >> |v_k(o)|$, $k \neq k^*$. This is achieved by determining the dependence of $N_{\tau^*}$ on $v_k^*(o)$ in this limit. As $|v_k^*(o)| \to +\infty$ $\tau_k^* \sim \frac{L}{|v_{k^*}(o)|}$ and for $|v_{k^*}(o)|$ sufficiently large, it is clear that there can not be more than one collision between any pair of trajectories chosen from $\{1,2,\ldots,\hat{k^*},\ldots,N\}$ in a time interval $\tau_k^*$. Furthermore trajectory $k^*$ no other trajectory more than twice. So for such $v_{k^*}(o)$,

$$N_{\tau^*} \leq 2(N-1) + \binom{N-1}{2} \qquad (6.25)$$

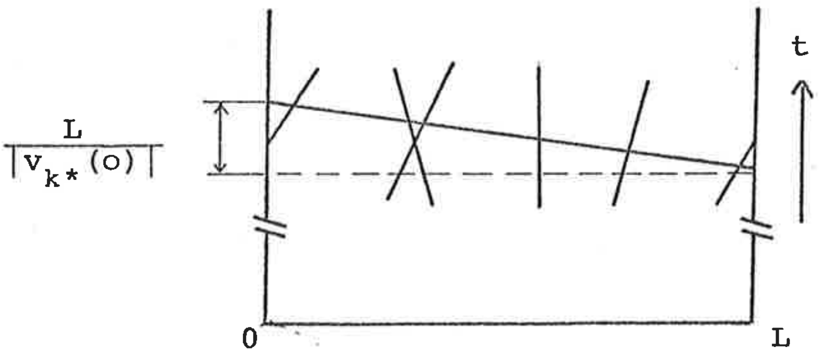



Fig. 5.4: The large $|v_{k^*}(o)|$ regime

The above analysis is now applied to the calculation of ensemble averages. By analogy with (2.1) $A_{jk}(t|x_i(o),v_i(o))$ is defined to be the probability that particle $j$ is on trajectory $k$ at a time $t$ (given a specific set of initial conditions). Then

$$A_{jk}(t|x_i(o),v_i(o))$$

$$= \sum_{n1=-\infty}^{+\infty} \sum_{n2=-\infty}^{+\infty} \cdots \sum_{nN=-\infty}^{+\infty} C^{|n1|+|n2|+\ldots+|nN|}(j,k|x_i(o),v_i(o))$$

$$\times\, r_{n1}(1,k,t)\; r_{n2}(2,k,t) \;\ldots\; r_{nN}(N,k,t)$$

$$= \frac{1}{N} + \sum_{n1=-\infty}^{+\infty} \sum_{n2=-\infty}^{+\infty} \cdots \sum_{nN=-\infty}^{+\infty} \left(C^{|n1|+|n2|+\ldots+|nN|}(j,k|x_i(o),v_i(o)) - \frac{1}{N}\right)$$

$$\times\ r_{n1}(1,k,t)\ r_{n2}(2,k,t)\ \ldots\ r_{nN}(N,k,t) \tag{6.26}$$

The ensemble average of section 5.2 is used, thus

$$F_{N,L} = \sum_{k=1}^{N} \langle f(v_1;x_k+v_kt,v_k)\ A_{jk}(t|x_i,v_i)\rangle_{N,L}$$

$$= \left(\frac{(N-1)!}{L^{N-1}} \int_o^L dx_N \int_o^{x_N} dx_{N-1} \ldots \int_o^{x_3} dx_2\right)\left(\prod_{i=1}^{N} \int_{-\infty}^{+\infty} dv_i h(v_i)\right)$$

$$\times \left(\frac{1}{N} \sum_{k=1}^{N} f(v_1;x_k + v_kt,\ v_k)\right.$$

$$+ \sum_{k=2}^{N} (f(v_1;x_k + v_kt,\ v_k) - f(v_1;v_1t,v_1))$$

$$\times \sum_{n1=-\infty}^{+\infty} \sum_{n2=-\infty}^{+\infty} \ldots \sum_{nN=-\infty}^{+\infty} (C^{|n1|+|n2|+\ldots+|nN|}(j,k|x_i,v_i) - \frac{1}{N})$$

$$\left.\times\ r_{n1}(1,k,t)\ r_{n2}(2,k,t)\ \ldots\ r_{nN}(N,k,t)\right) \tag{6.27}$$

where we have used the identity

$$\sum_{k=1}^{N} \cdot \left(\sum_{n1=-\infty}^{+\infty} \sum_{n2=-\infty}^{+\infty} \sum_{nN=-\infty}^{+\infty}\right)(C^{|n1|+|n2|+\ldots+|nN|}(j,k|x_i,v_i) - \frac{1}{N})$$

$$\times\ r_{n1}(1,k,t)\ r_{n2}(2,k,t)\ \ldots\ r_{nN}(N,k,t)$$

$$= \sum_{k=1}^{N} (C^{n_t}(j,k|x_i,v_i) - \frac{1}{N}) = 0 \tag{6.28}$$

from (6.6) where $n_t$ is the total number of collisions between trajectories up to a time $t$. In particular for the v.c.f.'s (6.27) becomes

$$F_{N,L} = \langle v_1(o)v_j(t)\rangle_{N,L}$$

$$= \frac{1}{N}\langle v_1(o)^2\rangle +$$

$$\left(\frac{(N-1)!}{L^{N-1}}\int_o^L dx_N \int_o^{x_N} dx_{N-1}\cdots\int_o^{x_3} dx_2\right)\left(\prod_{i=1}^{N}\int_{-\infty}^{+\infty} dv_i h(v_i)\right)$$

$$\times \left(v_1 \sum_{k=2}^{N}(v_k - v_1)\sum_{n1=-\infty}^{+\infty}\sum_{n2=-\infty}^{+\infty}\cdots\sum_{nN=-\infty}^{+\infty}\left(C^{|n1|+|n2|+\ldots+|nN|}(j,k|x_i,v_i) - \frac{1}{N}\right)\right.$$

$$\left. \times\, r_{n1}(1,k,t)\; r_{n2}(2,k,t)\;\ldots\; r_{nN}(N,k,t)\right) \qquad (6.29)$$

A crude asymptotic analysis for (5.29) in the limit as $t \to \infty$ is given below. In (6.29) the factor $(C^{|n1|+|n2|+\ldots+|nN|}(j,k|x_i,v_i) - \frac{1}{N})$ provides a cuttoff for those $(v_1,v_2,\ldots,v_N)$ outside the set

$$\{(v_1,v_2,\ldots,v_N):\ \text{for each } i, \text{ there exists } j \text{ such that } |v_i - v_j| = 0(\tfrac{L}{t})\} \qquad (6.30)$$

For outside this region, we can find $i=k^*$ such that $|v_{k^*} - v_j| \gg \frac{L}{t}$. Consequently for large $t$, $nk^*$ in $(C^{|n1|+|n2|+\ldots+|nN|}(j,k|x_i,v_i) - \frac{1}{N})$ for $k \neq k^*$ will be large compared with $N_{\tau^*}$, so this expression will be small. Also all the $ni$ in $(C^{|n1|+|n2|+\ldots+|nN|}(j,k^*|x_i,v_i) - \frac{1}{N})$ will be large compared with $N_{\tau^*}$, so this expression will also be small. The set (6.30) will have Gaussian measure

$0((\frac{L}{t})^{\frac{N}{2}})$ as $t \to \infty$ for $N$ even and $0((\frac{L}{t})^{\frac{N+1}{2}})$ as $t \to \infty$ for $N$ odd. So the decay of (6.29) to the equilibrium value $\frac{1}{N} \langle v_1(o)^2 \rangle$ will be of this form. For $N=2,3$, the factor $(v_k - v_1)$ in (5.29) produces an extra factor $0(\frac{L}{t})$ as $t \to \infty$ in the rate of decay.

# CHAPTER 6

# THE SOLUTION OF AN ELIMINATION PROBLEM IN KINETIC THEORY

## 6.1 INTRODUCTION

For an infinite classical system of particles with an arbitrary inter-particle potential, we examine the following special class of initial value problems (i.v.p.). The initial conditions are such that a particle, labelled "1" (say), has a specified initial distribution $f^{(1)}(\underline{z}_1;0)$ and the rest of the particles, labelled with an index $j$, are in equilibrium. The initial position and velocity of particle "1" could for example be fixed by choosing $f^{(1)}(\underline{z}_1;0)$ $= \delta(\underline{x}_1-\underline{x}')\delta(\underline{v}_1-\underline{v}')$.

The reduced distribution functions (r.d.f.) are defined through the grand canonical ensemble average $< - >_t^V$ for the corresponding finite systems of volume $V$ at time $t$ and then by taking the $V \to \infty$ limit. The average $< - >_t^V$ acts on functions of the variables $\underline{z}^j = (\underline{x}^j,\underline{v}^j)$ (denoting the position and velocity of the particle labelled "j") by integration over these variables with respect to suitable total distribution function measures. The n-particle r.d.f. is defined as

$$f^{(n)}(\underline{z}_1;\underline{z}_2;\ldots;\underline{z}_n;t)$$

$$= <\delta(\underline{z}_1-\underline{z}^1) \sum_{\substack{j\alpha\neq j\beta \\ j\alpha\neq 1}} \ {}_{\alpha\neq\beta} \ \delta(\underline{z}_2-\underline{z}^{j2}) \ \ldots \ \delta(\underline{z}_n-\underline{z}^{jn})>_t^V \qquad (1.1)$$

which gives the probability measure that the particle labelled "1" is at $\underline{z}_1$ and that some other particles are at $\underline{z}_2,\ldots,\underline{z}_n$. (1.1) is convergent for all time. From (1.1) and the specification above, the initial conditions on the $f^{(n)}$ are of the form: $f^{(1)}(\underline{z}_1;0)$ specified as above

$$f^{(n)}(\underline{z}_1;\underline{z}_2;\ldots;\underline{z}_n;0) = \rho_n(\underline{x}_1;\underline{x}_2;\ldots;\underline{x}_n)h_0(\underline{v}_2)\ldots h_0(\underline{v}_n)f^{(1)}(\underline{z}_1;0) \tag{1.2}$$

where $h_0(\ )$ is the Maxwellian distribution and $\rho_n(\ )$ is the n-particle equilibrium r.d.f. defined by

$$\rho_n(\underline{x}_1;\underline{x}_2;\ldots;\underline{x}_n)$$

$$= V\langle\delta(\underline{x}_1-\underline{x}^1)\sum_{\substack{j\alpha\neq j\beta\ \ \alpha\neq\beta \\ j\alpha\neq 1}}\delta(\underline{x}_2-\underline{x}^{j2})\ \ldots\ \delta(\underline{x}_n-\underline{x}^{jn})\rangle^V_{\text{equilibrium}} \tag{1.3}$$

Anstis[43,44] has shown that manipulation of (1.1) leads to the equations

$$f^{(1)}(1;t) = (1 + \sum_{m=1}^{+\infty} T^1_m(1;t))(S^1(1;t)f^{(1)}(1;0)) \tag{1.4}$$

$$f^{(n)}(1,2,\ldots,n;t) = (\sum_{m=0}^{+\infty} T^n_m(1,2,\ldots,n;t)(S^1(1;t)f^{(1)}(1;0)) \tag{1.5}$$

where

$$T^n_m(1,2,\ldots,n;t). =$$

$$\frac{1}{m!}\int d\underline{z}_1'\int d\underline{z}_2'\ldots\int d\underline{z}_m'\sum_{k=0}^{m}(-1)^{m-k}\binom{m}{k}S^{n+k}(1,2,\ldots,n,1',\ldots,k';t)$$

$$\rho_{n+m}(1,2,\ldots,n,1',\ldots,m')S^1(1;t)^{-1}$$

$$\times\ h_0(\underline{v}_2)\ \ldots\ h_0(\underline{v}_n)h_0(\underline{v}_1')\ \ldots\ h_0(\underline{v}_m')\ . \tag{1.6}$$

and we have written $i$ for $\underline{z}_i$ and $i'$ for $\underline{z}_i'$.

$S^q(1,2,...,q;t)$ is the q-particle streaming operator so $S^q(1,2,...,q;t)\ f(1,2,...,q) = f(1',2',...,q')$ where $\underline{z}_1', \underline{z}_2', ..., \underline{z}_q'$ are the coordinates of particles which at a time $t$ later under q-body dynamics are at $\underline{z}_1, \underline{z}_2, ..., \underline{z}_q$ (respectively). For finite $V$, (1.4) and (1.5) will be convergent for all time.

Our aim is to eliminate the expression $S^1(1;t)f^{(1)}(1;0)$ from (1.4) and (1.5) thus obtaining an expression for $f^{(n)}(1,2,...,n;t)$ in terms of $f^{(1)}(1;t)$ (termed as "upgrading" by Cohen[11]). The result for $n = 2$ may then be substituted into the first equation of the appropriate B.B.G.K.Y. hierarchy to obtain a closed equation for $f^{(1)}(1;t)$. Analogous non-linear problems have been solved using graph theoretic techniques for both the equilibrium case (see Uhlenbeck and Ford[84]) and the non-equilibrium case (Cohen[9]).

For the case of the one-dimensional hard "sphere" gas where $\rho_m(\ ) = \rho^{m-1}$ with $\rho$ equal to the mean density, (1.4) and (1.5) are shown to be convergent in the $V \to \infty$ limit for all time. The elimination problem is solved by rewriting (1.4) and (1.5) in terms of the corresponding cluster functions and operators and using graph theoretic techniques similar to those implemented by Cohen[9]. In the general case where $\rho_m(\ )$ does not factorize, more direct combinatorial methods are used to solve the elimination problem. Convergence of the series (1.4) and (1.5) may be assured at this stage by retaining finite $V$ and then letting $V \to \infty$ after we have solved the elimination problem. The convergence behaviour of the solution is considered in the next chapter. Unlike the special case above where $\rho_m(\ ) = \rho^{m-1}$, no cluster function structure is apparent here.

## 6.2 CLUSTER FORMULATION FOR THE ONE-DIMENSIONAL HARD "SPHERE" GAS*

The r.d.f.'s $f^{(n)}(\ ;t)$ are first expressed in terms of cluster operators corresponding to the streaming operators. This is essentially a combinatorial problem with an application of Liouville's theorem. Then these expressions are rewritten in terms of cluster functions corresponding to the $f^{(n)}(\ ;t)$ thus obtaining far neater expressions suitable for the application of graph theoretic methods.

First we give an alternative characterization of $T^1_m(1;t)$ through the identity

$$\sum_{k=0}^{m} (-1)^{m-k}\binom{m}{k} \int d\underline{z}_2 \ldots \int d\underline{z}_{1+m}\, S^{1+k}(1,2,\ldots,1+k;t)\,n(1,2,\ldots,1+m)$$
$$= \int d\underline{z}_2 \ldots \int d\underline{z}_{1+m}\, U^{1+m}(1,2,\ldots,1+m;t)\,n(1,2,\ldots,1+m) \qquad (2.1)$$

where $n(1,2,\ldots,1+m)$ is symmetric in the last m-variables. $U^m(\ ;t)$ are the cluster operators corresponding to the streaming operators $S^n(\ ;t)$ and are thus defined as (see Cohen [9])

$$U^m(1,2,\ldots,m;t) = \sum_{(1,2,\ldots,m\,\|\,\mathcal{L}_1,\ldots,\mathcal{L}_k)} (-1)^{k-1}(k-1)!\prod_{i=1}^{k} S^{\ell_i}(\mathcal{L}_i,t) \qquad (2.2)$$

where the sum is over all partitions of the labels $1,2,\ldots,m$ into non-empty sets $\mathcal{L}_i$ of size $\ell_i$ for $k = 1,2,\ldots,m$. We do not distinguish between different orderings of $\mathcal{L}_1,\ldots,\mathcal{L}_k$. The validity of (2.1) is shown by first proving

THEOREM 6.1. The signed and weighted number of times that a term $S^{1+m'}(1,\ldots,t)$ appears in the expansion (2.2) for $U^m(1,\ldots,m;t)$, $m \geqslant m' + 1$, is equal to $N(m,m') = (-1)^{m-1-m'}\binom{m-1}{m'}$.

---

* The vector notation $\underline{z}_i = (\underline{x}_i,\underline{v}_i)$ is retained indicating that much of the argument applies to systems of arbitrary dimension.

PROOF (i) for $m' = m-1$, the result is immediate.

(ii) for $m' < m-1$, the result is proved by induction on $m$. The result is easily verified for $m = 2$. We suppose it is true for $m = 2,3,\ldots,n-1$ and verify that it holds for $m = n$. The following representation of $U^n(\ ;t)$ is useful (see for example Cohen and Dorfman[24]).

$$U^n(1,2,\ldots,n;t) = S^n(1,2,\ldots,n;t)$$
$$- \Big\{U^1(1;t)S^{n-1}(2,3,\ldots,n;t) + \ldots + \sum_{2\leqslant i1<\ldots<ir\leqslant n} U^{r+1}(1,i1,\ldots,ir;t)S^{n-r-1}(2,\ldots,\hat{i1},\ldots,\hat{ir},\ldots,n;t) + \ldots$$
$$\ldots + \sum_{i=2}^{n} U^{n-1}(1,2,\ldots,\hat{i},\ldots,n;t)S^1(i;t)\Big\} . \tag{2.3}$$

Contributions to $S^{1+m'}(1,\ldots;t)$ terms in the expansion for $U^n(1,2,\ldots,n;t)$ come from terms $U^k(1,\ldots;t)S^{n-k}(\ldots;t)$ in (2.3) with $k = m'+1,\ldots,n-1$. The number of such terms $N(n,m')$ from the induction hypothesis and (2.3) is given by

$$- \left\{N(m'+1,m')\binom{n-1}{m'}+N(m'+2,m')\binom{n-1}{m'+1}+\ldots+N(n-1,m')\binom{n-1}{n-2}\right\}$$
$$= (-1)^{n-1-m'}\binom{n-1}{m'} \quad \text{as required.}$$

We have used the identity $\sum_{j=0}^{k}(-1)^j\binom{k}{j} = (1-1)^k = 0$ . □

To prove the result stated at the beginning of the section, it is now only necessary to note the following simple consequence of Liouville's theorem and the symmetry of $n(\quad)$. If $\Pi_i$ $i = 1,\ldots,p$ is a partition of $(2,\ldots,m+1)$ with $|\Pi_i| = \tau_i$ then

$$\int d\underline{z}_2 \ldots \int d\underline{z}_{1+m} S^{1+\tau_1}(1,\Pi_1;t)\prod_{i=2}^{p} S^{\tau_i}(\Pi_i;t)n(1,2,\ldots,m+1)$$
$$= \int d\underline{z}_2 \ldots\int d\underline{z}_{1+m} S^{1+\tau_1}(1,2,\ldots,\tau_1+1;t)n(1,2,\ldots,m+1) . \tag{2.4}$$

As a special case of (2.1), we have

$$T_m^1(1;t). = \int dz_1' \ldots \int dz_m' \, U^{1+m}(1,1',\ldots,m';t)$$

$$\times \rho_{1+m}(1,1',\ldots,m')S^1(1,t)^{-1} \prod_{i=2}^{m} h_0(\underline{v}_i') \quad . \qquad (2.5)$$

We now consider the related problem of producing an alternative characterization for $T_m^n(\ )$, $n > 1$, noting that the structure of the coefficients appearing in $T_m^n(\ )$ is independent of 'n'. New sets of streaming and cluster operators are defined with arguments chosen from the n-tuple $(1,2,\ldots,n)$ and the individual phase points $n+1, n+2, \ldots$ . If $\mathcal{R}$ denotes a set of these arguments then the streaming operators are given by

$$S_n^{|\mathcal{R}|}(\mathcal{R};t) = S^{|\mathcal{R}|+n-1}(\mathcal{R};t) \text{ if } (1,2,\ldots,n) \in \mathcal{R}$$

and (2.6)

$$S_n^{|\mathcal{R}|}(\mathcal{R};t) = S^{|\mathcal{R}|}(\mathcal{R};t) \quad \text{otherwise.}$$

The cluster operators are defined recursively by

$$S_n^{|\mathcal{R}|}(\mathcal{R};t) = \sum_{(\mathcal{R}\|\mathcal{R}_1,\ldots,\mathcal{R}_k)} \prod_{i=1}^{k} \mathcal{U}_n^{|\mathcal{R}_i|}(\mathcal{R}_i;t) \qquad (2.7)$$

where the sum is over all partitions of elements of $\mathcal{R}$. By comparison with the analysis leading to (2.5), we have

$$T_m^n(1,2,\ldots,n;t).$$

$$= \int dz_1' \ldots \int dz_m' \, \mathcal{U}_n^{1+m}((1,2,\ldots,n),1',\ldots,m';t)$$

$$\times \rho_{n+m}(1,\ldots,n,1',\ldots,m')S^1(1,t)^{-1} \prod_{i=2}^{n} h_0(\underline{v}_i) \prod_{i=1}^{m} h_0(\underline{v}_i') \, . \qquad (2.8)$$

$\mathcal{U}_n^{1+m}(\ ;t)$ may be characterized as a sum over certain products of cluster functions. We have immediately that

$$\mathcal{U}_n^1((1,2,\ldots,n);t) = S_n^1((1,2,\ldots,n);t) = S^n(1,2,\ldots,n;t)$$
$$= \sum_{(1,2,\ldots,n\|\mathcal{L}_1,\ldots,\mathcal{L}_k)} \prod_{i=1}^{k} U^{\ell_i}(\mathcal{L}_i;t) \quad (2.9)$$

From (2.7) and (2.9), it is clear that $\mathcal{U}_n^{1+m}(\ ;t)$ is represented as a sum over a subset of all possible products of cluster functions $U^p(\ ;t)$ which appear in the cluster expansion of $S_n^{1+m}(\ ;t)$. If $\Pi_k$, $k = 1,\ldots,p$, is a partition of the set $(1,2,\ldots,n)$, then a simple inductive argument shows that $\mathcal{U}_n^{1+m}(\ ;t)$ is a sum of terms like

$$U^{|\Pi_1|+\cdots}(\Pi_1,\ldots;t)\,U^{|\Pi_2|+\cdots}(\Pi_2,\ldots;t)\ldots U^{|\Pi_p|+\cdots}(\Pi_p,\ldots;t) \quad (2.10)$$

where the labels $1',2',\ldots,m'$ are distributed between these terms in all possible ways.

From (2.8) and (2.10), for the case where $\rho_m(\ ) = \rho^{m-1}$, (1.5) may be rewritten in the form

$$f^{(n)}(1,2,\ldots,n;t)$$
$$= \sum_{m=0}^{+\infty} \sum_{(1,2,\ldots,n\|\Pi_1,\ldots,\Pi_k)(1',2',\ldots,m'\|\mathcal{L}_1,\ldots,\mathcal{L}_k)_0}$$
$$\times \frac{1}{m!}\int d\underline{z}_1' \ldots \int d\underline{z}_m' \prod_{i=1}^{k} U^{|\Pi_i|+\ell_i}(\Pi_i,\mathcal{L}_i;t)$$
$$\times \prod_{i=2}^{n} \rho\, h_0(\underline{v}_i) \prod_{k=1}^{m} \rho\, h_0(\underline{v}_k') \cdot f^{(1)}(1;0) \quad (2.11)$$

where the sum is over all partitions of $1,2,\ldots,n$ into $\Pi_1,\ldots,\Pi_k$ all ordered partitions of $1',2',\ldots,m'$ into

$\mathcal{L}_1,\ldots,\mathcal{L}_k$ for $k = 1,\ldots,n$. The $\Pi_i$ are non-empty but the $\mathcal{L}_i$ may be empty. The total number of labellings of the $\mathcal{L}_i$ for given $\ell_i$ is equal to

$$\frac{\left(\sum_{i=1}^{k} \ell_i\right)!}{\prod_{i=1}^{k} \ell_i!}$$

and each gives an equal contribution to (2.11). So making a specific choice of labelling, we have

$$f^{(n)}(1,2,\ldots,n;t) = \sum_{(1,2,\ldots,n\|\Pi_1,\ldots,\Pi_k)}$$

$$\times \prod_{i=1}^{k} \left[ \sum_{\ell_i=0}^{+\infty} \frac{1}{\ell_i!} \int d\underline{z}_1' \ldots \int d\underline{z}_{\ell_i}' \; U^{|\Pi_i|+\ell_i}(\Pi_i,1',2',\ldots,\ell_i';t)\right.$$

$$\left. \times \prod_{k=1}^{\ell_i} \rho\, h_0(\underline{v}_k') \right] \prod_{i=2}^{n} \rho\, h_0(\underline{v}_i)\; f^{(1)}(1;0) \; . \qquad (2.12)$$

For a hard "sphere" system using conservation of kinetic energy, we have $U^{|\mathcal{L}|}(\mathcal{L};t) \prod_{i\in\mathcal{L}} h_0(\underline{v}_i) = 0$. So (2.12) may be simplified to

$$f^{(n)}(1,2,\ldots,n;t)$$

$$= \sum_{\Pi\subseteq\{2,\ldots,n\}} \left[ \sum_{j=0}^{+\infty} \frac{1}{j!} \int d\underline{z}_1' \ldots \int d\underline{z}_j' \; U^{|\Pi|+j+1}(1,\Pi,1',\ldots,j';t)\right.$$

$$\left. \times \prod_{k=1}^{j} \rho\, h_0(\underline{v}_k') \right] \prod_{i=2}^{n} \rho\, h_0(\underline{v}_i)\; f^{(1)}(1;0) \qquad (2.13)$$

The cluster functions corresponding to the $f^{(n)}$ are introduced in the following theorem which also provides the required expression for these cluster functions in terms of the cluster operators.

THEOREM 6.2. Define the functions $g^{(n)}(\ ;t)$ by

$$g^{(n)}(1,2,\ldots,n;t) = \sum_{\Pi \subseteq \{2,3,\ldots,n\}} (-1)^{n-1-|\Pi|}$$

$$\times\left(\prod_{i\in\{2,3,\ldots,n\}\setminus\Pi} \rho\, h_0(\underline{v}_i)\right) f^{|\Pi|+1}(1,\Pi;t). \qquad (2.14)$$

Then

$$g^{(n)}(1,2,\ldots,n;t)$$

$$= \sum_{\ell=0}^{+\infty} \frac{1}{\ell!} \int d\underline{z}_1' \ldots \int d\underline{z}_\ell' \; U^{\ell+n}(1,2,\ldots,n,1',\ldots,\ell';t)$$

$$\times \prod_{i=2}^{n} \rho\, h_0(\underline{v}_i) \prod_{k=1}^{\ell} \rho\, h_0(\underline{v}_k') \; f^{(1)}(1;0) \; . \qquad (2.15)$$

PROOF: For convenience of proof we take (2.15) as the definition of $g^{(n)}$ and prove (2.14). The result is easily verified for $n = 2$ and the general result is proved by induction. We suppose that (2.14) is true for $n = 2,\ldots,m-1$ and prove it valid for $n = m$. From (2.13), $g^{(m)}(\ ;t)$ may be written in the form

$$g^{(m)}(1,2,\ldots,m;t) = f^{(m)}(1,2,\ldots,m;t)$$

$$- \sum_{\Pi\subseteq\{2,\ldots,m\}(\neq\phi)} \sum_{j=0}^{+\infty} \frac{1}{j!} \int d\underline{z}_1' \ldots \int d\underline{z}_j' \; U^{|\Pi|+1}(1,\Pi,1',\ldots,j';t)$$

$$\times \prod_{k=1}^{j} \rho\, h_0(\underline{v}_k') \prod_{i=2}^{m} \rho\, h_0(\underline{v}_i) \; f^{(1)}(1;0) \; . \qquad (2.16)$$

Since $g^{(m)}(\ ;t)$ is symmetric in $(2,3,\ldots,m)$, it will suffice to determine from (2.16) the number of terms producing a factor $f^{(k+1)}(1,\ldots;t)$ and to show that this is equal to $M(k,m) = (-1)^{m-1-k}\binom{m-1}{k}$. From (2.16) this is equal to (by induction)

$$- \{M(k,m-1)\binom{m-1}{m-2} + M(k,m-2)\binom{m-1}{m-3} + \ldots + M(k,k+1)\binom{m-1}{k}\}$$

$$= (-1)^{m-1-k}\binom{m-1}{k} \quad \text{as required (c.f. THEOREM 6.1)} \quad \square \; .$$

So to solve the elimination problem for this special system, we may alternatively determine $g^{(n)}(\;;t)$ in terms of $g^{(1)}(\;;t)$. It is possible to show that the expressions for $f^{(n)}(\;;t)$ and $g^{(n)}(\;;t)$ are convergent in the $V \to \infty$ limit. For example, we show that the integrand of the $\ell^{th}$ term in (2.15) is zero for those $n+\ell$-particle configurations where there is a group of particles not containing $1,2,\ldots,n$ which interact only amongst themselves in the time interval $(0,t)$ i.e. disconnected collision events. This observation has been made previously by Cohen [11]. Let $A_i$ be a partition of the group of labels containing $1,2,\ldots,n$ with $1 \in A_{i1}$ and let $B_i$ be a partition of the other disconnected group. We use a representation of $U^{\ell+n}(\;;t)$ where all possible orderings of streaming operators occur, except that "1" must appear in the far left. Then all terms are of the form

$$(-1)^{p-1}S(A_{i1};t)S(A_{i2};t) \;\ldots\; S(A_{i\alpha};t)S(B_{i1};t) \;\ldots$$

or

$$(-1)^{p-2}S(A_{i1};t)S(A_{i2};t) \;\ldots\; S(A_{i\alpha},B_{i1};t) \;\ldots \quad .$$

These terms give equal and opposite contributions. Because of the Maxwellian factors the velocities are effectively restricted to a magnitude $O(v_{th})$ and so the spatial coordinates $\underline{x}_i$, $i > n$, are effectively restricted to within a distance $O(v_{th}t)$ of the set $\{\underline{x}_1,\underline{x}_2,\ldots,\underline{x}_n\}$. Noting also the ordering of spatial variables for the one-dimensional system, the series in (2.15) may be easily majorized in the $V \to \infty$ limit. A similar analysis is possible for $f^{(n)}( \;;t)$.

## 6.3 SOLUTION OF THE ELIMINATION PROBLEM FOR THE ONE-DIMENSIONAL HARD "SPHERE" GAS

From the relations (2.15) for $g^{(1)}(1,t)$ and $g^{(n)}(1,2,\ldots,n;t)$ in terms of $f^{1}(1;0)$, we obtain an expression for $g^{(n)}(1,2,\ldots,n;t)$ in terms of $g^{(1)}(1;t)$. This is achieved by constructing non-equilibrium Husimi-operator expansions for the cluster operators $U^{(m)}(1,2,\ldots,m;t)$ (c.f. Cohen [9]) appearing in (2.15). These operators are given a graph theoretic interpretation from which the solution to the elimination problem becomes obvious. The appropriate graph theoretic concepts are outlined by Uhlenbeck and Ford [84].

First we set up a correspondence between labelled Husimi trees and a set of non-commuting Husimi operators. The way the correspondence is set up is determined in part by the elimination problem to be solved. First consider the case where the Husimi tree consists of a single star, say an n-gon labelled (1,2,...,n). This graph then corresponds to an operator $V^{n}(1,2,\ldots,n;t)$. In general, to each star in the Husimi tree, there corresponds such an operator. Since these operators do not in general commute, an ordering convention is needed in dealing with a Husimi tree of more than one star. The most general Husimi tree may be decomposed as a number of sub-trees hung from the point labelled "1" (so that for each such subgraph "1" is not an articulation point). The operators associated with each such subgraph are grouped together. These groups of operators are ordered according to the minimum label (other than "1") associated with each subgraph (from left to right as the minimum label increases).

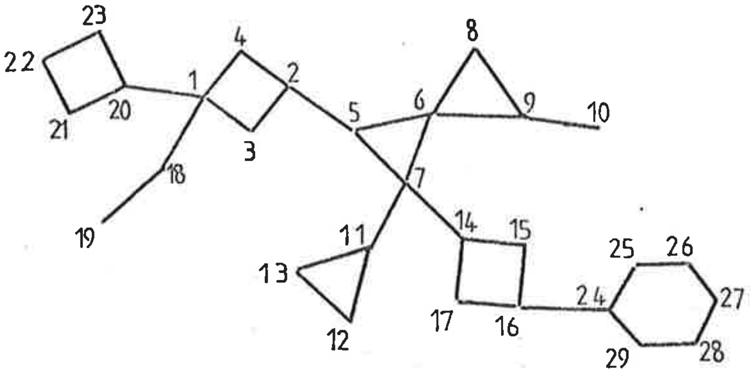
Now consider the ordering within each of the above mentioned subgraphs. The operator corresponding to the star including "1" appears to the left of all others. If there is only one star attached to this then the corresponding operator appears next to the right and so on out along the chain of stars away from the star containing "1". If when moving out along the chain a star is reached with more than two others attached, the procedure below must be implemented. We again group together the operators associated with each different subgraph attached to the end of this chain. The order of appearance (from left to right) is again determined by the minimum (non-equal) labels. The order within each subgraph is determined by the above rules except that the role of the point labelled "1" is now played by the point of attachment to the above chain.

Finally we prescribe a rule to determine the order of arguments within each operator $V^{n}(\ ;t)$. For a labelled star containing "1", we write $V^{\cdots}(1,\ldots;t)$. These operators are defined to be symmetric in all but the first argument. For the other operators the argument appearing first is that associated with the closest articulation point to "1".

The $V^{n}(\ ;t)$ operators are determined in terms of the cluster operators by requiring that the following relations hold:

$U^{n}(1,2,\ldots,n;t)U^{1}(1;t)^{-1}$

= sum over all distinct labelled Husimi trees of n-points with labels chosen from $(1,2,\ldots,n)$ (3.1) e.g.




corresponds to:

$$[(V^4_{(1,2,3,4;t)} V^2_{(2,5;t)} V^3_{(5,6,7;t)}) \ (V^3_{(6,8,9;t)} V^2_{(9,10;t)})$$
$$\times \ (V^2_{(7,11;t)} V^3_{(11,12,13;t)}) \ (V^2_{(7,14;t)} V^4_{(14,15,16,17;t)} V^2_{(16,24;t)}$$
$$\times \ V^6_{(24,25,26,27,28,29;t)})][V^2_{(1,18;t)} V^2_{(18,19;t)}]$$
$$\times \ [V^2_{(1,20;t)} V^4_{(20,21,22,23;t)}]$$

(2.15) may now be written as

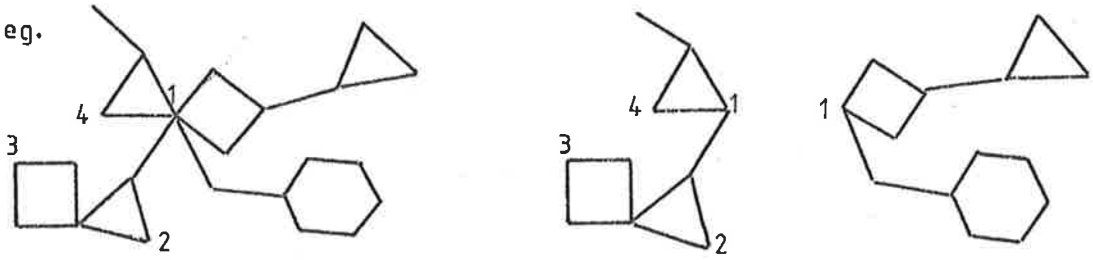
$$g^{(n)}(1,2,\ldots,n;t)$$
$$= \sum_{\ell=0}^{+\infty} \frac{1}{\ell!} \int d\underline{z}_{n+1} \ldots \int d\underline{z}_{n+\ell} \sum_{\mathrm{label}(n+1,\ldots,n+\ell)} \sum_{\mathrm{graphs}}$$
$$\times \ T^{n+\ell}_{\mathrm{root}(1,2,\ldots,n)} \left( \prod_{i=2}^{n+\ell} \rho \ h_0(\underline{v}_i)\right)(U^1(1;t) f^{(1)}(1;0)) \tag{3.2}$$

where $\sum_{\mathrm{graphs}}$ is the sum over all Husimi trees $T^{n+\ell}_{\mathrm{root}(1,2,\ldots,n)}$ of $n+\ell$ points with roots $1,2,\ldots,n$ and $\sum_{\mathrm{label}(\mathcal{L})}$ is the sum over all distinct labellings by $\mathcal{L}$ of the non-root points. $T^{n+\ell}_{\mathrm{root}(1,2,\ldots,n)}$ may be decomposed into subtrees hung from "1" for each of which "1" will not be an articulation point. Denote by $T^{1+\ell_2}_{\mathrm{root}(1)}$ the collection of these subtrees (of $1 + \ell_2$ points) which do not contain any of the points labelled $2,3,\ldots,n$. Then we have the unique decomposition

$$T^{n+\ell}_{\mathrm{root}(1,2,\ldots,n)} = T^{n+\ell_1,\mathrm{irred.}}_{\mathrm{root}(1,2,\ldots,n)} \cdot T^{1+\ell_2}_{\mathrm{root}(1)} \tag{3.3}$$

where $\mathcal{T}^{n+\ell_1,\text{irred.}}_{\text{root}(1,2,\ldots,n)}$ consists of the remainder of the subtrees making up $\mathcal{T}^{n+\ell}_{\text{root}(1,2,\ldots,n)}$ and $\ell_1 + \ell_2 = \ell$ .

eg.




$\mathcal{T}^{23}_{\text{root}(1,2,3,4)}$ $\mathcal{T}^{10,\text{irred.}}_{\text{root}(1,2,3,4)}$ $\mathcal{T}^{14}_{\text{root}(1)}$

Using the decomposition (3.3), (3.2) becomes

$$g^{(1)}(1;t)$$

$$= \sum_{\ell=0}^{+\infty} \frac{1}{\ell!} \int d\underline{z}_2 \ldots \int d\underline{z}_{1+\ell} \sum_{\text{label}(2,3,\ldots,\ell+1)} \sum_{\text{graphs}} \mathcal{T}^{1+\ell}_{\text{root}(1)}$$

$$\times \left( \prod_{i=2}^{1+\ell} \rho\, h_0(\underline{v}_i) \right) (U^1(1;t) f^{(1)}(1;0)) \tag{3.4}$$

and

$$g^{(n)}(1,2,\ldots,n;t)$$

$$= \sum_{\ell=0}^{+\infty} \frac{1}{\ell!} \sum_{(n+1,n+2,\ldots,n+\ell \| \mathcal{L}_1,\mathcal{L}_2)_0}$$

$$\times \prod_{i\in\mathcal{L}_1} \int d\underline{z}_i \sum_{\text{label}(\mathcal{L}_1)} \sum_{\text{graphs}} \mathcal{T}^{n+\ell_1,\text{irred.}}_{\text{root}(1,2,\ldots,n)} \left( \prod_{i\in\mathcal{L}_1} \rho\, h_0(\underline{v}_i) \right)$$

$$\times \prod_{i\in\mathcal{L}_2} \int d\underline{z}_i \sum_{\text{label}(\mathcal{L}_2)} \sum_{\text{graphs}} \mathcal{T}^{1+\ell_2}_{\text{root}(1)} \left( \prod_{i\in\mathcal{L}_2} \rho\, h_0(\underline{v}_i) \right)$$

$$\times \left( \prod_{i=2}^{n} \rho\, h_0(\underline{v}_i) \right) (U^1(1;t) f^{(1)}(1;0)) \tag{3.5}$$

where in (3.5) we have used that because of the way that the graph operator correspondence is set up, all operators associated with $T^{1+\ell_2}_{\mathrm{root}(1)}$ appear to the right of those associated with $T^{n+\ell_1,\mathrm{irred.}}_{\mathrm{root}(1,2,\ldots,n)}$ . It is clear that

$$\prod_{i\in\mathcal{L}_2} \int d\underline{z}_i \sum_{\mathrm{label}(\mathcal{L}_2)} \sum_{\mathrm{graphs}} T^{1+\ell_2}_{\mathrm{root}(1)} (\prod_{i\in\mathcal{L}_2} \rho\, h_0(\underline{v}_i))$$

$$\times\ (U^1(1;t)f^{(1)}(1;0)) \tag{3.6}$$

is independent of the choice of $\mathcal{L}_2$. Furthermore

$$\prod_{i\in\mathcal{L}_1} \int d\underline{z}_i \sum_{\mathrm{label}(\mathcal{L}_1)} \sum_{\mathrm{graphs}} T^{n+\ell_1,\mathrm{irred.}}_{\mathrm{root}(1,2,\ldots,n)} (\prod_{i\in\mathcal{L}_1} \rho\, h_0(\underline{v}_i))$$

$$\times\ (\prod_{i=2}^{n} \rho\, h_0(\underline{v}_i))h(1;t) \tag{3.7}$$

is independent of the choice of $\mathcal{L}_1$ for arbitrary $h(1;t)$. Using these results, (3.5) may be rewritten choosing a specific labelling from the $\frac{\ell!}{\ell_1!\ell_2!}$ possible ones as

$$g^{(n)}(1,2,\ldots,n;t)$$

$$= \sum_{\ell_1=0}^{+\infty} \frac{1}{\ell_1!} \int d\underline{z}_{n+1} \cdots \int d\underline{z}_{n+\ell_1} \sum_{\mathrm{label}(n+1,\ldots,n+\ell_1)} \sum_{\mathrm{graphs}}$$

$$\times\ T^{n+\ell_1,\mathrm{irred.}}_{\mathrm{root}(1,2,\ldots,n)} \prod_{i=2}^{n+\ell_1} \rho\, h_0(\underline{v}_i))$$

$$\times \sum_{\ell_2=0}^{+\infty} \frac{1}{\ell_2!} \int d\underline{z}'_1 \cdots \int d\underline{z}'_{\ell_2} \sum_{\mathrm{label}(1',2',\ldots,\ell'_2)} \sum_{\mathrm{graphs}} T^{1+\ell_2}_{\mathrm{root}(1)}$$

$$\times\ (\prod_{i=1}^{\ell_2} \rho\, h_0(\underline{v}'_i))(U^1(1;t)f^{(1)}(1;0)) \quad . \tag{3.8}$$

So from (3.4) and (3.6)

$$g^{(n)}(1,2,\ldots n;t)$$

$$= \sum_{\ell=0}^{+\infty} \frac{1}{\ell!} \int d\underline{z}_{n+1} \cdots \int d\underline{z}_{n+\ell}\, T^{n+\ell}(1,2,\ldots,n|n+1,\ldots,n+\ell;t)$$

$$\times \left(\prod_{i=2}^{n+\ell} \rho\, h_0(\underline{v}_i)\right) g^{(1)}(1;t) \tag{3.9}$$

where for a set of $\ell$ labels $\mathcal{L}$

$$T^{n+\ell}(1,2,\ldots,n|\mathcal{L};t) = \sum_{\text{label}(\mathcal{L})} \sum_{\text{graphs}} T^{n+\ell}_{\text{root}}(1,2,\ldots,n) \tag{3.10}$$

This is the required solution to the elimination problem.

## 6.4 CLUSTER AND STREAMING OPERATOR EXPANSIONS OF THE SOLUTION

The expansion (3.9) for $g^{(n)}(\ ;t)$ in terms of $g^{(1)}(\ ;t)$ has the disadvantage that the terms involve combinations of the $V^n(\ ;t)$ operators. It is more convenient to have an expansion in terms of cluster operators. This could be achieved by solving for $V^n(\ ;t)$ in terms of $U^m(\ ;t)$ recursively from (3.1). However a systematic inversion scheme is embodied in the following theorem.

<u>THEOREM 6.3.</u> If $T^{n+\ell}(1,2,\ldots,n|\mathcal{L};t)$ is defined as in (3.10) then

$$T^{n+\ell}(1,2,\ldots,n|\mathcal{L};t)$$

$$= \sum_{(n+1,n+2,\ldots,n+\ell\|\mathcal{L}_1|\mathcal{L}_2,\ldots,\mathcal{L}_k)_0} (-1)^{k-1} \tag{4.1}$$

$$\times\, U^{n+\ell_1}(1,2,\ldots,n,\mathcal{L}_1;t)\,U^1(1;t)^{-1}U^{1+\ell_2}(1,\mathcal{L}_2;t)$$

$$\times\, U^1(1;t)^{-1} \cdots U^{1+\ell_k}(1,\mathcal{L}_k;t)\,U^1(1;t)^{-1}$$

where the sum is over all ordered partitions of $n+1,\ldots,n+\ell$ into $\mathcal{L}_1,\ldots,\mathcal{L}_k$ where $\mathcal{L}_1$ may be empty and $\mathcal{L}_2,\ldots,\mathcal{L}_k$ are non-empty for $k = 1,2,\ldots,\ell+1$ .

PROOF The family of graphs associated with $T^{n+\ell}(1,2,\ldots,n|\mathcal{L};t)$ can be obtained by starting with all the graphs in the family associated with $U^{n+\ell}(1,2,\ldots,n,\mathcal{L};t)U^1(1;t)^{-1}$ and removing those containing a subtree hung from "1" which does not contain any of the points labelled $2,3,\ldots,n$. i.e.

$$T^{n+\ell'}(1,2,\ldots,n|n+1,\ldots,n+\ell';t)$$

$$= U^{n+\ell'}(1,2,\ldots,n+\ell';t)U^1(1;t)^{-1}$$

$$- \Big\{T^n(1,2,\ldots,n|t)U^{1+\ell'}(1,n+1,\ldots,n+\ell';t)U^1(1;t)^{-1} + \ldots$$

$$\ldots + \sum_{n+1\leq i1\leq\ldots\leq ir\leq n+\ell'} T^{n+r}(1,2,\ldots,n|i1,\ldots,ir;t)$$

$$\times\, U^{1+\ell'-r}(1,n+1,\ldots,\hat{i1},\ldots,\hat{ir},\ldots,n+\ell';t)U^1(1;t)^{-1} + \ldots$$

$$\ldots + \sum_{i=n+1}^{n+\ell'} T^{n+\ell'-1}(1,2,\ldots,n|n+1,\ldots,\hat{i},\ldots,n+\ell';t)$$

$$\times\, U^2(1,i;t)U^1(1;t)^{-1}\Big\} \quad . \qquad (4.2)$$

Note that (4.2) is ordered in the sense that the operators associated with the $T^{n+r}(\ \ )$ appear to the left of those associated with the $U^{1+\ell'-r}(\ \ )$. This is a consequence of our choice of graph-operator correspondence. (4.2) can be used recursively to obtain the required expansion (observing that $T^n(1,2,\ldots,n|t) = U^n(1,2,\ldots,n;t)U^1(1;t)^{-1}$). It can be verified directly that the theorem holds true for $\ell = 1$

(and 2,3 etc.). The proof of the general result shall be by induction. We suppose that it holds true for $\ell = 1,2,\ldots,\ell'-1$ and prove that it is true for $\ell = \ell'$.

Consider the number of terms in the expansion of $T^{n+\ell'}(1,2,\ldots,n|n+1,\ldots,n+\ell';t)$ which are of the form

$$U^{n+\ell_1}(1,2,\ldots,n,\ldots;t)U^1(1;t)^{-1}U^{1+\ell_2}(1,\ldots;t)U^1(1;t)^{-1}\ldots$$

$$\ldots U^{1+\ell_k}(1,\ldots;t)U^1(1;t)^{-1} \qquad (4.3)$$

for a given choice of $\ell_1,\ldots,\ell_k$. Contributions to (4.3) from (4.2) come from the terms

$$-T^{n+\ell'-\ell_k}(1,2,\ldots,n|i1,\ldots;t)U^{1+\ell_k}(1,n+1,\ldots,\hat{i1},\ldots,n+\ell';t)$$

$$\times U^1(1;t)^{-1} \qquad (4.4)$$

i.e. $\binom{\ell'}{\ell'-\ell_k}$ terms. By the induction hypothesis, the number of terms in $T^{n+\ell'-\ell_k}(1,2,\ldots,n|i1,\ldots;t)$ of the form

$$U^{n+\ell_1}(1,2,\ldots,n,\ldots;t)U^1(1;t)^{-1}U^{1+\ell_2}(1,\ldots;t)U^1(1;t)^{-1}\ldots$$

$$\ldots U^{1+\ell_{k-1}}(1,\ldots;t)U^1(1;t)^{-1}$$

is equal to

$$N_{k-1} = (-1)^{k-2}\frac{(\ell'-\ell_k)!}{\ell_1!\ell_2!\ldots\ell_{k-1}!}.$$

So the total number of contributions from (4.3) to (4.2) is equal to

$$N_k = (-1)\times\binom{\ell'}{\ell'-\ell_k}\times N_{k-1}$$

$$= (-1)^{k-1}\frac{\ell'!}{\ell_1!\ell_2!\ldots\ell_k!} \text{ as required.} \quad \square$$

As an application of this theorem, we may rewrite the solution (3.9) of the elimination problem as

$$g^{(n)}(1,2,\dots,n;t)$$

$$= \sum_{\ell=0}^{\infty} \frac{1}{\ell!} \int d\underline{z}_{n+1} \dots \int d\underline{z}_{n+\ell} \sum_{\overline{(n+1,n+2,\dots,n+\ell \| \mathcal{L}_1 | \mathcal{L}_2,\dots,\mathcal{L}_k)_0}} (-1)^{k-1}$$

$$\times\ U^{n+\ell_1}(1,2,\dots,n,\mathcal{L}_1;t)U^1(1;t)^{-1}U^{1+\ell_2}(1,\mathcal{L}_2;t)U^1(1;t)^{-1} \dots$$

$$\dots U^{1+\ell_k}(1,\mathcal{L}_k;t)U^1(1;t)^{-1} \left(\prod_{i=2}^{n+\ell} \rho\, h_0(\underline{v}_i)\right)g^{(1)}(1;t) \quad (4.5)$$

To obtain a streaming operator expansion of the solution of the elimination problem, we examine the structure of the $\ell^{th}$ term of (4.5) when the cluster operators are expanded in terms of streaming operators. The following simplified expansion is appropriate because of the nature of the functions acted on and using conservation of kinetic energy :

$$U^{1+\ell}(1,\mathcal{L};t)\left(\prod_{i\in\mathcal{L}} h_0(\underline{v}_i)h(1;t)\right) = \sum_{\mathcal{L}'\subseteq\mathcal{L}} (-1)^{\ell-\ell'} S^{1+\ell'}(1,\mathcal{L}';t)$$

$$\times \left(\prod_{i\in\mathcal{L}} h_o(\underline{v}_i)h(1;t)\right) . \quad (4.6)$$

This result is self evident using THEOREM 6.1 and symmetry arguments. The analysis is divided into several subcases

(I) let $\mathcal{L}^* \subseteq \{2,3,\dots,n\}$ with $|\mathcal{L}^*| = \ell^* > 0$; partition the labels $n+1,\dots,n+\ell$ into sets $\mathcal{L}_i$ $i = 1,2,\dots,k$. After substitition of (4.6) into the $\ell^{th}$ term of (4.5), we determine the number of times that the expression

$$S^{1+\ell^*+\ell_1}(1,\mathcal{L}^*,\mathcal{L}_1;t)S^1(1;t)^{-1}S^{1+\ell_2}(1,\mathcal{L}_2;t)S^1(1;t)^{-1} \dots$$

$$\dots S^{1+\ell_k}(1,\mathcal{L}_k;t)S^1(1;t)^{-1} \quad (4.7)$$

appears. The only contribution to (4.7) from (4.5) comes from the term

$$(-1)^{k-1}U^{n+\ell_1}(1,2,\ldots,n,\mathcal{L}_1;t)U^1(1;t)^{-1}U^{1+\ell_2}(1,\mathcal{L}_2;t)U^1(1;t)^{-1}\ldots$$

$$\ldots U^{1+\ell_k}(1,\mathcal{L}_k;t)U^1(1;t)^{-1} \quad . \tag{4.8}$$

The signed number of times that this term appears is given by

$$(-1)^{k-1} \times (-1)^{n-\ell^*-1} \quad .$$

(II) $\mathcal{L}_i$ $i = 1,\ldots,k$ as in (I). We determine the number of times that the expression

$$S^{1+\ell_1}(1,\mathcal{L}_1;t)S^1(1;t)^{-1}S^{1+\ell_2}(1,\mathcal{L}_2;t)S^1(1;t)^{-1}\ldots$$

$$\ldots S^{1+\ell_k}(1,\mathcal{L}_k;t)S^1(1;t)^{-1} \tag{4.9}$$

appears. Contributions to (4.9) come from the terms

$$(-1)^{k-1}U^{n+\ell_1}(1,2,\ldots,n,\mathcal{L}_1;t)U^1(1;t)^{-1}U^{1+\ell_2}(1,\mathcal{L}_2;t)U^1(1;t)^{-1}\ldots$$

$$\ldots U^{1+\ell_k}(1,\mathcal{L}_k;t)U^1(1;t)^{-1}$$

and

$$(-1)^{k}U^{n}(1,2,\ldots,n;t)U^1(1;t)^{-1}U^{1+\ell_1}(1,\mathcal{L}_1;t)U^1(1;t)^{-1}\ldots$$

$$\ldots U^{1+\ell_k}(1,\mathcal{L}_k;t)U^1(1;t)^{-1} \quad . \tag{4.10}$$

So the total number of times that (4.9) appears is given by

$$(-1)^{k-1} + (-1)^k = 0 \quad .$$

(III) let $\mathcal{L}^* \subseteq \{2,3,\ldots,n\}$ with $|\mathcal{L}^*| = \ell^* > 0$; partition '$\ell$-j' of the labels $n+1,n+2,\ldots,n+\ell$ into sets

$T_i, |T_i| = s_i$, $i = 1,2,\ldots,k$. We determine the number of times that the expression

$$S^{1+\ell^*+s_1}(1,\ell^*,T_1;t)S^1(1;t)^{-1}S^{1+s_2}(1,T_2;t)S^1(1;t)^{-1} \ldots$$

$$\ldots S^{1+s_k}(1,T_k;t)S^1(1;t)^{-1} \qquad (4.11)$$

The remaining 'j' labels are partitioned into sets $T_i', |T_i'| = s_i'$, $i = 1,2,\ldots,r$.

(a) $r \leqslant k$: in this case contributions to (4.11) associated with the partition $T_i'$ come from terms

$$(-1)^{k+(r-t)+1}U^{n+s_1+s_1'}(1,2,\ldots,n,T_1,T_1';t)U^1(1;t)^{-1}$$

$$\times U^{1+s_2+s_2'}(1,T_2,T_2';t)U^1(1;t)^{-1} \ldots$$

$$\ldots U^{1+s_t+s_t'}(1,T_t,T_t';t)U^1(1;t)^{-1}U^{1+s_{t+1}}(1,T_{t+1};t)U^1(1;t)^{-1}$$

$$\ldots U^{1+s_k}(1,T_k;t)U^1(1;t)^{-1}U^{1+s_{t+1}'}(1,T_{t+1}';t)U^1(1;t)^{-1} \ldots$$

$$\ldots U^{1+s_r'}(1,T_r';t)U^1(1;t)^{-1} \qquad (4.12)$$

& different positions of $T_1',\ldots,T_t'$ among the first "k" factors

& different positionings of the last "r-t" factors after the first factor

& different choices of "t" sets from $T_1',\ldots,T_r'$.

for $t = 0,1,\ldots,r$. The total number of such terms contributing to (4.12) is given by $k(k-1) \ldots (k-t+1) \cdot k(k+1) \ldots (k+(r-t)-1) \cdot \binom{r}{r-t}$ with a suitable interpretation for the case $t = 0$ and the case $t = k$ when

when $r = k$. We conclude that the total number of terms contributed to (4.11) by (4.12) is given, for $k \geqslant r$, by

$$M(s_i, s_i', n, \ell^*) = (-1)^{k-1} . (-1)^{n-\ell^*-1} . \prod_{i=1}^{r} (-1)^{s_i'} . k\left( \sum_{t'=0}^{r} T_{t'}^{r-1}(k) \right) \tag{4.13}$$

where

$$T_{t'}^{r-1}(k) = (-1)^{t'} \binom{r}{t'} (k+t'-1)(k+t'-2) \ldots (k+t'-r+1)$$

and from Appendix G, this expression is zero.

(b) $r > k$: in this case contributions to (4.11) associated with the partition $T_i'$ come from the terms described in (4.12), but here $t = 0,1,\ldots,k$. We conclude that the total number of terms contributed to (4.11) by (4.12) is given, for $r > k$, by

$$M(s_i, s_i', n, \ell^*) = (-1)^{r-1} \cdot (-1)^{n-\ell^*-1} \cdot \prod_{i=1}^{r} (-1)^{s_i'}$$
$$\times\; k \cdot (k+1) \ldots (r-1) \cdot \left( \sum_{t'=0}^{k} \hat{T}_{t'}^{r-1}(k) \right) \tag{4.14}$$

where

$$\hat{T}_{t'}^{r-1}(k) = (-1)^{t'} \binom{r}{r-k+t'} r \cdot (r+1) \ldots (r+t'-1) k(k-1) \ldots (t'+1)$$

with a suitable interpretation for cases $t' = 0$ and $t' = k$. From Appendix G, this expression is zero.

Using the results of (I), (II) and (III), it is clear that (4.5) may be rewritten as

$$f^{(n)}(1,2,\ldots,n;t)$$
$$= \sum_{\ell=0}^{\infty} \frac{1}{\ell!} \int d\underline{z}_{n+1} \ldots \int d\underline{z}_{n+\ell} \sum_{(n+1,n+2,\ldots,n+\ell \| \mathcal{L}_1 | \mathcal{L}_2,\ldots,\mathcal{L}_k)_0} (-1)^{k-1}$$
$$\times\; S^{n+\ell_1}(1,2,\ldots,n,\mathcal{L}_1;t) S^1(1;t)^{-1} S^{1+\ell_2}(1,\mathcal{L}_2;t) S^1(1;t)^{-1} \ldots$$
$$\ldots S^{1+\ell_k}(1,\mathcal{L}_k;t) S^1(1;t)^{-1} \left( \prod_{i=2}^{n+\ell} \rho\, h_0(\underline{v}_i) \right) f^{(1)}(1;t) \tag{4.15}$$

## 6.5 SOLUTION OF THE GENERAL ELIMINATION PROBLEM

Using (1.4) and (1.5), we obtain an expression for $f^{(n)}(1,2,\ldots,n;t)$ in terms of $f^{(1)}(1;t)$ by the following procedure. (1.4) is inverted to give

$$S^1(1;t)f^{(1)}(1;0) = (1 + \sum_{m=1}^{\infty} T_m^1(1;t))^{-1} f^{(1)}(1;t)$$

$$= (1 + \sum_{\ell=1}^{+\infty} \sum_{k=1}^{\ell} (-1)^k \sum_{\substack{m_i>0 \\ \sum_{i=1}^{k} m_i=\ell}} T_{m_1}^1(1;t)T_{m_2}^1(1;t)\ldots T_{m_k}^1(1;t)) \tag{5.1}$$

$$\times f^{(1)}(1;t)$$

for times $0 \leqslant t < t_c$ where the radius of convergence $t_c$ of the expansion in (5.1) is expected to be small because of the sensitivity of the operator $(1 + \sum_{m=1}^{\infty} T_m^1(1;t))^{-1}$ to small changes in $f^{(1)}(1;t)$. Qualitatively this is understood to be the case because very different initial states $f^{(1)}(1;0)$ approach the same equilibrium state. Upon substitution of (5.1) into (1.5), we obtain after some rearrangement

$$f^{(n)}(1,2,\ldots,n;t)$$

$$= (\sum_{\ell=0}^{+\infty} \sum_{k=1}^{\ell+1} (-1)^{k-1} \sum_{\substack{m_1 \geqslant 0 \;\; m_i>0,\; i>1 \\ \sum_{i=1}^{k} m_i=\ell}} T_{m_1}^n(1,2,\ldots,n;t)T_{m_2}^1(1;t)\ldots$$

$$\ldots T_{m_k}^1(1;t))f^{(1)}(1;t). \tag{5.2}$$

It is expected that the range of convergence with respect to time of (5.2) will be considerably greater than (5.1) because of the rearrangement of terms. So $t_c$ does not determine the range of convergence of the final solution and this is expected by comparison with the graph theoretic method where $t_c$ does not enter into the analysis.

Let us first examine the leading terms in (5.2) i.e. those of highest order in the streaming operators. The contribution from the term of $[\ell+(n-1)]^{th}$ order in density (the $\ell^{th}$ term in (5.2)) is then

$$\Big(\sum_{k=1}^{\ell+1} (-1)^{k-1} \sum_{\substack{m_1 \geq 0 \; m_i > 0,\; i>1 \\ \sum_{i=1}^{k} m_i = \ell}} \overset{*}{T}{}^{n}_{m_1}(1,2,\ldots,n;t)\overset{*}{T}{}^{1}_{m_2}(1;t) \ldots$$

$$\ldots \overset{*}{T}{}^{1}_{m_k}(1;t)\Big) f^{(1)}(1;t) \tag{5.3}$$

where

$$\overset{*}{T}{}^{p}_{m}(1,2,\ldots,p;t)\cdot =$$

$$\frac{1}{m!}\int d\underline{z}'_1 \ldots \int d\underline{z}'_m \; S^{p+m}(1,2,\ldots,p,1',\ldots,m';t)$$

$$\times \; \rho_{p+m}(1,2,\ldots,p,1',\ldots,m') S^1(1;t)^{-1}$$

$$\times \; h_0(\underline{v}_2) \ldots h_0(\underline{v}_p) h_0(\underline{v}'_1) \ldots h_0(\underline{v}'_m) \cdot \tag{5.4}$$

The total number of possible labellings of integration variables appearing in the streaming operators in (5.3) for a given choice of $m_1,\ldots,m_k$ with labels chosen from $(n+1,n+2,\ldots,n+\ell)$ is equal to $\frac{(m_1+m_2+\ldots+m_k)!}{m_1!m_2!\ldots m_k!}$ . Each of course will give an equal contribution to (5.3). Consequently an equivalent representation of (5.3) is

$$\frac{1}{\ell!}\int d\underline{z}_{n+1}\cdots\int d\underline{z}_{n+\ell}\sum_{(n+1,n+2,\ldots,n+\ell\|\mathcal{L}_1|\mathcal{L}_2,\ldots,\mathcal{L}_k)_0}(-1)^{k-1}$$

$$\times\, S^{n+\ell_1}(1,2,\ldots,n,\mathcal{L}_1;t)\rho_{n+\ell_1}(1,2,\ldots,n,\mathcal{L}_1)S^1(1;t)^{-1}$$

$$\times\, S^{1+\ell_2}(1,\mathcal{L}_2;t)\rho_{1+\ell_2}(1,\mathcal{L}_2)S^1(1;t)^{-1}$$

$$\times\,\ldots$$

$$\times\, S^{1+\ell_k}(1,\mathcal{L}_k;t)\rho_{1+\ell_k}(1,\mathcal{L}_k)S^1(1;t)^{-1}\prod_{j=2}^{n+\ell}h_0(\underline{v}_j)f^{(1)}(1;t) \quad (5.5)$$

where the sum has the same interpretation as in (4.1). Such a result is expected by comparison with the solution of the elimination problem for the one-dimensional hard "sphere" system in sections 6.2-4 we have shown that only leading terms with respect to the streaming operators contribute and the structure of the solution is similar to that of (5.5).

Next we consider all the remaining terms that are generated by (5.2) for a given $\ell$ . The streaming operator structure of these terms will be of the form

$$(-1)^{s-1}(-1)^{k_1-1}\ \ldots\ (-1)^{k_s-1}$$

$$\times\,\frac{(-1)^{\ell_1^2}}{(\ell_1^1+\ell_1^2)!}\binom{\ell_1^1+\ell_1^2}{\ell_1^1}S^{n+\ell_1^1}(1,2,\ldots,n,\mathcal{L}_1^1;t)$$

$$\times\,\rho_{n+\ell_1^1+\ell_1^2}(1,2,\ldots,n,\mathcal{L}_1^1,\mathcal{L}_1^2)\prod_{i=3}^{k_1}\frac{(-1)^{\ell_1^i}}{\ell_1^i!}\rho_{1+\ell_1^i}(1,\mathcal{L}_1^i)S^1(1;t)^{-1}$$

$$\times\,\frac{(-1)^{\ell_2^2}}{(\ell_2^1+\ell_2^2)!}\binom{\ell_2^1+\ell_2^2}{\ell_2^1}S^{1+\ell_2^1}(1,\mathcal{L}_2^1;t)$$

$$\times\,\rho_{1+\ell_2^1+\ell_2^2}(1,\mathcal{L}_2^1,\mathcal{L}_2^2)\prod_{i=3}^{k_2}\frac{(-1)^{\ell_2^i}}{\ell_2^i!}\rho_{1+\ell_2^i}(1,\mathcal{L}_2^i)S^1(1;t)^{-1}$$

$$\times \;\cdots\cdots\cdots$$

$$\times \frac{(-1)^{\ell_s^2}}{(\ell_s^1+\ell_s^2)!} \binom{\ell_s^1+\ell_s^2}{\ell_s^1} S^{1+\ell_s^1}(1,\mathcal{L}_s^1;t)$$

$$\times \rho_{1+\ell_s^1+\ell_s^2}(1,\mathcal{L}_s^1,\mathcal{L}_s^2) \prod_{i=3}^{k_s} \frac{(-1)^{\ell_s^i}}{\ell_s^i!} \rho_{1+\ell_s^i}(1,\mathcal{L}_s^i) S^1(1;t)^{-1} \quad (5.6)$$

where $\mathcal{L}_j = \dot{\bigcup}_{i=1}^{k_j} \mathcal{L}_j^i$ and $|\mathcal{L}_j^i| = \ell_j^i$. Also $k = k_1+\ldots+k_s$ . Let us now group together and sum terms of the above type for all possible partitions $\mathcal{L}_1^i$ of $\mathcal{L}_1$ (fixed). This is essentially a combinatorial problem. The total number of possible labellings of $\mathcal{L}_1^i$ $i = 2,\ldots,k_1$ from any set of $\sum_{i=2}^{k_1}\ell_1^i$ labels is equal to $\frac{(\ell_1^2+\ell_1^3+\ldots\ell_1^{k_1})!}{\ell_1^2!\ell_1^3!\ldots\ell_1^{k_1}!}$ . With this in mind, if we define

$$\omega(1,2,\ldots,m,\mathcal{L}^1 \| \mathcal{L}^*)$$

$$= \sum_{(\mathcal{L}^* \| \mathcal{L}^2 | \mathcal{L}^3 \ldots \mathcal{L}^k)_0} (-1)^{k-1} \rho_{n+\ell^1+\ell^2}(1,2,\ldots,m,\mathcal{L}^1,\mathcal{L}^2)$$

$$\times \prod_{i=3}^{k} \rho_{1+\ell^i}(1,\mathcal{L}^i) \quad (5.7)$$

then the sum of terms of the above type is given by

$$(-1)^{s-1}(-1)^{k_2-1} \ldots (-1)^{k_s-1}$$

$$\times \frac{(-1)^{\sum_{i=2}^{k_1}\ell_1^i}}{\ell_1^1!(\sum_{i=2}^{k_1}\ell_1^i)!} S^{n+\ell_1^1}(1,2,\ldots,n,\mathcal{L}_1^1;t)\,\omega(1,2,\ldots,n,\mathcal{L}_1^1 \| \bigcup_{i=2}^{k_1}\mathcal{L}_1^i) S^1(1;t)^{-1}$$

$$\times \;\cdots\cdots$$

$$\times \frac{(-1)^{\ell_s^1}}{(\ell_s^1+\ell_s^2)!} \binom{\ell_s^1+\ell_s^2}{\ell_s^1} S^{1+\ell_s^1}(1,\mathcal{L}_s^1;t)$$

$$\times \rho_{1+\ell_s^1+\ell_s^2}(1,\mathcal{L}_s^1,\mathcal{L}_s^2) \prod_{i=3}^{k_s} \frac{(-1)^{\ell_s^i}}{\ell_s^i!} \rho_{1+\ell_s^i}(1,\mathcal{L}_s^i) S^1(1;t)^{-1} \quad (5.8)$$

Similarly we may group together and sum terms for all possible partitions $\mathcal{L}_j^i$ of $\mathcal{L}_j$ (fixed) for $j = 2,\ldots,s$. The result is

$$(-1)^{s-1}(-1)^{\ell_1(2)}(-1)^{\ell_2(2)} \ldots (-1)^{\ell_s(2)}$$

$$\times \frac{1}{\ell_1(1)!\ell_1(2)!} S^{n+\ell_1(1)}(1,2,\ldots,n,\mathcal{L}_1(1);t)$$

$$\times \omega(1,2,\ldots,n,\mathcal{L}_1(1)\|\mathcal{L}_1(2))S^1(1;t)^{-1}$$

$$\times \frac{1}{\ell_2(1)!\ell_2(2)!} S^{1+\ell_2(1)}(1,\mathcal{L}_2(1);t)\omega(1,\mathcal{L}_2(1)\|\mathcal{L}_2(2))S^1(1;t)^{-1}$$

$$\times \ldots\ldots$$

$$\times \frac{1}{\ell_s(1)!\ell_s(2)!} S^{1+\ell_s(1)}(1,\mathcal{L}_s(1);t)\omega(1,\mathcal{L}_s(1)\|\mathcal{L}_s(2))S^1(1;t)^{-1} \tag{5.9}$$

where we have set $\mathcal{L}_j(1) = \mathcal{L}_j^1$, $\mathcal{L}_j(2) = \dot{\bigcup}_{i=2}^{k_j} \mathcal{L}_j^i$ so $\mathcal{L}_j = \mathcal{L}_j(1) \dot{\cup} \mathcal{L}_j(2)$. Also $\ell_j(1) = \ell_j^1$ and $\ell_j(2) = \sum_{i=2}^{k_j} \ell_j^i$. The total number of possible labellings of $\mathcal{L}_1(1)$, $\mathcal{L}_1(2)$, $\mathcal{L}_2(1)$, $\mathcal{L}_2(2),\ldots,\mathcal{L}_s(1),\mathcal{L}_s(2)$ from a set of labels $n+1,n+2,\ldots,n+\ell$ where $\ell = \sum_{j=1}^{s} \ell_j$ is equal to

$$\frac{(\ell_1(1)+\ell_1(2)+\ell_2(1)+\ell_2(2)+\ldots+\ell_s(1)+\ell_s(2))!}{\ell_1(1)!\ell_1(2)!\ell_2(1)!\ell_2(2)!\ldots\ell_s(1)!\ell_s(2)!} .$$

If we multiply the above expression by the appropriate Maxwellian factors and integrate over all variables in $\mathcal{L}_j$, $j = 1,\ldots,s$, it may be re-expressed as

$$\frac{1}{\ell!}\left(\prod_{j=n+1}^{n+\ell}\int d\underline{z}_j\right)$$

$$\sum_{(n+1,n+2,\ldots,n+\ell\|\mathcal{L}_1(1)\mathcal{L}_1(2)\ldots\hat{\mathcal{L}}_p(2)\ldots\mathcal{L}_s(2)|\mathcal{L}_p(2)\mathcal{L}_2(1)\ldots\mathcal{L}_s(1))_0}$$

$$\times\ (-1)^{S-1}(-1)^{\ell_1(2)}(-1)^{\ell_2(2)}\ \ldots\ (-1)^{\ell_s(2)}$$

$$\times\ S^{n+\ell_1(1)}(1,2,\ldots,n,\mathcal{L}_1(1);t)\,\omega(1,2,\ldots,n,\mathcal{L}_1(1)\|\mathcal{L}_1(2))\,S^1(1;t)^{-1}$$

$$\times\ S^{1+\ell_2(1)}(1,\mathcal{L}_2(1);t)\,\omega(1,\mathcal{L}_2(1)\|\mathcal{L}_2(2))\,S^1(1;t)^{-1}$$

$$\times\ \ldots$$

$$\times\ S^{1+\ell_s(1)}(1,\mathcal{L}_s(1);t)\,\omega(1,\mathcal{L}_s(1)\|\mathcal{L}_s(2))\,S^1(1;t)^{-1}$$

$$\times\ \prod_{i=2}^{n+\ell} h_0(\underline{v}_i)\ . \tag{5.10}$$

where the sum is over all ordered partitions of $n+1,n+2,\ldots,n+\ell$ into sets $\mathcal{L}_j(1)$, $\mathcal{L}_j(2)$, $1 \leq j \leq s$ where $\ell_1(1) \geq 0$ so $\mathcal{L}_1(1)$ may be empty, $\ell_j(1) > 0$ for $j = 2,\ldots,s$. Also $\ell_j(2) \geq 0$ for $j = 1,\ldots,s$ but at least one of the $\mathcal{L}_p(2)$ must be non-empty.

From (5.5) and (5.10), the solution to the elimination problem is given by

$f^{(n)}(1,2,\ldots,n;t)$

$$= \sum_{\ell=0}^{\infty}\frac{1}{\ell!}\left(\prod_{j=n+1}^{n+\ell}\int d\underline{z}_j\right)\sum_{(n+1,n+2,\ldots,n+\ell\|\mathcal{L}_1|\mathcal{L}_2,\ldots,\mathcal{L}_k)_0}(-1)^{k-1}$$

$$\times\ S^{n+\ell_1}(1,2,\ldots,n,\mathcal{L}_1;t)\,\rho_{n+\ell_1}(1,2,\ldots,n,\mathcal{L}_1)\,S^1(1;t)^{-1}$$

$$\times\ S^{1+\ell_2}(1,\mathcal{L}_2;t)\,\rho_{1+\ell_2}(1,\mathcal{L}_2)\,S^1(1;t)^{-1}$$

$$\times\ \ldots\ldots$$

$$\times \cdots$$

$$\times\ S^{1+\ell_k}(1,\mathcal{L}_k;t)\,\rho_{1+\ell_k}(1,\mathcal{L}_k)\,S^1(1;t)^{-1}\prod_{i=2}^{n+\ell} h_o(\underline{v}_i)\,f^{(1)}(1;t)$$

$$+\sum_{\ell=0}^{\infty}\frac{1}{\ell!}\left(\prod_{j=n+1}^{n+\ell}\int dz_j\right)$$

$$\times \sum_{(n+1,n+2,\ldots,n+\ell\|\mathcal{L}_1(1)\mathcal{L}_1(2)\ldots\hat{\mathcal{L}}_p(2)\ldots\mathcal{L}_k(2)|\mathcal{L}_p(2)\mathcal{L}_2(1)\ldots\mathcal{L}_k(1))_0}$$

$$\times\ (-1)^{k-1}(-1)^{\ell_1(2)}(-1)^{\ell_2(2)}\ \ldots\ (-1)^{\ell_k(2)}$$

$$\times\ S^{n+\ell_1(1)}(1,2,\ldots,n,\mathcal{L}_1(1);t)\,\omega(1,2,\ldots,n,\mathcal{L}_1(1)\|\mathcal{L}_1(2))\,S^1(1;t)^{-1}$$

$$\times\ S^{1+\ell_2(1)}(1,\mathcal{L}_2(1);t)\,\omega(1,\mathcal{L}_2(1)\|\mathcal{L}_2(2))\,S^1(1;t)^{-1}$$

$$\cdots$$

$$\times\ S^{1+\ell_k(1)}(1,\mathcal{L}_k(1);t)\,\omega(1,\mathcal{L}_k(1)\|\mathcal{L}_k(2))\,S^1(1;t)^{-1}$$

$$\times\prod_{i=2}^{n+\ell} h_0(\underline{v}_i)\,f^{(1)}(1;t)\,. \tag{5.11}$$

For the special case where $\rho_m(\ ) = \rho^{m-1}$, it is easily shown that (5.11) reduces to the result derived previously. In fact this result is given by just the first term in (5.11). The second is zero since $\omega(1,2,\ldots,m,\mathcal{L}^1\|\mathcal{L}^*) = 0$ if $\rho_m(\ ) = \rho^{m-1}$ because

$$\sum_{(\mathcal{L}^*\|\mathcal{L}^2|\mathcal{L}^3\ldots\mathcal{L}^k)_0}(-1)^{k-1} = 0\ . \tag{5.12}$$

(5.12) is proved by comparison with the Mayer cluster expansion, i.e. if

$$\rho_\ell(1,2,\ldots,\ell) = \sum_{(1,2,\ldots,\ell\|\mathcal{L}_1,\ldots,\mathcal{L}_k)}\prod_{i=1}^{k}\mu_{\ell k}(\mathcal{L}_k)\,,$$

then

$$\mu_{\ell}(1,2,\ldots,\ell) = \sum_{(1,2,\ldots,\ell \| \mathcal{L}_1,\ldots,\mathcal{L}_k)} (-1)^{k-1}(k-1)!$$

$$\times \prod_{i=1}^{k} \rho_{\ell k}(\mathcal{L}_k) .$$

Clearly $\mu_{\ell}(\ \ ) = 0$ if $\rho_m(\ \ ) = \rho^{m-1}$ for $\ell > 1$ so

$$\sum_{(1,2,\ldots,\ell \| \mathcal{L}_1,\ldots,\mathcal{L}_k)} (-1)^{k-1}(k-1)! = 0 \quad . \qquad (5.13)$$

There is a one-to-one correspondence of terms in (5.12) and (5.13). The extra factor of (k-1)! appears in (5.13) because we have not distinguished in the sum between different orderings of partitions.

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The methods of this chapter are applied to the non-linear problem in Appendix H

# CHAPTER 7

# THE ANALYSIS AND APPLICATIONS OF THE SOLUTION TO THE ELIMINATION PROBLEM

## 7.1 INTRODUCTION

The solution to the elimination problem for $n = 2$, i.e. $f^{(2)}(1,2;t) = T(1,2\;;t)f^{(1)}(1;t)$ obtained in the last chapter may be used to obtain a closed kinetic equation for $f^{(1)}(1;t)$ by substitution into the first hierarchy equation. This necessitates the consideration of $f^{(2)}(1,2;t)$ only for phase points $\underline{z}_1$ and $\underline{z}_2$ such that the corresponding particles are interacting (at a time $t$).

To prove the convergence of the integrals associated with the terms in the expansion of $T(1,2;t)$, we consider first combinations of streaming operators of the form

$$\overline{\sum_{(3,4,\ldots,2+\ell\|\mathcal{L}_1|\mathcal{L}_2,\ldots,\mathcal{L}_k)_0}} (-1)^{k-1} S^{2+\ell_1}(1,2,\mathcal{L}_1;t)S^1(1;t)^{-1}$$

$$\times\, S^{1+\ell_2}(1,\mathcal{L}_2;t)S^1(1;t)^{-1} \ldots S^{1+\ell_k}(1,\mathcal{L}_k;t)S^1(1;t)^{-1} \qquad (7.1)$$

(denoted $U^{2+\ell}(1,2|3,\ldots,2+\ell;t)$) acting on a class of functions $h(1,2,\ldots,2+\ell) = h(\underline{z}_1,\underline{v}_2,\ldots,\underline{v}_{2+\ell})$ which satisfy the following condition. $h(1,2,\ldots,2+\ell)$ should be invariant under a kinetic energy conserving transformation on the velocities $\underline{v}_2,\underline{v}_3,\ldots,\underline{v}_{2+\ell}$. For $\underline{z}_1,\underline{z}_2$ as above, the only non-vanishing contributions to (7.1) are shown to be associated with phase points corresponding to certain "connected" collision sequences between $2+\ell$ particles in the time interval $(0,t)$. Cohen[11] has placed a similar interpretation on contributions to the combinations of streaming operators which appear in the solution to the non-linear elimination problem.

The above mentioned analysis is carried out in detail first for a hard sphere potential and for the lowest order terms. Here the concept of collisions is well defined and there are no genuine multiple collisions (where a group of more than two particles is mutually interacting at one time). In the enumeration of contributing events, certain non-interacting and hypothetical collision events appear (c.f. the work by Sengers [7] on the Choh-Uhlenbeck equation). General results are then obtained for an arbitrary short range interparticle potential which could allow bound states.

The above analysis is used to prove the convergence of the expansion for $T(1,2;t)$, for the one dimensional hard "sphere" case and to examine the lowest order terms in density for the corresponding three dimensional case. Finally, the case of an arbitrary short range potential is considered. It is argued that the existence of bound states should not markedly affect the convergence behaviour.

Similar collisional interpretations of streaming or related operators have appeared in other work on kinetic theory. The binary collision expansion (Yang and Lee [19]) enables an easy interpretation in terms of collision sequences (Cohen [11]). The dominant contributions come from "ring events" where two collisions of particles 1 and 2 are connected by a series of uncorrelated binary collisions between the other particles. These are also the dominant terms in our analysis. Weinstock[23] has given a collisional interpretation of non-equilibrium Husimi type operators which is again similar to ours.

Finally we discuss the usefulness and limitations of using the expression $f^{(1)}(1,2;t) = T(1,2;t)f^{(1)}(1;t)$ to obtain kinetic equations. The equations should be valid for short times for arbitrary potentials, but resummation may be necessary before the equations can be used to determine long time behaviour. For hard sphere potentials, a method is described for extracting a closed equation for the delta-function part of $f^{(1)}(1;t)$.

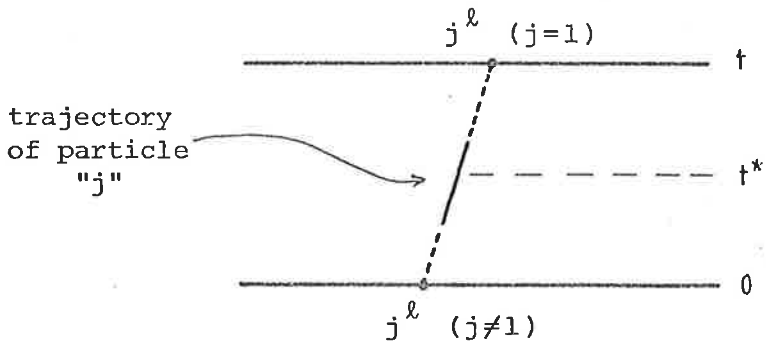
## 7.2 THE 3- AND 4-PARTICLE TERMS FOR A HARD SPHERE POTENTIAL

We enumerate all possible collision sequences between $n(=3,4)$ particles in a time interval $(0,t)$ for a hard sphere potential in 3 dimensions. For lower dimensions, all possible collisions will be a subset of these. We always assume that the last collision to occur before time "t" is between particles "1" and "2". By carrying out this analysis for low $m$, we hope to give some insight into a general rule determining which collision sequences give a non-zero contribution to $U^n(1,2|3,\ldots,n;t)h(1,2,\ldots,n)$ for arbitrary $n$.

First a description is given of the method of evaluation of the effect of products of streaming operators of the form (7.1) acting on a function $h(1,2,\ldots,n)$ of the class described. A criterion is developed to show the equivalence of certain classes of collision sequences with regard to the evaluation of $U^n(1,2|3,\ldots,n;t)h(1,2,\ldots,n)$.

It is also convenient to set up a notation to describe positions and velocities of particles at various intermediate stages of the collision sequence. Choose a time $t^* \in (0,t)$.

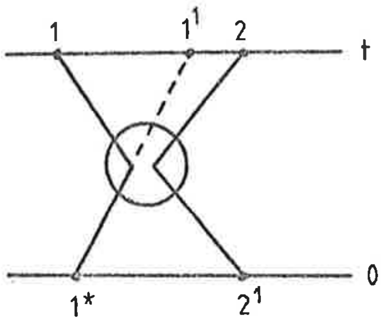
Let us consider a point on the trajectory of particle "j" at a time $t^*$. Now suppose that by following this point in a time increasing direction from a time $t^*$ to time $t$ along the trajectory of particle "j" and/or the trajectories of particles connected directly or indirectly to "j" through interaction, at most "$\ell$" collisions are encountered. Then for particle $j$, the phase point $j^\ell = (\underline{x}_j^\ell, \underline{v}_j^\ell)$ is defined as follows. $\underline{v}_j^\ell = \underline{v}_j(t^*)$, the velocity of particle $j$ at a time $t^*$ and $\underline{x}_j^\ell = \underline{x}_j(t^*) - \underline{v}_j(t^*)t^*$ for $j \neq 1$ and $\underline{x}_1^\ell = \underline{x}_1(t^*) + \underline{v}_1(t^*)(t-t^*)$.




- Note that the spacial dependence of $j^\ell$ for $j \neq 1$ is not important since $h(1,2,...,n)$ is independent of $\underline{x}_j$ for $j \neq 1$. For convenience, the segment of the trajectory of particle $j$ shown in the above diagram is also denoted by $j^\ell$.

The above ideas are first clarified by considering some very simple collision events. Certain other concepts are introduced. The effect of the streaming operator to the far left is evaluated first. We then continue from left to right evaluating the effect of each streaming operator in turn.

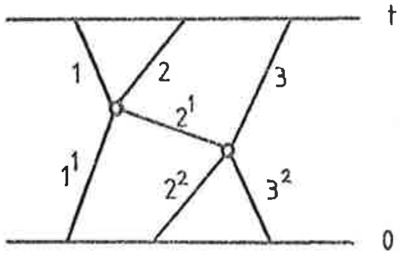
(i)




$$S^2(1,2;t)S^1(1;t)^{-1}h(1,2)$$
$$= S^1(1^*,t)^{-1}h(1^*,2^1)$$
$$= h(1^1,2^1)$$

In the following we shall set $S^{1+\ell}(1,\mathcal{L};t) = S^{1+\ell}(1,\mathcal{L};t)S^1(1;t)^{-1}$ for a set of $\ell$ labels $\mathcal{L}$.

(ii)



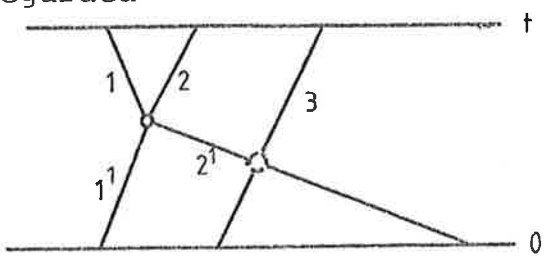

$$S^3(1,2,3;t)h(1,2,3)$$
$$= h(1^1,2^2,3^2)$$
$$= h(1^1,2^1,3\ )$$

noting that kinetic energy is conserved on collision between 2 and 3 and using the invariance property of $h(\ \ )$.

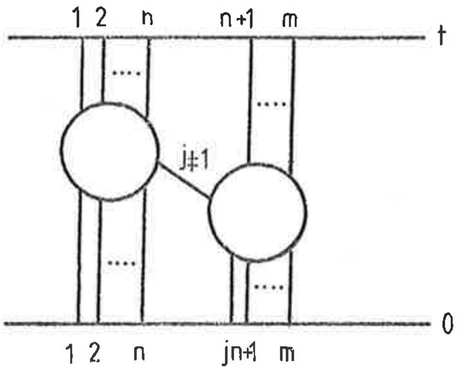
$$S^2(1,2;t)S^2(1,3;t)h(1,2,3)$$
$$= S^2(1^1,3;t)h(1^1,2^1,3)$$
$$= h(1^1,2^1,3)$$

except for the special cases mentioned below.

From this example, the following general rule may be discovered. For purposes of calculating the effect of streaming operators, the above diagram may be regarded as equivalent to:

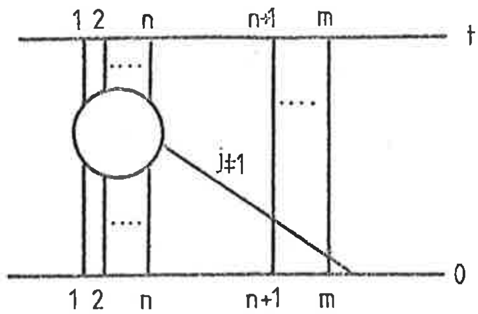



i.e. the collision between particles 2 and 3 is neglected. Such a collision has been termed non-interacting by Sengers [7]. This property may be generalized to the m-particle case in the following sense. A general class of collision events may be represented schematically by the following diagram:

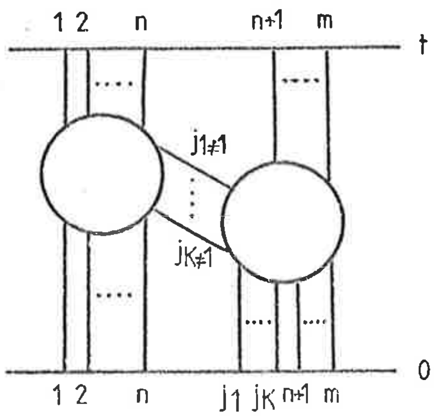


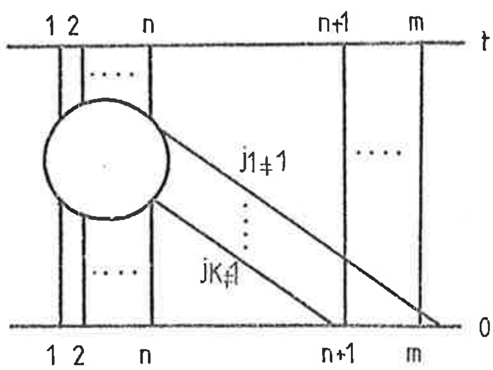

The details of the collision sequences within the circles are not specified. Only the direction of transfer in time of particle "j" from one group of particles to another is important.

Again using conservation of kinetic energy on collision and the invariance property for h( ), it becomes clear that for purposes of evaluating the effect of streaming operators, the above diagram may be regarded as equivalent to:



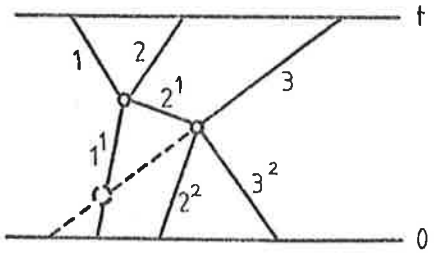

i.e. we neglect all collisions between particles j, n+1, n+2,...,m. Similarly, the following classes of diagrams are in this sense equivalent:

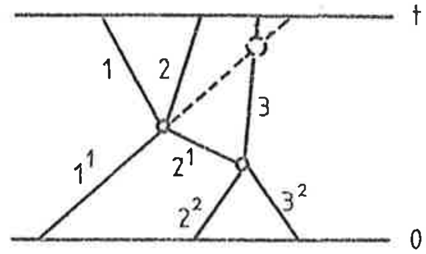


This result is useful in simplifying the enumeration of collision events.

(iii) There are some special cases for the collision sequence in (ii) where the above analysis of streaming operator effects is not valid. Following Sengers [7], these cases are termed "hypothetical" collisions. There are two basic types as exemplified below.

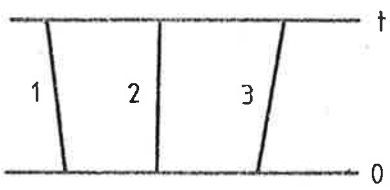


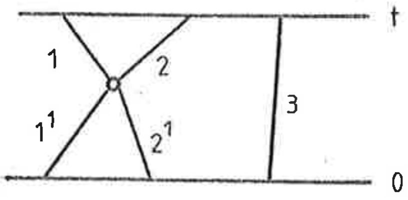



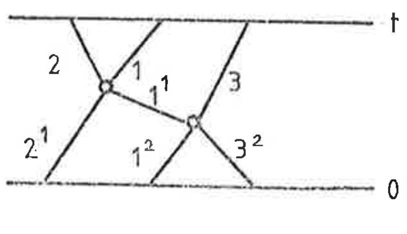

For both a) and b), again $S^3(1,2,3;t)h(1,2,3) = h(1^1,2^1,3)$ but $S^2(1,2;t)S^2(1,3;t)h(1,2,3) = S^2(1^1,3;t)h(1^1,2^1,3) \neq h(1^1,2^1,3)$. It is not necessary to consider b) for our analysis since the collision between "1" and "2" must be the last collision before time $t$.

For the case $n = 3$, we enumerate all possible collision sequences and extract those which give a non-zero contribution to $U^3(1,2|3;t)h(1,2,3)$

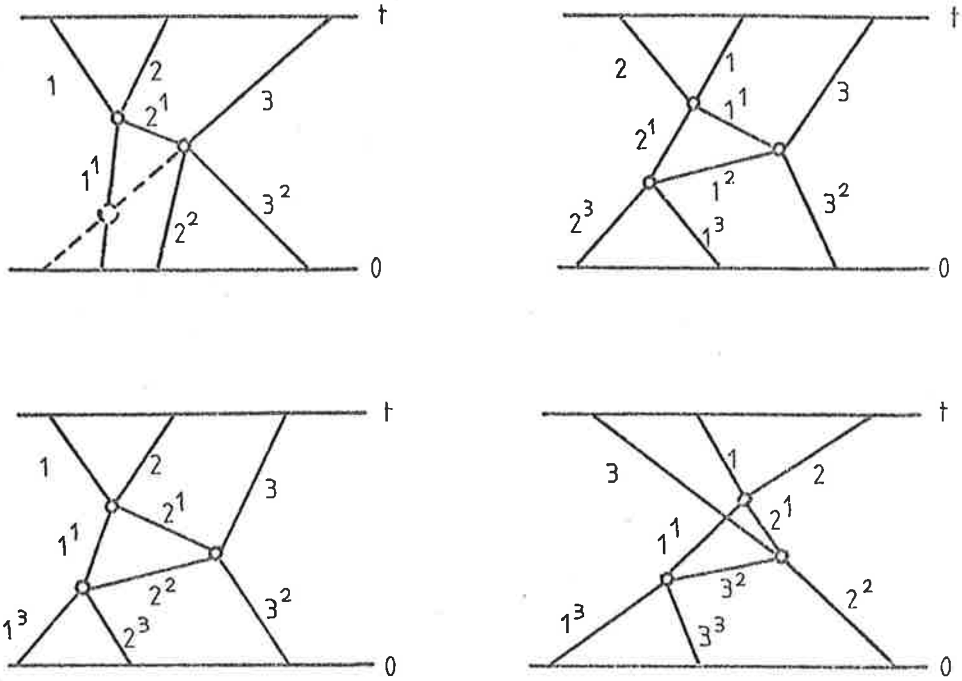
Zero contribution:



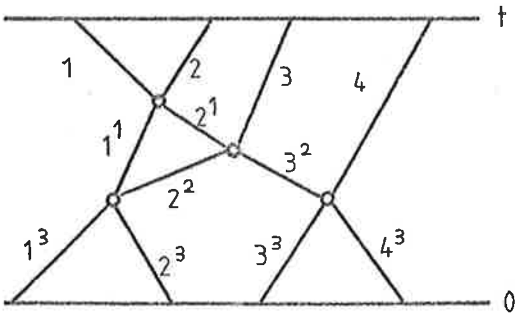



Non-zero contribution:




Finally, let us examine the rather more complex case $m = 4$. We shall first give an example of the analysis of a typical 4-particle collision event, namely:



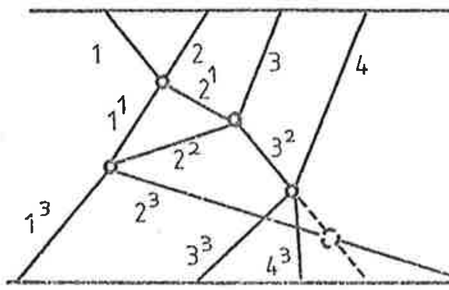

The reason for taking account of the last collision between "3" and "4" shall become obvious in the following analysis. We shall evaluate $U^4(1,2|3,4;t)h(1,2,3,4)$ for the above diagram.

a) $S^4(1,2,3,4;t)h(1,2,3,4) = h(1^3,2^3,3^3,4^3) = h(1^3,2^3,3^2,4)$.

b) $S^3(1,2,3;t)S^2(1,4;t)h(1,2,3,4)$

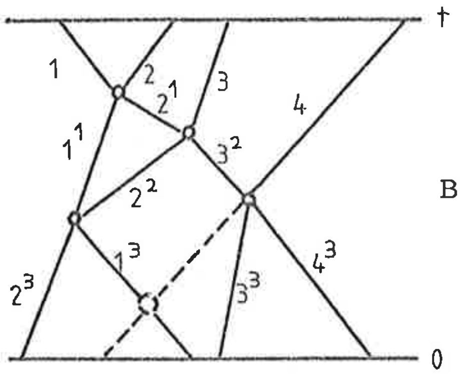
$= S^2(1^3,4;t)h(1^3,2^3,3^2,4)$

except for A.

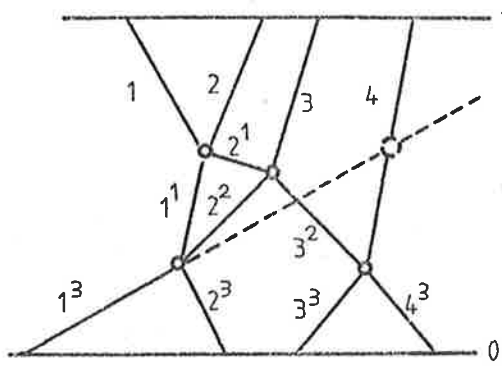



A

$= h(1^3,2^3,3^2,4)$ except for B,C.




B



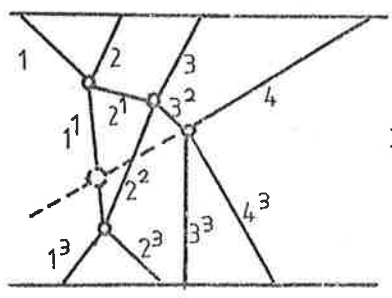

C

c) $S^3(1,2,4;t)S^2(1,3;t)h(1,2,3,4)$

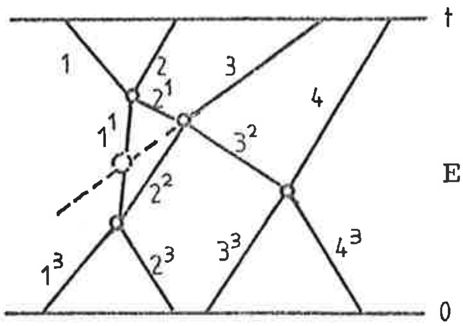
$= S(1^1,3;t)h(1^1,2^1,3,4)$

except for D .

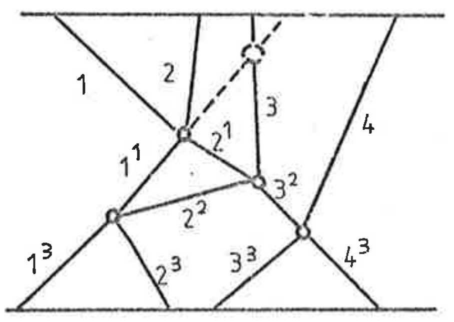
$= h(1^1,2^1,3,4)$ except for E,F .




D




E



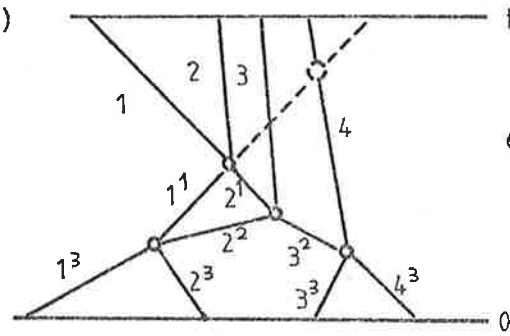

F

d) $S^2(1,2;t)S^3(1,3,4;t)h(1,2,3,4)$

$= S^3(1^1,3,4;t)h(1^1,2^1,3,4)$

$= h(1^1,2^1,3,4)$

except for D,E,F,G.




G

e) $S^2(1,2;t)S^2(1,3;t)S^2(1,4;t)h(1,2,3,4)$

$= S^2(1^1,3;t)S^2(1^1,4;t)h(1^1,2^1,3,4)$

$= S^2(1^1,4;t)h(1^1,2^1,3,4)$ except for E,F.

$= h(1^1,2^1,3,4)$ except for D,G.

f) $S^2(1,2;t)S^2(1,4;t)S^2(1,3;t)h(1,2,3,4)$

$= S^2(1^1,4;t)S^2(1^1,3;t)h(1^1,2^1,3,4)$

$= S^2(1^1,3;t)h(1^1,2^1,3,4)$ except for D,G

$= h(1^1,2^1,3,4)$ except for E,F.

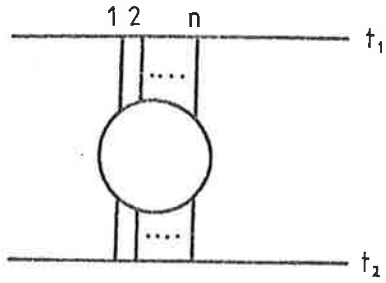
By inspection it is clear that neglecting A,B,...,G, there is zero contribution to $U^4(1,2|3,4;t)h(1,2,3,4)$. Further analysis shows that there is also a zero contribution from D,E and F. There is however a non-zero contribution from A,B,C and G . If the last collision before time t is between "1" and "2", then also G may be neglected.

All possible 4-particle collision events may be analyzed in a similar fashion. A list of all relevant contributing events is given in Appendix I.

## 7.3 CATEGORIZATION OF n-BODY COLLISION SEQUENCES FOR SHORT RANGE POTENTIALS

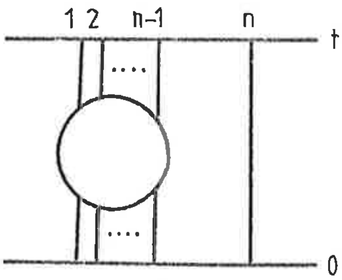
In this section we categorize certain classes of n-body collision events which give a non-zero contribution to $U^n(1,2|\ldots,n;t)h(1,2,\ldots,n)$. A concept of "connectedness" somewhat similar to that introduced by Green[85] shall be of use here. The schematic representation of collision events used by Green[85] is also adopted here (see section 7.2). For a collision sequence to give a non-zero contribution, we show that there can be no subgroup of particles which do not interact with the rest, i.e. the collision sequence must be connected. Also if genuine m-body collisions are given the weight of m binary collisions, then we show that the n-particles must undergo at least n collisions (counting real and hypothetical collisions).

As in section 7.2, we let




denote a collision sequence between times $t_1$ and $t_2$ involving particles 1,2,...,n. The details are not specified. There may be hypothetical collisions involved in this sequence. A number of classes of collision sequences are examined below.

(i)




Let $\{A_j : j=1,\dots,p\}$ be an ordered partition of $\{3,4,\dots,n-1\}$. We group the terms in $U^n(1,2|3,\dots,n;t)h(1,2,\dots,n)$ into pairs

$$(-1)^{p-1} S^{\cdots}(1,2,A_1;t)\dots S^{\cdots}(1,A_j;t) S^2(1,n+1;t)$$

$$S^{\cdots}(1,A_{j+1};t)\dots S^{\cdots}(1,A_p;t)h(\dots)$$

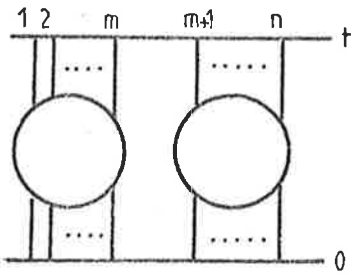
and

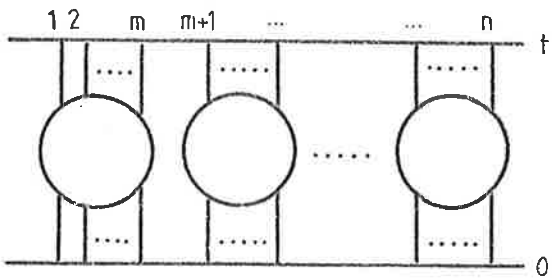
$$(-1)^p S^{\cdots}(1,2,A_1;t)\dots S^{\cdots}(1,n+1,A_j;t) S^{\cdots}(1,A_{j+1};t) \dots$$

$$\dots S^{\cdots}(1,A_p;t)h(\dots) \qquad (3.1)$$

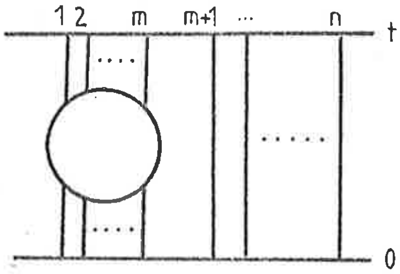
which give opposite contributions.

(ii)



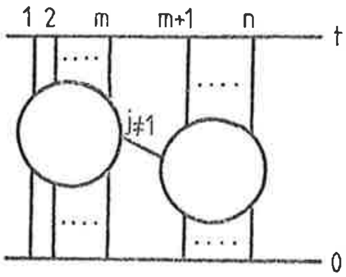



The discussion of section 7.2 shows that (using the invariance property of h( ) and conservation of kinetic energy) (ii) may be regarded as equivalent to

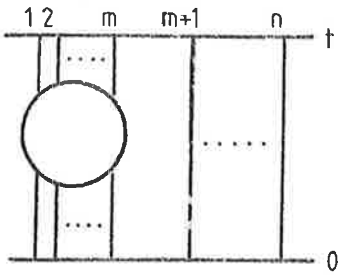



which may be regarded as a member of the class (i) and thus will not contribute.

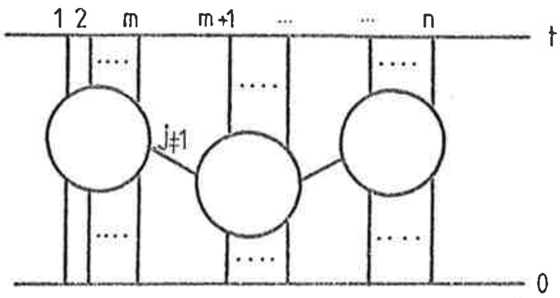
(iii)



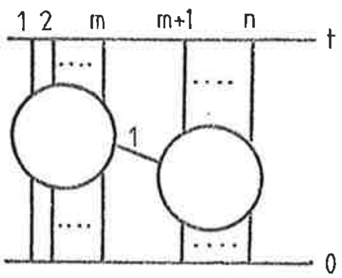

which is equivalent to




from the discussion of section 7.2 and thus from (ii) gives zero contribution. Note that (iii) includes collision events like




(iv)




Let $\{A_j : j=1,2,\ldots,p\}$ be an ordered partition of $\{3,4,\ldots,m\}$ and let $\{B_j : j=1,2,\ldots,p'\}$ be an ordered partition of $\{m+1,\ldots,n\}$

Again we group the terms in $U^n(1,2|3,\ldots,n;t)h(1,2,\ldots,n)$ into pairs which give opposite contributions as follows:

$$(-1)^{\ell-1}S^{\cdots}(1,2,A_1;t)S^{\cdots}(1,A_2;t)\ldots S^{\cdots}(1,A_j;t)S^{\cdots}(1,B_1;t)\ldots$$

$$\ldots\ h(\ldots)$$

and

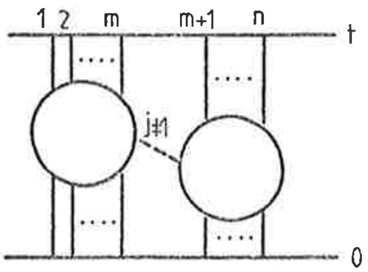
$$(-1)^{\ell}S^{\cdots}(1,2,A_1;t)S^{\cdots}(1,A_2;t)\ldots S^{\cdots}(1,A_j,B_1;t)\ldots h(\ldots) \tag{3.2}$$

where $\ell$ equals the number of streaming operators $S^{\cdots}(\ldots)$ in the first expression. The factors appearing to the right of the streaming operator containing the labels $B_1$ are of the form $S^{\cdots}(1,A_k;t)$, $S^{\cdots}(1,B_{k'};t)$ and $S^{\cdots}(1,A_k,B_{k'};t)$ for $k > j$ and $k' > 1$. The result follows from the identity

$$S^{\cdots}(1,2,A_1;t)S^{\cdots}(1,A_2;t)\ldots S^{\cdots}(1,A_j;t)S^{\cdots}(1,B_1;t)\cdot\underline{z}_j$$

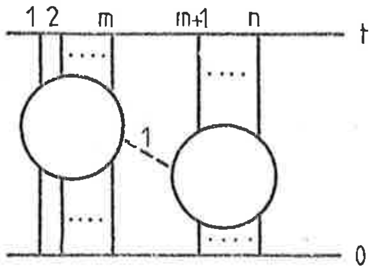
$$= S^{\cdots}(1,2,A_1;t)S^{\cdots}(1,A_2;t)\ldots S^{\cdots}(1,A_j,B_1;t)\cdot\underline{z}_j \tag{3.3}$$

(v)



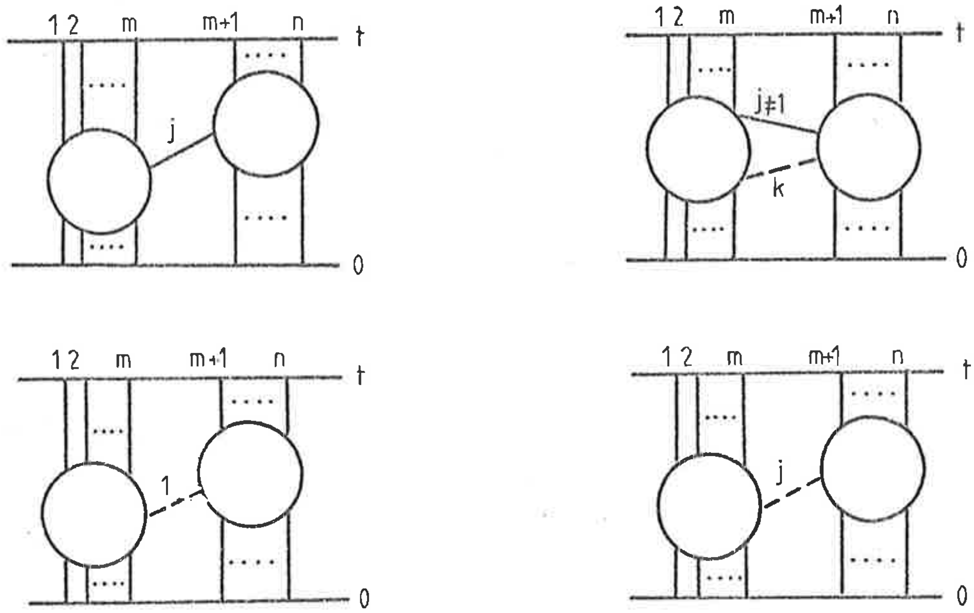

The discussion of section 7.2 shows that (v) is equivalent to the disconnected diagram shown in (iii) and thus gives zero contribution.

(vi)



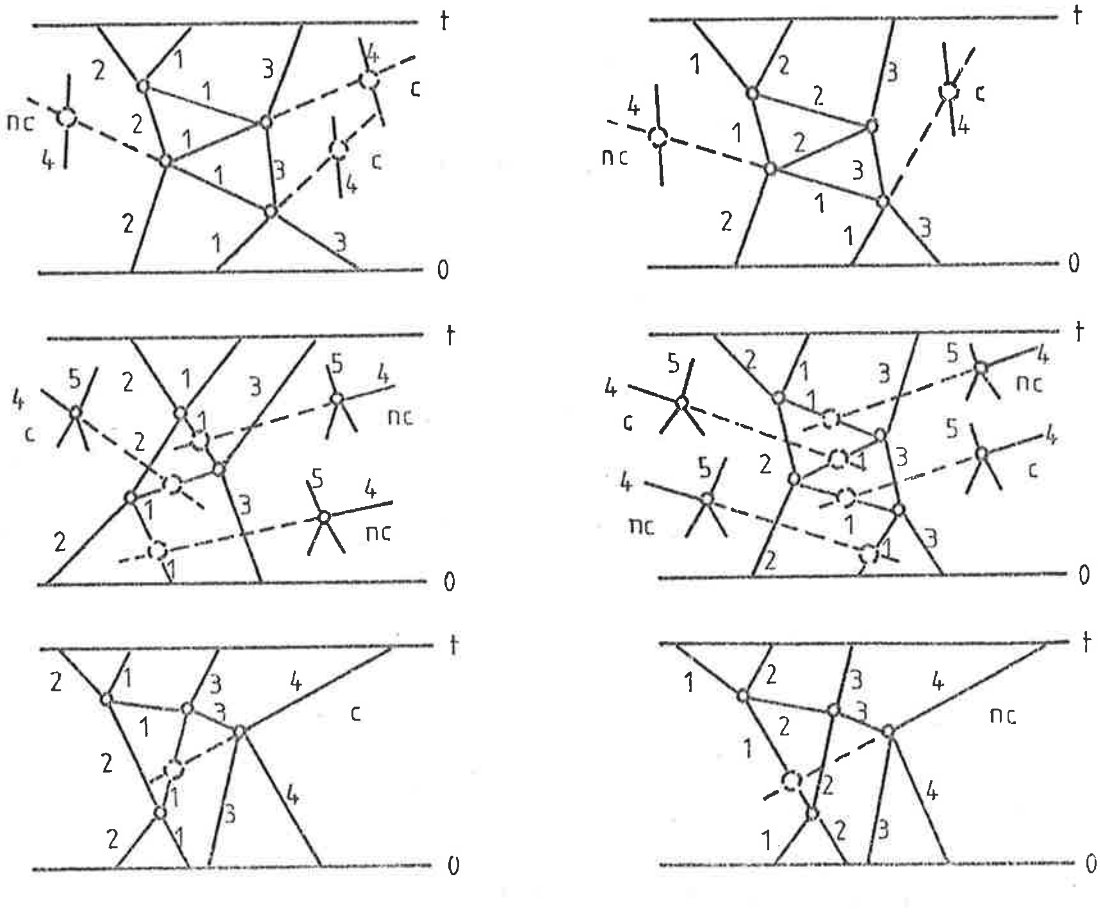

The method of analysis and results of (iv) are also applicable to this case.

Finally we give some examples of classes of collision sequences which do not necessarily give a vanishing contribution to $U^n(1,2|3,\ldots n;t)h(1,2,\ldots,n)$:

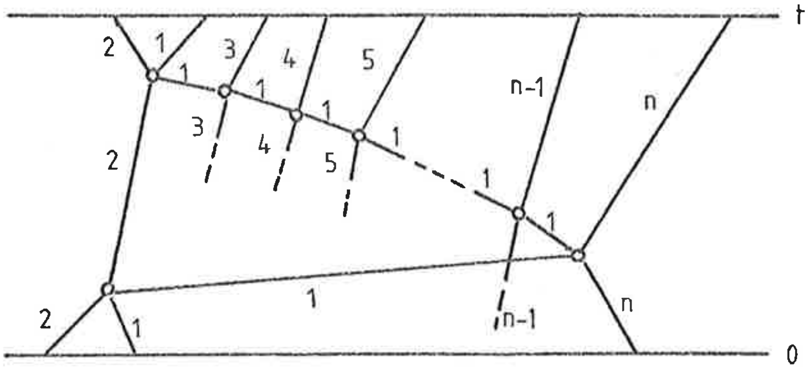



The situation is particularly complex with the last three cases shown as indicated by the following examples:

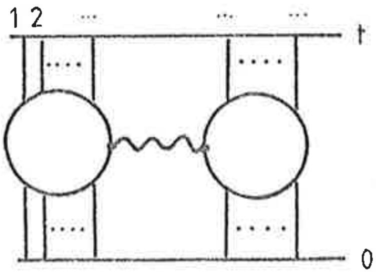
c = contributing nc = not contributing



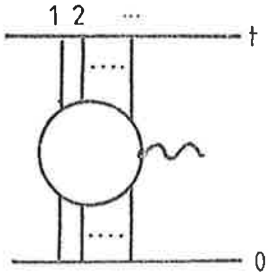
Next we determine the minimum number of collisions between n particles necessary to give a non-vanishing contribution to $U^n(1,2|3,...,n;t)h(1,2,...,n)$. We know that only connected collision sequences contributed. Therefore the number of collisions, with the described weighting on genuine multiple collisions, must be at least n-1. This is a simple consequence of the following graph theoretical results (see Wilson[86]): let a graph have n points, k components and m lines, then $n-k \leqslant m$. For our application $k = 1$, n is the number of particles and m is the number of distinct pairs of particles that have interacted. An example of a contributing collision sequence with exactly n collisions is the "ring" event



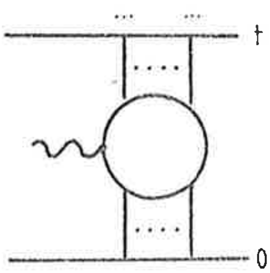

It remains to prove that all collision sequences with exactly "n-1" collisions vanish. Firstly we note that it is always possible to represent a connected collision sequence (other than a genuine n-body collision) in the form



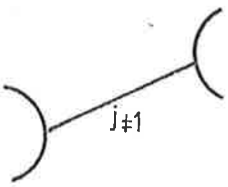

where

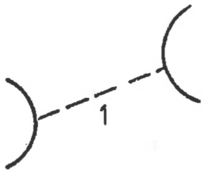



and

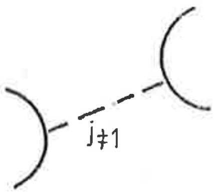


are connected. The possibility of this choice is easily verified by graph theoretical considerations. Suppose firstly that  consists of $c > 1$ connecting collisions (real and/or hypothetical). Using the graph theoretical result above to determine a lower bound for the number of collisions in each of the above connected components, we conclude that the total number of collisions must be at least $n+c-2 \geqslant n$, as required. Secondly, we suppose that  consists of a single connecting particle. If the contribution of this collision sequence to $U^n(1,2|3,...,n;t)h(1,2,...,n)$ is not to vanish, then  must be of the form

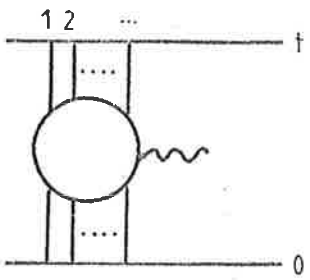


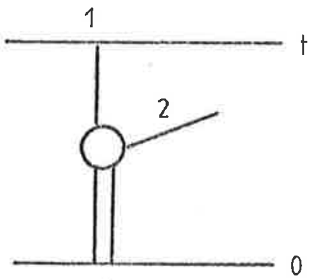

or

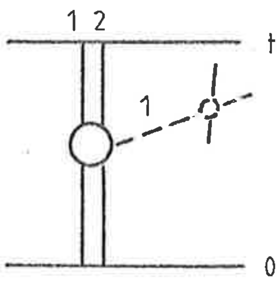


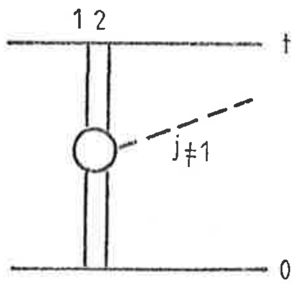

If this is the case we reapply the above considerations to




. By continually repeating this procedure, we show that either there must be $\geqslant n$ collisions or that one of the following cases arises




However since we have prescribed that "1" and "2" must be interacting at time $t$, none of these cases are allowed.

In conclusion, the n-particle collision sequences which contribute to $U^n(1,2|3,\ldots,n;t)h(1,2,\ldots,n)$ must have at least n collisions (real and/or hypothetical and with genuine multiple collisions weighted in the prescribed way).

## 7.4 CONVERGENCE CONSIDERATIONS FOR THE SOLUTION TO THE ELIMINATION PROBLEM

The results of the preceding sections may be applied to the analysis of terms in the expression $f^{(2)}(1,2;t) = T(1,2;t)f^{(1)}(1;t)$ for configurations where particles "1" and "2" are interacting at a time t . In particular we wish to show that for each term in the expansion of $T(1,2;t)$, the integrals are convergent. An order of magnitude estimate (in terms of "t") is to be made for each of these terms and, if possible, an estimate of the range of convergence with respect to time determined for the series.

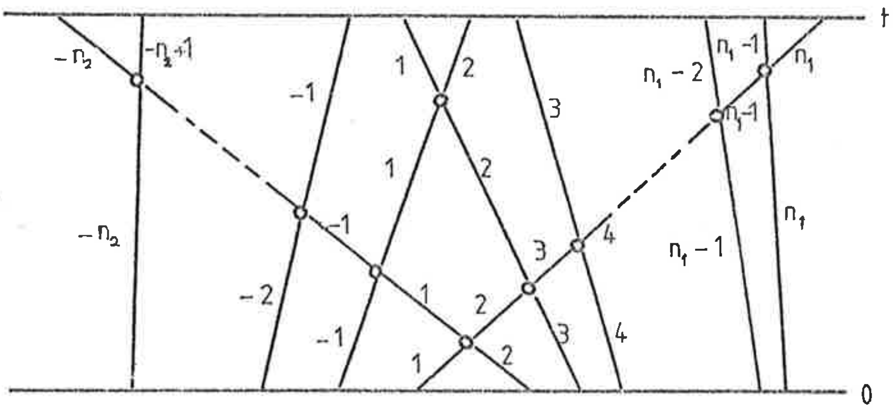
For the one-dimensional hard "sphere" gas $T(1,2;t)$ assumes a particularly simple form. From (4.15) of chapter 6

$$f^{(2)}(1,2;t) = \sum_{\ell=0}^{\infty} \frac{\rho^{\ell+1}}{\ell!} \int d\underline{z}_3 \int d\underline{z}_4 \cdots \int d\underline{z}_{2+\ell}$$

$$\times\, U^{2+\ell}(1,2|3,\ldots,2+\ell;t) \prod_{i=2}^{2+\ell} h_0(\underline{v}_i) f^{(1)}(1;t) \quad (4.1)$$

where "$\rho$" is the mean particle density. The function $h(1,2,\ldots,2+\ell) = \prod_{i=1}^{2+\ell} h_0(\underline{v}_i) f^{(1)}(1;t)$ satisfies the invariance condition of section 7.1. So the analysis of the previous sections is applicable if we consider $f^{(2)}(1,2;t)$ evaluated at precollision points $x_2 = x_1 - \epsilon\,\mathrm{sgn}(v_2-v_1)$ in the limit $\epsilon \to 0$.

The convergence of the integrals is proved from the connectivity condition of section 7.3 (c.f. section 6.2). Because of the Maxwellian factors in (4.1), the velocities are effectively restricted to a magnitude $O(v_{th})$ so the spatial coordinates $x_i$, $i > 2$ are effectively restricted to within a distance $O(v_{th}t)$ of $\{x_1, x_2\}$. Also using the ordering constraint on the spatial coordinates, we conclude that the effective region of integration for the $\ell^{th}$ term of (4.1) has size $O(\frac{(v_{th}^2 t)^{\ell}}{\ell!})$. The order of magnitude of the integrand is expected to be $O(1)$ because of partial cancellation from various terms in $U^{2+\ell}(1,2|3,\ldots,2+\ell;t)$. The above estimate agrees with that made by Anstis [43] for the corresponding velocity distribution functions. It is not possible to obtain a better estimate as may be seen by examination of the collision sequence




$$n_1+n_2 = \ell+2$$

We now consider the corresponding expressions for the 3-dimensional hard sphere gas. Specifically we shall examine the convergence of the integrals associated with the lowest order terms for given powers of density. Order of magnitude estimates are also made on these terms. The following results are needed from equilibrium statistical mechanics (see Uhlenbeck and Ford [84])

$$\rho_2(1,2) = \rho\, e^{-\phi_{12}}(1+\rho \int dz_3\, (e^{-\phi_{13}}-1)(e^{-\phi_{23}}-1)+\ldots)$$

$$\rho_3(1,2,3) = \rho^2\, e^{-\phi_{123}}(1+\rho \int dz_4[(e^{-\phi_{14}}-1)(e^{-\phi_{24}}-1)(e^{-\phi_{34}}-1) + (e^{-\phi_{14}}-1)(e^{-\phi_{24}}-1)+(e^{-\phi_{14}}-1)(e^{-\phi_{34}}-1) + (e^{-\phi_{24}}-1)(e^{-\phi_{34}}-1)] + \ldots)$$

$$\rho_4(1,2,3,4) = \rho^3\, e^{-\phi_{1234}}(1+\ldots) \qquad (4.2)$$

where $e^{-\phi_{12\ldots q}} = \exp(-\sum_{i<j=1}^{q} \phi_{ij})$ where $\phi_{ij}$ is the inter-particle potential between particles "i" and "j". The analysis of the expansion for $f^{(2)}(1,2;t)$ shall only be for phase points $\underline{z}_1,\underline{z}_2$ at time $t$ such that the particles "1" and "2" are about to collide. For hard sphere potentials we shall make use of the commutation result (see Ernst et al.[87]).

$$S^n(1,2,\ldots,n;t)e^{-\phi_{12\ldots n}} = e^{-\phi_{12\ldots n}}S^n(1,2,\ldots,n;t) \qquad (4.3)$$

The 3-particle $(\ell=1)$ term has been examined previously by Anstis[44]. We have that

$$\int d\underline{z}_3\, (S^3(1,2,3;t)\rho_3(1,2,3)S^1(1;t)^{-1}-S^2(1,2;t)\rho_2(1,2)S^1(1;t)^{-1} \times S^2(1,3;t)\rho_2(1,3)S^1(1;t)^{-1})h_0(\underline{v}_2)h_0(\underline{v}_3)f^{(1)}(1;t)$$

$$- \int d\underline{z}_3\, S^2(1,2;t)\omega(1,2\|3)S^1(1;t)^{-1}h_0(\underline{v}_2)h_0(\underline{v}_3)f^{(1)}(1;t)$$

$$= \rho^2 \int d\underline{z}_3\, e^{-\phi_{123}}(S^3(1,2,3;t)S^1(1;t)^{-1}-S^2(1,2;t)S^1(1;t)^{-1} \times S^2(1,3;t)S^1(1;t)^{-1})h_0(\underline{v}_2)h_0(\underline{v}_3)f^{(1)}(1;t)$$

$$+ \rho^2 \int d\underline{z}_3 (e^{-\phi_{13}}e^{-\phi_{23}}-S^1(1;t)e^{-\phi_{13}}S^1(1;t)^{-1})(S^2(1,3;t)S^1(1;t)^{-1}-1) \times h_0(\underline{v}_2)h_0(\underline{v}_3)f^{(1)}(1;t)$$

$$+ \rho^2 \int d\underline{z}_3 (e^{-\phi_{13}}e^{-\phi_{23}}-S^1(1;t)e^{-\phi_{13}}S^1(1;t)^{-1}S^1(2;t)e^{-\phi_{23}}) \times h_0(\underline{v}_2)h_0(\underline{v}_3)f^{(1)}(1;t)$$

$$+ O(\rho^3)\,. \qquad (4.4)$$

Convergence of the integral in the first term may be proved using the connectivity condition discussed previously. Collision sequences contributing to this term must have at least three collisions (including the collision between "1" and "2" at time $t$). An estimate of the phase space volume of const + $O(\frac{t_c}{t})$ has been made for such events (see Cohen[10]) where $t_c$ is the collision time $\approx$ (range of $\phi_{ij}$)/$v_{th}$. The second and third terms in (4.4) are clearly convergent and bounded in time.

The terms of order $\rho^3$ in (4.4) may be written in the form

$$\rho^3 \int d\underline{z}_3 \int d\underline{z}_4 [e^{-\phi_{123}} S^3(1,2,3;t) - S^1(1;t)S^1(2;t)e^{-\phi_{123}}](e^{-\phi_{14}}-1)$$

$$\times (e^{-\phi_{24}}-1)(e^{-\phi_{34}}-1)S^1(1;t)^{-1}h_0(\underline{v}_2)h_0(\underline{v}_3)h_0(\underline{v}_4)f^{(1)}(1;t)$$

$$+ \rho^3 \int d\underline{z}_3 \int d\underline{z}_4 [(e^{-\phi_{123}}-e^{-\phi_{12}})S^3(1,2,3;t) + e^{-\phi_{12}}(S^3(1,2,3;t)$$

$$- S^1(1;t)S^1(2;t)][(e^{-\phi_{14}}-1)(e^{-\phi_{24}}-1) + (e^{-\phi_{14}}-1)(e^{-\phi_{34}}-1)$$

$$+ (e^{-\phi_{24}}-1)(e^{-\phi_{34}}-1)]S^1(1;t)^{-1} h_0(\underline{v}_2)h_0(\underline{v}_3)h_0(\underline{v}_4)f^{(1)}(1;t)$$

$$- \rho^3 \int d\underline{z}_3 \int d\underline{z}_4 \; e^{-\phi_{12}} S^1(1;t)S^1(2;t)(e^{-\phi_{14}}-1)(e^{-\phi_{24}}-1)S^1(1;t)^{-1}$$

$$\times [e^{-\phi_{13}}(S^2(1,3;t)S^1(1;t)^{-1}-1) - (S^1(1;t)e^{-\phi_{13}}S^1(1;t)^{-1}$$

$$- e^{-\phi_{13}})]h_0(\underline{v}_2)h_0(\underline{v}_3)h_0(\underline{v}_4)f^{(1)}(1;t)$$

$$+ \rho^3 \int d\underline{z}_3 \int d\underline{z}_4 \; e^{-\phi_{12}}(S^2(1,3;t) - S^1(1;t))S^1(2;t)e^{-\phi_{13}}(e^{-\phi_{14}}-1)$$

$$\times (e^{-\phi_{24}}-1)S^1(1;t)^{-1}h_0(\underline{v}_2)h_0(\underline{v}_3)h_0(\underline{v}_4)f^{(1)}(1;t). \qquad (4.5)$$

The factors $(e^{-\phi_{14}}-1)$ and/or $(e^{-\phi_{24}}-1)$ ensure that the integral over $\underline{z}_4$ converges. The factors $S^2(1,3;t)-S^1(1;t)$, $S^3(1,2,3;t)-S^2(1,2;t)$ and $S^3(1,2,3;t)(e^{-\phi_{34}}-1)$ ensure that $\underline{z}_3$ is effectively confined to a region of phase space of size $O((v_{th}^2 t)^3)$. This gives an estimate of the size of terms in (4.5).

Other terms of order $\rho^3$ come from the 4-particle $(\ell = 2)$ term of (5.11), chapter 6. These may be rearranged so that one term contains a factor $U^4(1,2|3,4;t)$ which produces a convergent contribution associated with connected 4-particle collision sequences of at least four collisions. From Cohen's analysis these contributions will be of order $O((v_{th}^2 t_c)\ell n(\frac{t}{t_c}))$. The convergence of the remaining terms is assured by the inclusion of factors containing suitable combinations of streaming operators and of potential terms. These terms dominate the long time behaviour.

For a general short range potential, it is easiest to check convergence for each term ($\ell$ fixed) of (5.11) by examination of (5.2). In this expression appear the operators $T_{m_1}^2(1,2;t)$ and $T_{m_i}^1(1;t)$. An analysis similar to that at the end of section 6.2 shows that the only contributions to the integrals appearing in these operators come from phase points associated with collision sequences connected to "1" and/or "2" for $T_{m_1}^2(1,2;t)$ and connected to "1" for $T_{m_i}^1(1;t)$. The convergence of the integrals is therefore easily verified. For this analysis the existence of bound states is not significant. Therefore we do not expect the range of convergence of (5.11) to depend significantly on this feature of the interparticle potential. However the nature of (5.11) will be affected by the existence of bound states. It is also quite easy to prove that the first term (and therefore the second term) of (5.11) converge separately. Consider a disconnected collision sequence where there is a group of particles not interacting with "1" or "2" in the time interval (0,t). Let $A_i$ be a partition of the group of labels attached to { 1,2 } and let $B_i$ be a partition of the other disconnected group. In the first term of (5.11), we group together products of streaming operators of the form

$$(-1)^{p-1} S^{\cdot\cdot}(1,2,A_1;t)\,\rho_{\cdot\cdot}(1,A_1)\,S^1(1;t)^{-1} S^{\cdot\cdot}(1,A_2;t)\,\rho_{\cdot\cdot}(1,A_2)\,S^1(1;t)^{-1}\ldots$$

$$S^{\cdot\cdot}(1,A_j;t)\,\rho_{\cdot\cdot}(1,A_j)\,S^1(1;t)^{-1} S^{\cdot\cdot}(1,B_1;t)\,\rho_{\cdot\cdot}(1,B_1)\,S^1(1;t)^{-1}\ldots$$

or

$$(-1)^{p-2} S^{\cdot\cdot}(1,2,A_1;t)\,\rho_{\cdot\cdot}(1,A_1)\,S^1(1;t)^{-1} S^{\cdot\cdot}(1,A_2;t)\,\rho_{\cdot\cdot}(1,A_2)\,S^1(1;t)^{-1}\ldots$$

$$S^{\cdot\cdot}(1,A_j,B_1;t)\,\rho_{\cdot\cdot}(1,A_j,B_1)\,S^1(1;t)^{-1}\ldots \tag{4.6}$$

The sum contribution from these two terms is of the order $\rho_{\cdot\cdot}(1,A_j,B_1) - \rho_{\cdot\cdot}(1,A_j)\,\rho_{\cdot\cdot}(1,B_1)$ which approaches zero as the distance between the sets of phase points corresponding to $A_j$ and $B_1$ becomes large. So the corresponding integral will converge provided the equilibrium correlations diminish sufficiently quickly for large separations.

## 7.5 A KINETIC EQUATION FOR $f^{(1)}(1;t)$

The usefulness of the expression $f^{(2)}(1,2;t)=T(1,2;t)f^{(1)}(1;t)$ will depend on the range of convergence of the series expansion and the accuracy to which the series may be approximated by retaining the first few terms. For times short compared with the mean free time, we certainly expect the approximation to be good. We expect the range of convergence to decrease with increased mean density and with increased range of the inter-particle potential. Bound state effects should show up for times greater than the period of orbit for the bound particle motion.

Without resummation of terms in the expression for $f^{(2)}(1,2;t)$ , the resulting kinetic equation is not expected to be useful in describing the long time behaviour of $f^{(1)}(1;t)$. This is because the $\ell^{th}$ term of (5.11) (chapter 6) involves isolated $\ell+2$-particle collision sequences. As pointed out by Cohen [10] and others, such terms will produce unmanageable long time behaviour so there is a need to resum to include many particle effects in all terms. Physically this represents a many-particle damping of isolated $\ell+2$-particle collision sequences occurring over long times. A resummation of this type has been achieved using a binary collision expansion formulation (see Kawasaki and Oppenheim [22]). A resummation closer to that described above has been discussed by Cohen [11].

For the one dimensional hard "sphere" gas, the kinetic equation which results from retaining the first two terms in $T(1,2;t)$ is given below. For the velocity distribution function

$$h^{(1)}(v;t) = \int dx\ f^{(1)}(x,v;t) \tag{5.1}$$

we have

$$\frac{\partial}{\partial t} h^{(1)}(v_1;t) = U_{reg}(v_1;t|h^{(1)}) + U_\delta(v_1;t)h^{(1)}(v_1;t) \tag{5.2}$$

where $U_{reg}(v_1;t|h)$ involves integration over $h(v;t)$ with respect to the variable $v$ and

$$U_\delta(v_1;t) = - n \int dv_2 |v_1-v_2| h_0(v_2)$$

$$+ n^2 t \int dv_2 \int dv_3 \, H((v_2-v_1)(v_1-v_3)) |v_1-v_2| |v_1-v_3| h_0(v_2) h_0(v_3)$$

$$= - n\alpha(v_1) + n^2 t \, \beta(v_1) \qquad \text{(say)} \qquad (5.3)$$

(5.2) has been solved using iterative techniques by Anstis [43]. Where the initial conditions are such that $h^{(1)}(v_1;t)$ has a delta function component $\delta(v_1-v')$, we make the decomposition $h^{(1)}(v_1;t) = h_\delta^{(1)}(v';t)\delta(v_1-v') + h_{reg}^{(1)}(v_1;t)$ into delta-function and regular parts. An equation for $h_\delta^{(1)}(v';t)$ may be extracted from (5.2):

$$\frac{\partial}{\partial t} h_\delta^{(1)}(v';t) = U_\delta(v';t) h_\delta^{(1)}(v';t)$$

$$= (-n\alpha(v') + n^2 t\beta(v')) h_\delta^{(1)}(v';t) \qquad (5.4)$$

which has the solution

$$h_\delta^{(1)}(v';t) = \exp(-\alpha(v')(nt) + \tfrac{1}{2}\beta(v')(nt)^2) h_\delta^{(1)}(v';0) \qquad (5.5)$$

so clearly the usefulness of (5.5) is limited to times much shorter than the mean free time. The inclusion of higher order terms from $T(1,2;t)$ will only introduce higher order polynomial terms in $t$. Thus the need for resummation is clear.

This method of extracting a kinetic equation for the delta-function part $h_\delta^{(1)}$ is also applicable to hard sphere potentials in higher dimensions and to the non-Markovian kinetic equations corresponding to these potentials. For the non-Markovian case with a hard sphere potential where $f^{(2)}(1,2;t)$ is expressed in the form $f^{(2)}(1,2;t) = \rho_2(1,2)h_0(v_2)f^{(1)}(1;t) + \int_0^t dt'\ M(1,2;t-t')f^{(1)}(1;t')$, a Volterra integral equation of the convolution type is obtained for $h_\delta^{(1)}$. This may be solved using Laplace transform techniques. For example in the one dimensional case, retaining the three body terms in the equation derived by Anstis [43], we obtain for the Laplace transform $\hat{h}_\delta^{(1)}(s)$ of $h_\delta^{(1)}(t)$ an expression of the form

$$\hat{h}_\delta^{(1)}(s) = \frac{h_\delta^{(1)}(0)}{s+n\alpha(v')-n^2\gamma(v',s)} \quad . \tag{5.6}$$

The r.h.s. has a branch along the negative real axis and poles in the negative half-plane. Asymptotic contributions to $h_\delta^{(1)}(t)$ for large $t$ may be determined using Plemelj type relations.

# APPENDIX A

To be amenable to physical interpretation, the r.d.f.'s must satisfy several constraints. These must of course be satisfied by the initial conditions. This being the case, it is then possible to show that, under time evolution governed by the hierarchy equations, these constraints are satisfied for all times. Existence, uniqueness and boundedness of the solutions of the hierarchy equations shall be assumed here. These results may be obtained rigorously by a suitable adaptation of the function-analytic techniques of Chapter 3.

(i) Asymptotic Liouville Property

$$\lim_{\epsilon\to 0} f_j^{(n)}(x_1^{\pm},v_2;x_1,v_1;z_3;\ldots;z_n;t)$$

$$= \lim_{\epsilon\to 0} f_j^{(n)}(x_1,v_1;x_1^{\mp},v_2;z_3;\ldots;z_n;t)$$

$$\text{where } x_1^{\pm} = x_1 \pm \epsilon\,\mathrm{sgn}(v_2-v_1)$$

As indicated in Chapter 2, this result is a consequence of the properties of the n-particle Liouville operator appearing on the r.h.s. of the hierarchy equation for $f_j^{(n)}$ and the nature of the dynamics for this system (a pair of particles interchange velocities upon collision).

(ii) Impenetrability Condition

$$\lim_{\epsilon\to 0} f_j^{(n)}(x_1\pm\epsilon, v_2; x_1, v_1; z_3; \ldots; z_n; t)$$

$$= \lim_{\epsilon\to 0} f_{j\mp 1}^{(n)}(x_1, v_1; x_1\pm\epsilon, v_2; z_3; \ldots; z_n; t)$$

To prove this result, we suppose that the $f_j^{(n)}$ are decomposable at t = 0 as appropriate sums over $f_{i1\ i2\ \ldots\ in}^{(n)}$ (the n-particle r.d.f.'s for particles i1 i2 ... in) with i1 = j (cf. (2.9)), i.e. we must have physical initial conditions. We examine the appropriate equations for $f_{i1\ i2\ \ldots\ in}^{(n+m)} = \sum_{\substack{j\alpha\neq j\beta\ \alpha\neq\beta \\ j\alpha\neq i\beta}} f_{i1\ \ldots\ in\ j1\ \ldots\ jm}^{(n+m)}$ and then obtain the required result for $f_j^{(n)}$ by summation over i2,...,in. From (2.7)

$$\left(\frac{\partial}{\partial t} + K_{i1\ i2\ \ldots\ in}^{(n+m)}\right) f_{i1\ i2\ \ldots\ in}^{(n+m)}(z_1; \ldots; z_{n+m}; t)$$

$$= \sum_{\alpha=1}^{n} \lim_{\epsilon\to 0} \int_{-\infty}^{+\infty} dv\,|v-v_1|\cdot$$

$$\Big(f_{i1\ i2\ \ldots\ in}^{(n+m+1)}(z_1; \ldots; z_n; x_\alpha^+, v; z_{n+1}; \ldots z_{n+m}, t)$$

$$- f_{i1\ i2\ \ldots\ in}^{(n+m+1)}(z_1; \ldots; z_n; x_\alpha^-, v; z_{n+1}; \ldots; z_{n+m}; t)\Big)$$

where $x_\alpha^\pm = x_\alpha \pm \epsilon\ \mathrm{sgn}(v-v_1)$ and where we have used symmetry of $f_{i1\ i2\ \ldots\ in}^{(n+m')}$ in the last m' variables. $K_{i1\ i2\ \ldots\ in}^{(n+m)}$ is the (n+m)-particle Liouville operator which takes into account all interactions between the labelled particles $i1 \ldots in$ and interactions between the unlabelled particles and any of $i1 \ldots in$.

<u>support considerations</u>: At $t = 0$, if for example $i1 < i2 < \ldots < in$, then $f^{(n+m)}_{i1\ i2\ \ldots\ in}$ is non-zero only for $x_1 \leqslant x_2 \leqslant \ldots \leqslant x_n$. From the above definition of $K^{(n+m)}_{i1\ i2\ \ldots\ in}$, it is clear that the above equation is invariant on such ordered regions of phase space. So the above constraint on supp $f^{(n+m)}_{i1\ i2\ \ldots\ in}$ extends to times $t > 0$.

<u>representation of $f^{(n)}_{i1\ i2\ \ldots\ in}$</u>: If we consider the two hierarchies of functions $f^{(n+m)}_{i1\ i2\ \ldots\ in}(z_1;\ldots;z_{n+m};t)$ and

$$\int dz\, f^{(n+m+1)}_{i1\ i2\ \ldots\ in\ k}(z_1;\ldots;z_n;z;z_{n+1};\ldots;z_{n+m};t)$$

$$+ \sum_{\alpha=n+1}^{n+m} f^{(n+m)}_{i1\ i2\ \ldots\ in\ k}(z_1;\ldots;z_n;z_\alpha;z_{n+1};\ldots;\hat{z}_\alpha;\ldots;z_{n+m};t),$$

they have identical initial conditions and may be shown to satisfy the same set of hierarchy equations. Consequently they are identical for all $t > 0$. In particular

$$f^{(n)}_{i1\ i2\ \ldots\ in}(z_1;\ldots;z_n;t) = \int dz\, f^{(n+1)}_{i1\ i2\ \ldots\ in\ k}(z_1;\ldots;z_n;z;t)$$

<u>$f^{(n)}_{ij}$ as $|x_1-x_2| \to 0$</u>: $f^{(n)}_{ij}$ is decomposable as a sum over $f^{(n)}_{i\,j\ i3\ \ldots\ in}$. Suppose $|i-j| > 1$. Then we may write this sum in two parts. In the first, we suppose that for each

k between i and j that $i\alpha \neq k$, $\alpha = 3,4,\ldots,n$. In this case using the support considerations and representation of $f^{(n)}_{i\,j\,i3\,\ldots\,in}$ mentioned above

$$f^{(n)}_{i\,j\,i3\,\ldots\,in}(z_1;\ldots;z_n;t)$$

$$= \int_{\min(x_1,x_2)}^{\max(x_1,x_2)} dx \int_{-\infty}^{+\infty} dv\ f^{(n+1)}_{ij\ i3\ \ldots\ in\ k}(z_1;\ldots;z_n;z;t)$$

for such k. So $f^{(n)}_{i\,j\,i3\,\ldots\,in}(x_1,v_1;x_1\pm\epsilon,v_2;z_3;\ldots;z_n;t) = O(\epsilon)$ as $\epsilon \to 0$ since $f^{(n)}_{i\,j\,i3\,\ldots\,in\,k}$ is bounded and the delta-function parts will not contribute to the integral.
In the second part of the sum, there exists k between i and j and $\alpha \in \{2,3,\ldots,n\}$ such that $i\alpha = k$. From the support considerations $f^{(n)}_{i\,j\,i3\,\ldots\,in}(x_1,v_1;x_1\pm\epsilon,v_2;z_3;\ldots;z_n;t) = 0$ for $\epsilon$ sufficiently small.

Therefore

$$\lim_{\epsilon\to 0} f^{(n)}_{j}(x_1\pm\epsilon,v_2;x_1,v_1;z_3;\ldots;z_n;t)$$

$$= \lim_{\epsilon\to 0} f^{(n)}_{jj\mp 1}(x_1\pm\epsilon,v_2;x_1,v_1;z_3;\ldots;z_n;t) \tag{*}$$

where we have interchanged the limit and the sum. Since the spatial derivatives of $f^{(n)}_{i\,j\,i3\,\ldots\,in}$ are uniformly bounded, each term in the sum remains either positive or negative for sufficiently small $\epsilon$. Thus we may split the sum into positive and negative convergent parts (in fact the negative part will be empty). Then Dini's theorem may be applied to justify the interchange of the limit and the sum. The impenetrability result follows easily from (*).

(iii) Symmetry Condition (direct verification)

$$f_j^{(n)}(z_1;\ldots;z_\alpha;\ldots;z_\beta;\ldots;t) = f_j^{(n)}(z_1;\ldots;z_\beta;\ldots;z_\alpha;\ldots;t)$$

$$\text{for } \alpha,\beta \in \{2,3,\ldots,n\}$$

We suppose the above is true at $t = 0$. Now $f_j^{(n+m)}(z_1;\ldots;z_\alpha;\ldots;z_\beta;\ldots;t)$ and $f_j^{(n+m)}(z_1;\ldots;z_\beta;\ldots;z_\alpha;\ldots;t)$ for $m \geqslant 0$ satisfy the same hierarchy equations and have identical initial conditions. So by the uniqueness of solutions, they are identical for all times.

(iv) Compatibility Condition

$$f_j^{(n)}(z_1;\ldots;z_n;t) = M_z\, f_j^{(n+1)}(z_1;\ldots;z_n;z;t)$$

where the mean $M_z = \lim_{L'\to\infty}\left(\frac{1}{2\rho L'}\int_{-L'}^{+L'} dx\right)\int_{-\infty}^{+\infty} dv$, $\rho > 0$ is a constant which will in fact be the mean particle number (see Doplicher et al.[88] for a higher dimensional analogue of the mean).

We suppose that the above condition holds at $t = 0$, then show it is true for all time. To achieve this, we simply show that $M_z\, f_j^{(n+m+1)}(z_1;\ldots;z_n;z;z_{n+1};\ldots;z_{n+m};t)$, $m \geqslant 0$ satisfy the same set of hierarchy equations as $f_j^{(n+m)}(z_1;\ldots;z_{n+m};t)$ by applying $M_z$ to the equations

$$\left(\frac{\partial}{\partial t} + K_j^{(n+m+1)}\right) f_j^{(n+m+1)}(z_1;\dots;z_n;z;z_{n+1};\dots;z_{n+m};t)$$

$$= \lim_{\epsilon\to 0} \int_{-\infty}^{+\infty} dv' |v'-v_1| \cdot$$

$$\left(f_{(j)}^{(n+m+2)}(z_1;x_1^-,v';z_2;\dots;z_n;z;z_{n+1};\dots;z_{n+m};t) - f_j^{(n+m+2)}(z_1;x_1^-,v';\dots \quad \dots;z_{n+m};t)\right)$$

where $x_1^- = x_1 - \epsilon \operatorname{sgn}(v'-v_1)$.

If we write $K_j^{(n+m+1)} = K_j^{(n+m)} + v \frac{\partial}{\partial x} - \frac{\partial}{\partial x} \phi(|x-x_1|) \cdot \left(\frac{\partial}{\partial v} + \frac{\partial}{\partial v_1}\right)$, then it is easy to verify that for a suitably well behaved class of functions

$$M_z K_j^{(m+n+1)} = K_j^{(m+n)} M_z$$

Using this identity the required result is easily proved.

(v) Existence of Mean Particle Number, Momentum and Energy

$\sum_{j=-\infty}^{+\infty} f_j^{(1)}(x,v;t)$ for each v and $\int_{-\infty}^{+\infty} dv\, v^k \sum_{j=-\infty}^{+\infty} f_j^{(1)}(x,v;t)$ for $k = 0,1,2$ should be (c-1) summable to positive constants on $x \in (0,\infty)$ and $(-\infty,0)$.

$$\text{Now } \left(\frac{\partial}{\partial t} + K_j^{(n)}\right)\left(\sum_{j=-\infty}^{+\infty} f_j^{(n)}(z_1;\dots;z_n;t)\right) = 0$$

$$\text{so } \sum_{j=-\infty}^{+\infty} f_j^{(n)}(z_1(t);\dots;z_n(t);t) = \sum_{j=-\infty}^{+\infty} f_j^{(n)}(z_1(0);\dots;z_n(0);0)$$

where the characteristics of $\left(\frac{\partial}{\partial t} + K_j^{(n)}\right)$ are given by $(z_j(t),t)$. In particular

$$\sum_{j=-\infty}^{+\infty} f_j^{(1)}(x_1,v_1;t) = \sum_{j=-\infty}^{+\infty} f_j^{(1)}(x_1-v_1t,v_1;0)$$

If we suppose (c-1) summability holds for the initial conditions, then the above identity automatically guarantees (c-1) summability for $\sum_{j=-\infty}^{+\infty} f_j^{(1)}(x,v,t)$ for each v. (c-1) summability of the other expressions also holds as may be proved using a suitable upper bound on initial conditions and the Lebesgue dominated convergence theorem to show that

$$\lim_{L'\to\infty} \frac{1}{L'} \int_0^{L'} dx \int_{-\infty}^{+\infty} dv \sum_{j=-\infty}^{+\infty} f_j^{(1)}(x-vt,v;0)$$

$$= \int_{-\infty}^{+\infty} dv \lim_{L'\to\infty} \frac{1}{L'} \int_0^{L'} dx \sum_{j=-\infty}^{+\infty} f_j^{(1)}(x-vt,v;0)$$

(vi) <u>Normalization of $f_j^{(1)}$</u>

$$\int dz_1\; f_j^{(1)}(z_1;t) = 1 \quad \text{for all } t > 0$$

From the first hierarchy equation

$$\frac{\partial}{\partial t}\left(\int dz_1 f_j^{(1)}(z_1;t)\right)$$

$$= \int dx_1 \lim_{\epsilon\to 0} \int dv_1 \int dv_2\; |v_2-v_1|\cdot$$

$$\left(f_j^{(2)}(x_1^-,v_2;x_1,v_1;t) - f_j^{(2)}(x_1,v_1;x_1^-,v_2;t)\right)$$

and since

$$\int dv_1 \int dv_2 \ |v_2 - v_1| \cdot f_j^{(2)}(x_1, v_1; x_1^-, v_2; t)$$

$$= \int dv_1 \int dv_2 \ |v_2 - v_1| \cdot f_j^{(2)}(x_1, v_2; x_1^+, v_1; t)$$

the above integral is clearly zero using (i) and the Lebesgue dominated convergence theorem to justify the interchange of $\lim_{\epsilon \to 0}$ and $\int dv_1 \int dv_2$.

## APPENDIX B

We show that $D^{reg}_{\beta,1(\infty)}$ are Banach spaces with respect to the appropriate norms. The proof effectively combines the proofs of completeness of bounded, piecewise continuous functions (with fixed discontinuities) under the ess sup norm and of the sequence spaces $\iota^1$ $(\iota^\infty)$. The proofs that $D^{\delta}_{\beta,1(\infty)}$ are Banach spaces may be constructed similarly.

(i) Consider the space of bounded, piecewise continuous functions (with discontinuities at fixed $x_i - v_i t$) denoted by $\left(\overline{H}^{(n)}_{\sim reg}\right)_j (z_1;\ldots;z_n)$ such that

$$\left\| \left(\overline{H}^{(n)}_{\sim reg}\right)_j \right\|^{reg}_{j,n} = \underset{\substack{x_i \quad i \geq 1 \\ v_i \quad i \geq 2}}{\text{ess sup}} \left| \frac{\left(\overline{H}^{(n)}_{\sim reg}\right)_j (z_1;\ldots;z_n)}{\overline{f}^{(1)}_{j+\delta j}\left(x_1{}^1{}_{max}, v_1; 0\right) \prod_{i=2}^{n} \rho h_0(v_i)} \right| < \infty$$

If we consider a Cauchy sequence $\left\{\left(\overline{H}^{(n)}_{\sim reg}\right)^m_j\right\}^\infty_{m=1}$, the corresponding analysis for continuous functions under the sup norm may be adapted to show that this sequence converges pointwise to a function $\left(\overline{H}^{(n)}_{\sim reg}\right)_j$ say (except possibly on a fixed set of discontinuities). We may then show that $\left(\overline{H}^{(n)}_{\sim reg}\right)_j$ is an element of the above space and that

$$\left\| \left(\overline{H}^{(n)}_{\sim reg}\right)^m_j - \left(\overline{H}^{(n)}_{\sim reg}\right)_j \right\|^{reg}_{j,n} \to 0 \text{ as } m \to \infty$$

(ii) Consider a direct sum of "P + 1" Banach spaces of the type considered in (i). Elements of this space are denoted by

$$\bar{H}^{(n)}_{\sim reg} = \begin{bmatrix} \bar{H}^{(n)}_{reg\ 0} \\ \bar{H}^{(n)}_{reg\ 1} \\ \cdot \\ \cdot \\ \cdot \\ \bar{H}^{(n)}_{reg\ P} \end{bmatrix}$$

With a choice of norm

$$\| \bar{H}^{(n)}_{\sim reg} \|^{reg}_{n} = \max_{0 \leq j \leq P} \| \left( \bar{H}^{(n)}_{\sim reg} \right)_j \|^{reg}_{j,n}$$

this space is automatically Banach.

(iii) Consider the space $D^{reg}_{\beta,\infty}$. If $\{\bar{H}_{\sim reg\ m}\}_{m=1}$ is a Cauchy sequence in $D^{reg}_{\beta,\infty}$, then from (ii) it follows that the sequence converges componentwise to $\bar{H}_{\sim reg}$. By analogy with the corresponding proof for $\iota^{\infty}$, we may show that $\bar{H}_{\sim reg} \in D^{reg}_{\beta,\infty}$ and that $\| \bar{H}_{\sim reg\ m} - \bar{H}_{\sim reg} \|^{reg}_{\beta,\infty} \to 0$ as $m \to \infty$.

(iii)' Consider the space $D^{reg}_{\beta,1}$. An adaptation of (iii) modelled on the proof of completeness of $\iota^{1}$ shows that $D^{reg}_{\beta,1}$ is Banach.

## APPENDIX C.

We describe here the meaning of the expression

$$\underset{\sim}{f}_{reg}(s) = \sum_{m=o}^{\infty} \left( \int_o^s ds_m \underset{\approx}{C}(s_m) \int_o^{s_m} ds_{m-1} \underset{\approx}{C}(s_{m-1}) \ldots \int_o^{s_2} ds_1 \underset{\approx}{C}(s_1) \right) \underset{\sim}{f}_{reg}(s=o) \tag{C1}$$

appearing in 3.2 and in a specialized form in 2.6. This is essentially a solution of the hierarchy equations by interation and successive terms in the above expression are obtained from successive iterations*. Let the characteristics of $\left(\frac{\partial}{\partial t} + K_j^{(m)}\right)$ be parameterized as previously by

$$z_i = z_i^m \,(s, z_{j,o}^m) \quad i,j = 1,2,\ldots,m \;;\; t=s$$

where $z_i^m \,(o, z_{j,o}^m) = z_{i,o}^m$

Now

$$\begin{aligned} & f_{regj}^{(n)} \left(z_1^n \,(s, z_{k,o}^n); \ldots; z_n^n \,(s, z_{k,o}^n) \;;\; s\right) \\ = \; & f_{regj}^{(n)} \left(z_1^n \,(o, z_{k,o}^n); \ldots; z_n^n \,(o, z_{k,o}^n) \;;\; o\right) \\ + \; & \int_o^s ds_1 \lim_{\epsilon \to o} \int_{-\infty}^{+\infty} dv_{n+1} \left| v_{n+1} - v_1^n \,(s_1, z_{k,o}^n)\right| \\ \times \; & \left\{ f_{reg(j)}^{(n+1)} \left(z_1^n(s_1, z_{k,o}^n);\; x_1^n(s_1, z_{k,o}^n)^-, v_{n+1}; z_2^n(s_1, z_{k,o}^n); \ldots; s_1\right) \right. \\ & \left. - f_{regj}^{(n+1)} \left(z_1^n(s_1, z_{k,o}^n); \ldots \ldots; s_1\right) \right\} \end{aligned} \tag{C2}$$

where $(x_1^n)^- = x_1^n - \epsilon \,\mathrm{sgn}(v_{n+1} - v_1^n)$

and

$$f_{regj'}^{(n+1)} \left(z_1^n(s_1, z_{k,o}^n);\; x_1^n(s_1, z_{k,o}^n)^-,\; v_{n+1}; z_2^n(s_1, z_{k,o}^n); \ldots; s_1\right)$$

---

* For convenience we neglect the jump condition here.

$$= f^{(n+1)}_{regj'}\left(z_1^{n+1}(o,z_{k,o}^{n+1});\ z_{n+1}^{n+1}(o,z_{k,o}^{n+1});\ z_2^{n+1}(o,z_{k,o}^{n+1});\ldots;o\right)$$

$$+ \int_o^{s_1} ds_2 \lim_{\epsilon\to o} \int_{-\infty}^{+\infty} dv_{n+2} \left| v_{n+2} - v_1^{n+1}(s_2;z_{k,o}^{n+1})\right|$$

$$\times \left\{ f^{(n+2)}_{reg(j')}\left(z_1^{n+1}(s_2,z_{k,o}^{n+1});x_1^{n+1}(s_2,z_{k,o}^{n+1})^-,v_{n+2};z_{n+1}^{n+1}(s_2,z_{k,o}^{n+1});\right.\right.$$

$$\left. z_2^{n+1}(s_2,z_{k,o}^{n+1});\ldots;s_2\right)$$

$$\left. - f^{(n+2)}_{regj'}\left(z_1^{n+1},(s_2;z_{k,o}^{n+1});\ldots \ldots;s_2\right)\right\}$$

(C3)

where $z_i^{n+1}(s_1,z_{k,o}^{n+1}) = z_i^n(s_1;z_{k,o}^n) \quad i = 1,2,\ldots,n$

$$z_{n+1}^{n+1}(s_1,z_{k,o}^{n+1}) = \left(x_1^n(s_1,z_{k,o}^n)^-,\ v_{n+1}\right) \qquad \text{(C4)}$$

and $(x_1^{n+1})^- = x_1^{n+1} - \epsilon\, \mathrm{sgn}(v_{n+1}-v_1^{n+1})$

The $m = o$ term of (C1) is given by the first term on the r.h.s. of (C2). If (C3) is substituted into the second term of (C2), then the $m = 1$ term of (C1) involving $f^{(n+1)}_{reg(j)}(\ldots;o)$ and $f^{(n+1)}_{regj}(\ldots;o)$ appears.

The terms $m \geqslant 2$ of (C1) may be obtained in a similar way.

The above results may be applied in section 2.6 where the characteristics of $\left(\frac{\partial}{\partial t} + K_j^{(m)}\right)$ have the simplified form

$$x_i = v_{i,o}s + x_{i,o}$$

$$v_i = v_{i,o}$$

$$t = s$$

# APPENDIX D

## SPECTRAL ANALYSIS OF $\underset{\approx}{C}_o^\delta$ IN $\iota^2$

A direct sequence space analysis may be employed noting that $\iota^2$ is a reflexive space (and in fact a Hilbert space). This enables us to make more specific statements about the spectrum from the general theory. However here we shall develop alternative methods. Let $L^2(o,2\pi)$ be the (Hilbert) space of Lebesgue square integrable functions on $[o,2\pi]$. This space is congruent to $\iota^2$ i.e. there exists an isometric isomorphism $J : \iota^2 \to L^2(o,2\pi)$. If $\underset{\sim}{y} \in \iota^2$ then it may be represented by a function $Y = J\underset{\sim}{y} \in L^2(o,2\pi)$ and a bounded linear operator $\underset{\approx}{G}$ on $\iota^2$ is represented by a bounded linear operator $G = J\underset{\approx}{G}J^{-1}$ on $L^2(o,2\pi)$. Using the isometric and isomorphic properties of J, it is easy to show that $\sigma(G) = \sigma(\underset{\approx}{G})$, or more specifically that $P\sigma(G) = P\sigma(\underset{\approx}{G})$, $C\sigma(G) = C\sigma(\underset{\approx}{G})$ and $R\sigma(G) = R\sigma(\underset{\approx}{G})$.

Next let us determine the operator $C_o^\delta$ on $L^2(o,2\pi)$ corresponding to the matrix operator $\underset{\approx}{C}_o^\delta$ on $\iota^2$. J may be realized in the following way. For any $\underset{\sim}{y} \in \iota^2$, $Y = J\underset{\sim}{y} \in L^2(o,2\pi)$ is given by

$$Y(\eta) = \sum_{j=-\infty}^{+\infty} e^{\hat{i}j\eta} y_j \qquad \eta \in [o,2\pi]$$

Let $\underset{\sim}{y} = \underset{\approx}{C}_o^\delta \underset{\sim}{x}$, then in component form this equation becomes

$$y_j = \gamma_{\rho h} x_{j-1} + \beta_{\rho h} x_{j+1}$$

Applying the transform $\sum_{j=-\infty}^{+\infty} e^{\hat{i}j\eta}$. to this equation gives

$$Y(\eta) = (\gamma_{\rho h} e^{\hat{i}\eta} + \beta_{\rho h} e^{-\hat{i}\eta}) \,.\, X(\eta) \qquad \eta \in [o,2\pi]$$

where $Y = J\underset{\sim}{y}$ and $X = J\underset{\sim}{x}$. We conclude that $C_o^\delta$ is given by the normal, multiplicative operator

$$C_o^\delta = \gamma_{\rho h} e^{\hat{i}\eta} + \beta_{\rho_h} e^{-\hat{i}\eta} \qquad \eta \in [o,2\pi]$$

Such an operator is called a factor transform and a sufficient condition for it to be a bounded linear operator on $L^2(o,2\pi)$ is that it be essentially bounded and measurable as a function of $\eta$ on $[o,2\pi]$. (c.f. Hille[63] for the $L^2(-\infty,+\infty)$ case). Thus $C_o^\delta$ satisfies the required condition.

Let $E = \{\lambda \in C \;:\; \lambda = \gamma_{\rho h} e^{\hat{i}\theta} + \beta_{\rho h} e^{-\hat{i}\theta} \;:\; \theta \in [o;2\pi)\}$ if $\lambda \notin E$, then $\lambda - C_o^\delta$ is continuous and bounded away from zero for $\eta \in [o,2\pi]$. Consequently $\lambda - C_o^\delta$ is invertible and therefore $\lambda \notin \sigma(C_o^\delta)$. So $\sigma(C_o^\delta) \subseteq E$. From the general theory of normal operators $R\sigma\,(C_o^\delta) = \emptyset$ (see Dunford and Schwartz[52]). Thus it remains to determine $P\sigma(C_o^\delta)$ and $C\sigma(C_o^\delta)$.

Suppose $\lambda \in E$ and $(\lambda - C_o^\delta).X(\eta) = o$ in $L^2[o,2\pi]$. Since $\lambda - C_o^\delta$ is a continuous function of $\eta$ and only equal to zero at one point $\eta = \lambda$, it follows that $X(\eta) = o$ a.e. is the only $L^2(o,2\pi)$ solution of the above equation. Thus $P\sigma(C_o^\delta) = \emptyset$.

Again choose $\lambda \in E$, specifically $\lambda = \gamma_{\rho h} e^{\hat{i}\eta^*} + \beta_{\rho h} e^{-\hat{i}\eta^*}$ for some $\eta^* \in [o,2\pi)$ and let $Y(\eta) \in L^2(o,2\pi)$ be continuous and non-zero at $\eta = \eta^*$. Suppose

$$Y(\eta) = (\lambda - C_o^\delta) X(\eta)$$

where $\eta \in [o,2\pi)$. Then $X(\eta) = Y(\eta) / (\lambda - \gamma_{\rho h} e^{\hat{i}\eta} - \beta_{\rho h} e^{-\hat{i}\eta})$ $\notin L^2(o,2\pi)$. $\lambda - C_o^\delta$ is not invertible, so $\lambda \in \sigma(C_o^\delta)$.

In conclusion

$$P\sigma(C_o^\delta) = P\sigma(\underset{\approx}{C}_o^\delta) = \emptyset = R\sigma(C_o^\delta) = R\sigma(\underset{\approx}{C}_o^\delta)$$

and $$C\sigma(C_o^\delta) = C\sigma(\underset{\approx}{C}_o^\delta) = E$$

## APPENDIX E

We consider here an asymptotic analysis of the expression

$$\sum_{m=-\infty}^{+\infty} \int_o^{\frac{L}{t}} dv_k h(v_k+\frac{mL}{t})\; e^{-\hat{\imath}mu}\cdot\hat{Q}[u,v_kt,t]\cdot[\frac{1}{L}\int_o^L dx_n R[u,v_kt-x_n,t]]^{N-2}$$

$$= \int_o^{\frac{L}{t}} dv_k\cdot(\sum_{m=-\infty}^{+\infty} \frac{t}{L}\, e^{-\hat{\imath}(2\pi m-u)\cdot\frac{v_kt}{L}}\, e^{-\frac{1}{2}(\frac{v_{th}t}{L})^2\cdot(2\pi m-u)^2})$$

$$\times \sum_{n=-\infty}^{+\infty} -\frac{t}{L}v_{TH}{}^2(e^{\hat{\imath}u}-1)\, e^{-\hat{\imath}(2\pi n-u)\cdot\frac{v_kt}{L}}\, e^{-\frac{1}{2}(\frac{v_{th}t}{L})^2(2\pi n-u)^2})$$

$$\times \prod_{i=1}^{N-2} (\sum_{p_i=-\infty}^{+\infty} \frac{2(1-\cos u)}{(2\pi p_i-u)^2}\, e^{-\hat{\imath}(2\pi p_i-u)\cdot\frac{v_kt}{L}}\, e^{-\frac{1}{2}(\frac{v_{th}t}{L})^2(2\pi p_i-u)^2})$$

$$= -\;(\frac{v_{th}t}{L})^2(e^{\hat{\imath}u}-1)(2(1-\cos u))^{N-2}$$

$$\times \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \sum_{\substack{p_i=-\infty \\ i\epsilon\{1,2,\ldots,N-2\}}}^{+\infty} \left(\prod_{i=1}^{N-2} \frac{1}{(2\pi p_i-u)^2}\right)$$

$$\times \int_o^{\frac{L}{t}} dv_k\; e^{-\hat{\imath}\frac{v_kt}{L}((2\pi m-u)+(2\pi n-u)+\sum_{i=1}^{N-2}(2\pi p_i-u))}$$

$$\times\; e^{-\frac{1}{2}(\frac{v_{th}t}{L})^2((2\pi m-u)^2+(2\pi n-u)^2+\sum_{i=1}^{N-2}(2\pi p_i-u)^2)}\;.$$

We should note that the integral over $v_k$ is zero iff

$$(2\pi m-u) + (2\pi n-u) + \sum_{i=1}^{N-2} (2\pi p_i-u) = 2\pi\kappa$$

with $\kappa$ a non-zero integer. So the problem is to minimize

$$(2\pi m-u)^2 + (2\pi n-u)^2 + \sum_{i=1}^{N-2} (2\pi p_i-u)^2$$

where $m, n, p_i$ are integers and $u \varepsilon \{\frac{2\pi}{N}\cdot l \;:\; l = 1,2,\ldots,N-1\}$ and where the integral over $v_k$ is non-zero. We list the solutions to this problem below:

(a) $u = \frac{2\pi}{N}$ and $m=1,\ n=0,\ p_i=0$

or $m=0,\ n=1,\ p_i=0$

or $m=0,\ n=0,\ p_{i^*}=1$ for some $i^* \varepsilon \{1,2,\ldots,N-2\}$

$p_i = 0$ for $i \neq i^*$ .

(b) $u = \frac{2\pi}{N} \cdot (N-1)$ and $m=0,\ n=1,\ p_i=1$

or $m=1,\ n=0,\ p_i=1$

or $m=1,\ n=1,\ p_{i^*}=0$ for some $i^* \varepsilon \{1,2,\ldots,N-2\}$

$p_i = 1$ for $i \neq i^*$ .

The contributions of solutions from (b) to $\langle v_1(o)v_j(t)\rangle_{N,L}$ are complex conjugate to the corresponding contributions of solutions from (a).

A similar analysis is applicable to expressions of the form

$$\sum_{m=-\infty}^{+\infty} \int_o^{\frac{L}{t}} dv_1 \left(v_1+\frac{mL}{t}\right)^2 h\left(v_1+\frac{mL}{t}\right) e^{-\hat{\imath}mu} \cdot \left\{\frac{1}{L} \int_o^L dx_n R[u, v_1 t - x_n]\right\}^{N-1} .$$

# APPENDIX F

We shall consider here expressions of the form

$$\text{(I)} \quad \frac{1}{x}\int_o^x dx_n \underset{\sim}{R}[u,w,x_n,t] \quad \text{and}$$

$$\text{(II)} \quad \frac{1}{L-x}\int_x^L dx_n \underset{\sim}{R}[u,w,x_n,t]$$

where

$$\underset{\sim}{R}[u,w,x_n,t] = \int_{-\infty}^{+\infty} dv_n h(v_n) \prod_{\pm} \underset{\sim}{S}[u,w\pm(x_n+v_nt)]$$

Since $\underset{\sim}{S}[u,w]$ is separately continuous in the first variable and piecewise continuous in the second, it follows that $\underset{\sim}{R}[u,w,x_n,t]$ is continuous in the variables $w$ and $x_n$. From this result follows the continuity of (I) and (II) with respect to $(w,x)$ on $(-\infty,+\infty) \times [0,L]$. Also from (3.3),

$$\underset{\sim}{R}[u,w+2L,x_n,t] = e^{2\hat{\imath}u} \underset{\sim}{R}[u,w,x_n,t]$$

and an analogous result holds for (I) and (II).

We shall examine the asymptotic behaviour of (I) for large $t$. Results for (II) follow using the formula:

$$\frac{1}{L-x}\int_o^L dx_n \; \underset{\sim}{R}[u,w,x_n,t] = \frac{L}{L-x}\left(\frac{1}{L}\int_o^L dx_n \; \underset{\sim}{R}[u,w,x_n,t]\right)$$

$$- \frac{x}{L-x}\left(\frac{1}{x}\int_o^x dx_n \; \underset{\sim}{R}[u,w,x_n,t]\right)$$

Clearly it is necessary only to examine (I) for $w \in [0,2L]$. In so doing, it is most convenient to examine several separate subcases.

(A) $w \in \left[0, \frac{L}{2}\right]$. We first calculate

$$\underset{\sim}{F}[u,x,w,v_nt] = \frac{1}{x}\int_o^x dx_n \prod_{\pm} \underset{\sim}{S}[u,w\pm(x_n+v_nt)].$$

A number of subcases are enumerated. In the following $H(\ )$ denotes the Heaviside step function

(i) $0 < v_n t < w$ :

$$\underset{\sim}{F} = H(x-(w-v_n t))e^{2\hat{\imath}u}\left[\frac{(w-v_n t)+(x-(w-v_n t))e^{-\hat{\imath}u}}{x}\right]$$

$$+H((w-v_n t)-x)\ e^{2\hat{\imath}u}.$$

(ii) $w < v_n t < L - w$ : $\underset{\sim}{F} = e^{2\hat{\imath}u}$ .

(iii) $L - w < v_n t < L + w$ :

$$\underset{\sim}{F} = H(x-(2L-w-v_n t))\ e^{2\hat{\imath}u}\left[\frac{(2L-w-v_n t)e^{-\hat{\imath}u}+(x-(2L-w-v_n t))}{x}\right]$$

$$+ H((2L - w - v_n t) - x)\ e^{2\hat{\imath}u}.$$

(iv) $L + w < v_n t < 2L - w$ :

$$\underset{\sim}{F} = H(x-(2L-v_n t+w))\ e^{2\hat{\imath}u}\left[\frac{2w+(x-2w)e^{-\hat{\imath}u}}{x}\right]$$

$$+ H((2L-v_n t+w)-x))H(x-(2L-w-v_n t))\ e^{2\hat{\imath}u}$$

$$\times\ \left[\frac{(2L-w-v_n t)e^{-\hat{\imath}u}+x-(2L-w-v_n t)}{x}\right]$$

$$+ H((2L - w - v_n t) - x)\ e^{2\hat{\imath}u}.$$

(v) $2L - w < v_n t < 2L$ :

$$\underset{\sim}{F} = H(x-(2L-v_n t+w))\ e^{2\hat{\imath}u}\ \left[\frac{(2L+w-v_n t)+(x-(2L+w-v_n t))e^{-\hat{\imath}u}}{x}\right]$$

$$+ H((2L - v_n t + w)-x)e^{2\hat{\imath}u}$$

From these results, we can write down an expression for

$$\frac{1}{x}\int_0^x dx_n\ \underset{\sim}{R}[u,w,x_n,t] = \int_{-\infty}^{+\infty} dv_n h(v_n)\ \underset{\sim}{F}[u,x,w,v_n t].$$

The integral over an infinite velocity range may be converted to a sum of integrals over a finite range. Using a Poisson sum formula, the dominant term as $t \to \infty$ may be extracted.

(B) $w \in \left[\frac{L}{2}, L\right]$. A similar analysis is necessary for this case.

(C) $w \in \left[L, \frac{3L}{2}\right]$ and (D) $w \in \left[\frac{3L}{2}, 2L\right]$. The results for these cases may be obtained from (A) and (B) as follows. Using (3.3) and the identity $\underset{\sim}{S}[u,-w] = e^{\hat{\imath}u} \underset{\sim}{S}[-u,w]$, we may prove that

$$\underset{\sim}{F}[u,x,2L - w,v_n t] = e^{4\hat{\imath}u} \underset{\sim}{F}[-u,x,w,v_n t] .$$

So

$$\frac{1}{x} \int_o^x dx_n \ \underset{\sim}{R}[u,2L-w,x_n,t] = e^{4\hat{\imath}u} \frac{1}{x} \int_o^x dx_n \ \underset{\sim}{R}[-u,w,x_n,t] .$$

# APPENDIX G

THEOREM 1 Let $T_s^{r-1}(k) = (-1)^s \binom{r}{s}(k+s-1)(k+s-2)\ldots(k+s-r+1)$ for $k \geqslant r$, then $\sum_{s=0}^{r} T_s^{r-1}(k) = 0$.

PROOF We show first by induction that for $0 \leqslant t \leqslant r-1$

$$\sum_{s=0}^{t} T_s^{r-1}(k) = (-1)^t \binom{r-1}{t}(k+t)(k+t-1)\ldots(k+1)(k-1)\ldots$$

$$\ldots(k+t-r+1) \qquad \text{(G.1)}$$

with a suitable interpretation for the cases $t = 0$ and $t = r-1$. The result of the theorem is then obvious since

$$\sum_{s=0}^{r-1} T_s^{r-1}(k) = -T_r^{r-1}(k) \quad . \qquad \text{(G.2)}$$

(G.1) is clearly true for $t = 0$. So assuming (G.1) true for $t = w$, we prove that it is true for $t = w+1$ $(0 \leqslant w \leqslant r-2)$.

Now

$$\sum_{s=0}^{w+1} T_s^{r-1}(k) = \sum_{s=0}^{w} T_s^{r-1}(k) + T_{w+1}^{r-1}(k)$$

$$= (-1)^{w+1}(k+w)(k+w-1)\ldots(k+1)(k-1)\ \ldots$$

$$\ldots\ (k+w-r+2)\left(\binom{r}{w+1}k-\binom{r-1}{w}(k+w-r+1)\right).$$

Since $\binom{r}{w+1}-\binom{r-1}{w} = \binom{r-1}{w+1}$ and $(r-w+1)\binom{r-1}{w} = (w+1)\binom{r-1}{w+1}$, we have $\binom{r}{w+1}k-\binom{r-1}{w}(k+w-r+1) = \binom{r-1}{w+1}(k+w+1)$. So the desired result is obtained.

<u>THEOREM 2</u> Let $\hat{T}_s^{r-1}(k) = (-1)^t \binom{r}{r-k+t} r(r+1)\dots(r+t-1).k(k-1)\dots$ $\dots(t+1)$ for $r > k$ with a suitable interpretation for the cases $t = 0$ and $t = k$. Then $\sum_{s=0}^{k} \hat{T}_s^{r-1}(k) = 0$.

<u>PROOF</u> We show first by induction that for $0 \leqslant t \leqslant k-1$

$$\sum_{s=0}^{t} \hat{T}_s^{r-1}(k) = (-1)^t \binom{r-1}{r-k+t} (r+t)(r+t-1)\dots$$

$$\dots r.(k-1)(k-2)\dots(t+1)$$

with a suitable interpretation for the case $t = k-1$. The result of the theorem is then obvious since

$$\sum_{s=0}^{k-1} \hat{T}_s^{r-1}(k) = - \hat{T}_k^{r-1}(k) \quad .$$

The analysis for the proof by induction is rather similar to the above theorem and is thus omitted.

# APPENDIX H

Methods similar to those implemented in chapter 6 are used here to solve the non-linear elimination problem studied by Cohen [9] . The problem is stated below. For $s = 1,2,...$

$$G^s(1,2,\ldots,s;t) = (U^s(1,2,\ldots,s;t)\prod_{i=1}^{s} U^1(i;t)^{-1})\prod_{i=1}^{s} D^1(i;t)$$

$$+ \frac{\rho}{1!}\int d\underline{z}_{s+1}(U^{s+1}(1,2,\ldots,s+1;t)\prod_{i=1}^{s+1} U^1(i;t)^{-1})\prod_{i=1}^{s+1} D^1(i;t)$$

$$+ \frac{\rho^2}{2!}\int d\underline{z}_{s+1}\int d\underline{z}_{s+2}(U^{s+2}(1,2,\ldots,s+2;t)\prod_{i=1}^{s+2} U^1(i;t)^{-1})$$

$$\times \prod_{i=1}^{s+2} D^1(i;t)$$

$$+ \ldots.$$

Our aim is to take these equations for $s = 1$ and $s = 2$ and to eliminate $D^1(\ ;t)$ thus obtaining an expression for $G^2(\ ;t)$ in terms of $G^1(\ ;t)$.

Using graph theoretic techniques, Cohen has given the solution

$$G^2(1,2\ ;t) = \sum_{\ell=0}^{\infty} \rho^\ell \int d\underline{z}_3 \ldots \int d\underline{z}_{2+\ell}\ T^{2+\ell}_{irred}(1,2\ |3,\ldots,2+\ell;t)$$

$$\times \prod_{i=1}^{2+\ell} G^1(i;t)$$

where $T^{2+\ell}_{irred}(1,2\ |\mathcal{L};t)$ is equal to the sum over all distinct labelled (1,2)-irreducible graphs of $2+\ell$ points with labels chosen from $\{1,2,\mathcal{L}\}$. The same ordering and labelling convention for operators associated with trees as developed in chapter 6 may be adopted. Here we set the sum of all labelled Husimi trees of n-points equal to $\mathcal{U}^n(1,2,\ldots,n;t) = U^n(1,2,\ldots,n;t)\prod_{i=1}^{n} U^1(i;t)^{-1}$. Our aim is to express $\mathcal{T}^{2+\ell}_{irred}(1,2|\mathcal{L};t)$ in terms of cluster operators. The following relation is obvious from the graph theoretic interpretation (c.f. (4.2) of chapter 6)

$$\mathcal{T}^n_{irred}(1,2\ |3,\ldots,n;t) = \mathcal{U}^n(1,2,\ldots,n;t)$$

$$- \Big\{\mathcal{T}^{n-1}_{irred}(1,2|3,\ldots,n-1;t)\,(\mathcal{U}^2(1,n;t)+\mathcal{U}^2(2,n;t) + \ldots$$

$$\ldots + \mathcal{U}^2(n-1,n;t) \quad \text{and rearrangements among } 3,4,\ldots,n$$

$$+ \ldots$$

$$+ \mathcal{T}^{n-r}_{irred}(1,2|3,\ldots,n-r,t)$$

$$\times \Big(\sum_{1\leqslant i1\leqslant\ldots\leqslant ir\leqslant n-r}\ \sum_{(n-r+1,\ldots,n\|\phi|\mathcal{L}_1,\ldots,\mathcal{L}_r)_0}$$

$$\times \prod_{\alpha=1}^{r} \mathcal{U}^{1+\ell_\alpha}(i\alpha,\mathcal{L}_\alpha;t) \quad \text{and rearrangements among } 3,4,\ldots,n$$

$$+ \ldots \Big\}$$

An induction argument shows that

$$\mathcal{T}^n_{irred}(1,2\ |3,\ldots,n) = \sum_{\text{linked}} (-1)^{k-1}\mathcal{U}^{2+\ell_1}(1,2,\ldots;t)$$

$$\times \quad \mathcal{U}^{1+\ell_2}(\ldots;t)\ldots\mathcal{U}^{1+\ell_k}(\ldots;t)$$

where $\sum_{i=1}^{k}\ell_i = n-2$ and the sum is over all distinct labelled products of $\mathcal{U}^{\cdot\cdot}(\ )$ operators such that each $\mathcal{U}^{\cdot\cdot}(\ )$ is linked by one argument to one further to the left. Furthermore for each $\mathcal{U}^{\cdot\cdot}(\ )$ there must be a unique chain linking it to $\mathcal{U}^{2+\ell_1}(1,2,\ldots;t)$.

An alternative combinatorial method of solution starts by inverting the equation for $s = 1$. If we write this as

$$G^1(1;t) = D^1(1;t) + \frac{\rho}{1!} C_2(1,2';t)D^1(1;t)D^1(2';t)$$

$$+ \frac{\rho^2}{2!} C_3(1,2',3';t)D^1(1;t)D^1(2';t)D^1(3';t)$$

$$+ \dots$$

then we set

$$D^1(1;t) = G(1;t) + \rho C_2'(1,2';t)G^1(1;t)G^1(2';t)$$

$$+ \rho^2 C_3'(1,2',3';t)G^1(1;t)G^1(2';t)G^1(3';t)$$

$$+ \dots$$

Substitution of the second expression into the first and examination of terms of $n^{th}$ order yields

$$\frac{1}{0!} C_n'(1,2',3',\dots,n';t) + \dots$$

$$+ \frac{1}{j!} C_j'(1,2',\dots,j';t)\left( \sum_{s=1}^{\min(j,n-j)} \sum_{1 \leqslant i_1 \leqslant \dots \leqslant i_s \leqslant j} \sum_{\substack{r_k \\ \sum_{k=1}^{s} r_k = n-j}} \cdot \prod_{k=1}^{s} C_{1+r_k}(i_k', (r_1+\dots+r_{k-1}+1)', \dots, (r_1+\dots+r_k)';t)\right)$$

$$+ \dots$$

$$+ \frac{1}{n!} C_n(1,2',\dots,n';t) = 0.$$

Using this relation as the basis for a proof by induction, we may show that

$$C_n'(1,2',\dots,n';t) \cdot$$

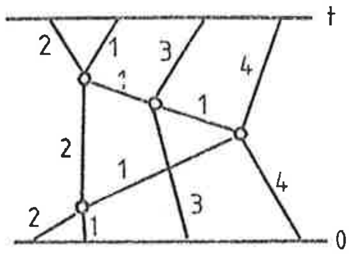
$$= \frac{1}{n!} \int d\underline{z}_2' \dots \int d\underline{z}_n' \sum_{\text{linked}} (-1)^k U^{1+\ell_1}(1,\dots;t)\, U^{1+\ell_2}(\dots;t)$$

$$\times U^{1+\ell_k}(\dots;t) \cdot$$

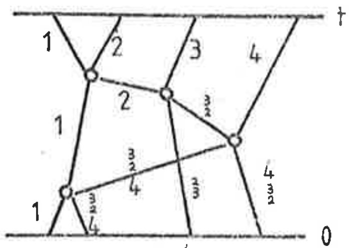
where $\sum_{i=1}^{k} \ell_i = n-1$ and where the sum has the same interpretation as above. On substitution into the equation for $s = 2$, we obtain the same result as above.

# APPENDIX I

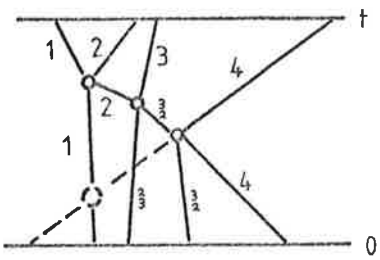
The following is a list of 4-particle collision sequences contributing to $U^4(1,2|3,4;t)h(1,2,3,4)$ for a hard sphere potential. In all diagrams, the possibility of further collisions between 2,3 and 4 is allowed. Where a further collision or collisions involving particle 1 gives a contributing event (not covered by another case), this is mentioned explicitly. In addition to the diagrams shown below, those obtained by interchanging particles 3 and 4 also give contributing events. + (i,j) denotes a further collision between i and j and + ... denotes further collisions still (if possible).

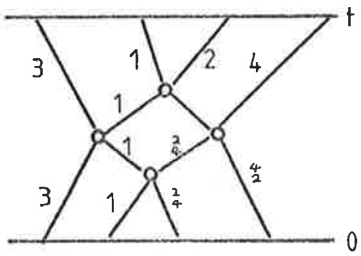


+ (1,4) or (1,3) + ...

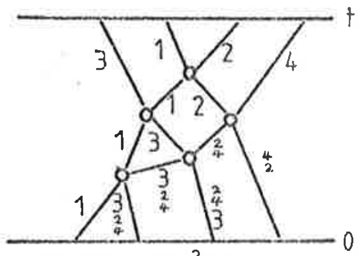


$+ (1, \substack{2\\3}) \text{ or } (1, \substack{4\\3\\2}) + \cdots$

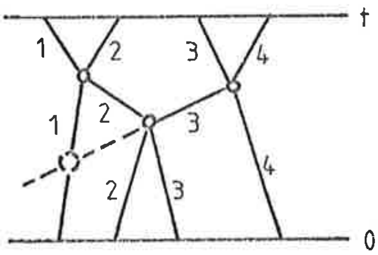


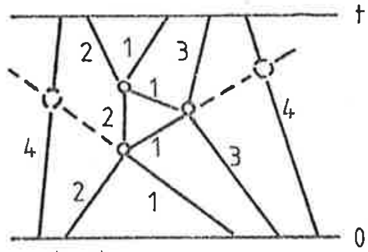


$+ (1,3) \text{ or } (1, \substack{4\\2}) + \cdots$

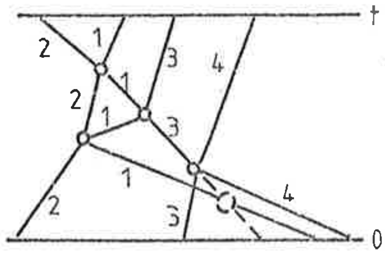


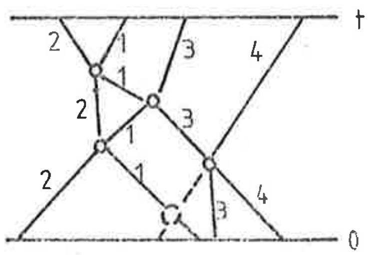
$+ (1, \substack{4\\2}) \text{ or } (1, \substack{2\\4\\3}) + \cdots$

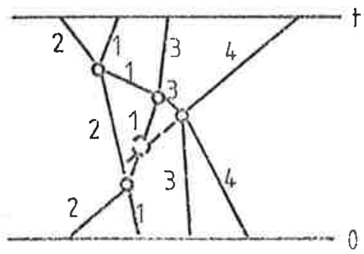


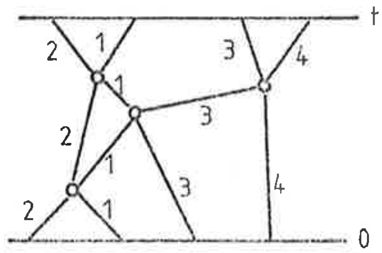


+ (1,4) + ...

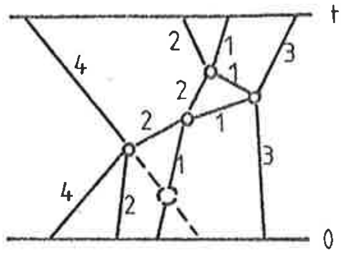


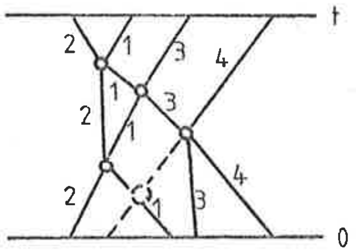


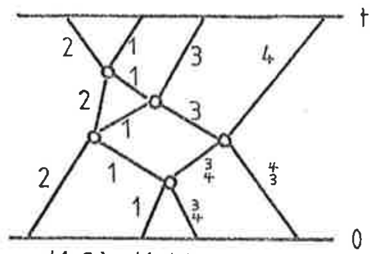




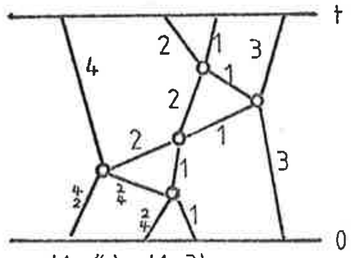
+ (1,3) + (1,4) + ...



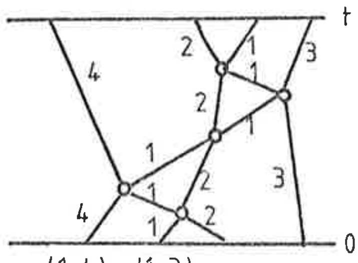




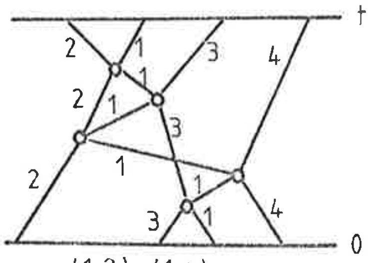
$+(1,2)+(1,\substack{4\\3})+\cdots$



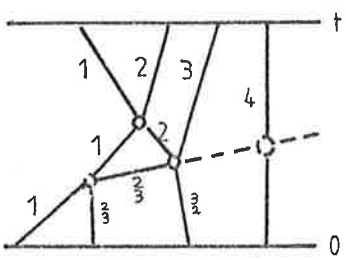
$+(1,\substack{4\\2})+(1,3)+\cdots$



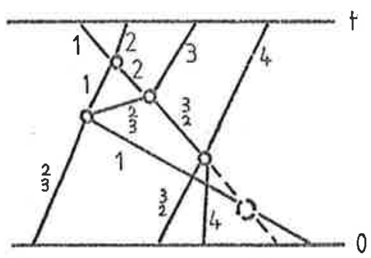
$+(1,4)+(1,3)+\cdots$

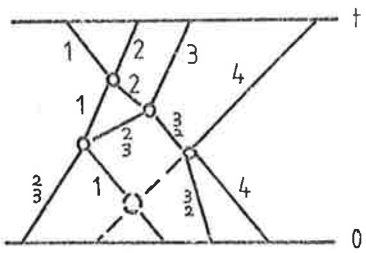


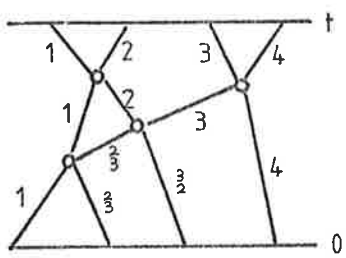
$+(1,2)+(1,4)+\cdots$



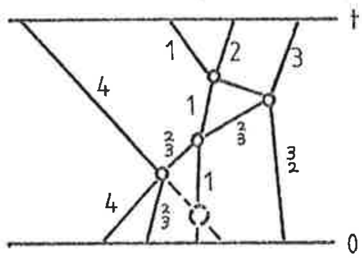
$+(1,4)+\cdots$

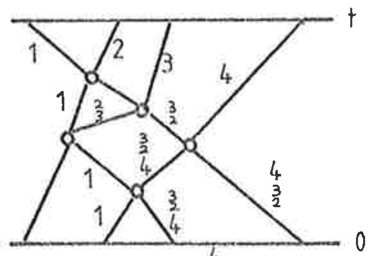




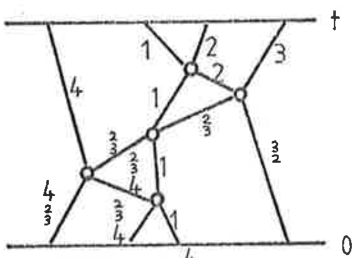


$+(1,\substack{3\\2})+(1,4)+\cdots$

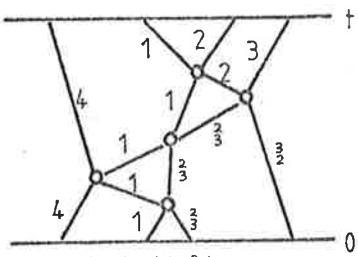




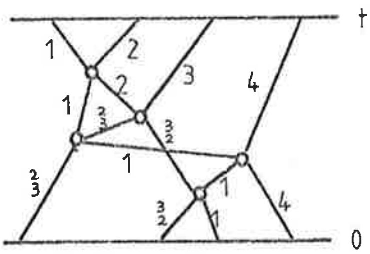
$+(1,\substack{2\\3})+(1,\substack{4\\3\\2})+\cdots$



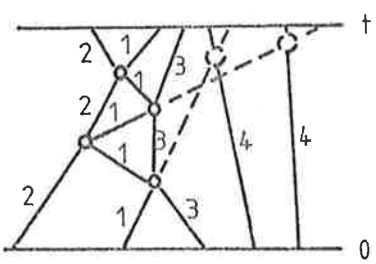
$+(1,\substack{3\\2})+(1,\substack{4\\2\\3})+\cdots$

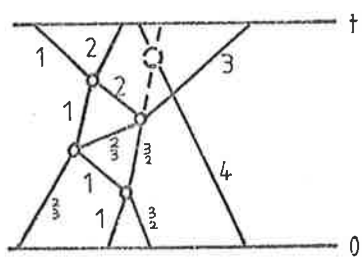


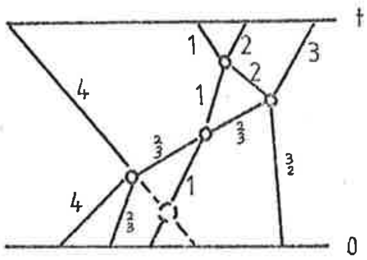
$+(1,4)+(1,\substack{3\\2})+\cdots$



$+(1,4)+(1,\substack{2\\3})+\cdots$







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