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ASPECTS OF THE KINETIC EQUATIONS FOR A SPECIAL ONE-DIMENSIONAL SYSTEM

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Abstract

Some initial value problems are considered which arise in the treatment of a one-dimensional gas of point particles interacting with a "hard-core" potential.

Two basic types of initial conditions are considered. For the first, one particle is specified to be at the origin with a given velocity. The positions in phase space of the remaining background of particles are represented by continuous distribution functions. The second problem is a periodic analogue of the first.

Exact equations for the delta-function part of the single particle distribution functions are derived for the non-periodic case and approximate equations for the periodic case. These take the form of differential operator equations. The spectral and asymptotic properties of the operators associated with the two cases are examined and compared. The behaviour of the solutions is also considered.

1. Introduction

Because of its relative simplicity, the non-equilibrium behaviour of the above-mentioned statistical mechanical system has been examined previously in some detail. Jepsen [10] developed methods applicable to the calculation of various ensemble averages.These methods depended crucially on the simple dynamics associated with a system having a "hard-core" interaction and have been applied to an infinite system with a background of particles in equilibrium at the initial time. This special case has also been treated by Lebowitz and Percus [11] using a distribution function formalism. They consider also the kinetic equation associated with the time evolution of the system.† Our work utilizes methods developed by Anstis *et al.* [1] based on solving the hierarchy equations by factorization techniques. We shall cover the more general problem where the background of particles may be distributed inhomogeneously at the initial time (for both the periodic and non-periodic cases). The use of methods involving the hierarchy equations to derive governing time evolution equations lends itself more readily to comparison with treatments of more general systems. The results are presented in a way suggestive of generalization to other systems. The relationship between the behaviour of the system which we consider and a system of hard-rods of non-zero diameter a has been discussed by Anstis *et al.* [1].

2. The hierarchy equations

For any configuration associated with the initial ensemble, we label the particles with an index $j \in \{\dots, -2, -1, 0, 1, \dots\}$ increasing from left to right. We make the convention that the particle specified to be at the origin at the initial time is labelled by $j = 0$. This ordering is then preserved for all times.

Since we are dealing with a spatially infinite system, we may choose to employ either the grand canonical ensemble in the infinite volume limit or the canonical ensemble in the thermodynamic limit.

The relevant reduced distribution functions associated with either of the above ensembles are defined below. Let $z_i(t) = (g_i(t), v_i(t))$ denote the position and velocity of particle i at a time $t \geqslant 0$. The n-particle distribution functions are defined as

$$f_{j_1}^{(n)}(z^1; z^2; \dots; z^n; t) = \sum_{\substack{j_2,\dots,j_n=-\infty \\ j_\alpha \neq j_\beta,\, \alpha\neq\beta;\, j_\alpha \neq j}}^{+\infty} f_{j_1 j_2 \dots j_n}^{(n)}(z^1; z^2; \dots; z^n; t) \tag{2.1}$$

with

$$f_{j_1 j_2 \dots j_n}^{(n)}(z^1; z^2; \dots; z^n; t) = \text{“lim”}\langle \delta(z^1 - z_{j_1}(t)) \dots \delta(z^n - z_{j_n}(t))\rangle_V$$

where “lim” represents a suitable limit to infinite volume and where $\langle - \rangle_V$ is the appropriate ensemble average for a finite region V. (See Appendix A.) It follows that $f_j^{(n)}$ is symmetric in the variables $z^2, \dots, z^n$.

These functions satisfy a coupled hierarchy of equations very similar to the *BBGKY* hierarchy. For the case of the grand canonical ensemble, these equations may be derived using the methods of Anstis *et al.* [1]. The work of Bogoliubov [2] may be generalized to derive identical equations for the case of the canonical ensemble in the thermodynamic limit.

† Gervois and Pomeau [7] have examined aspects of the corresponding semi-infinite system.

After considerable simplification, using the special properties of the interparticle potential, these equations take the form:

$$\left(\frac{\partial}{\partial t}+K_j^{(n)}\right)f_j^{(n)}(z_1;\, z_2;\, \dots;\, z_n;\, t)$$

$$= \lim_{\varepsilon\to 0}\int dv_{n+1}|v_{n+1}-v_1|\times\{f_{(j)}^{(n+1)}(z_1;\, g_1^-, v_{n+1};\, z_2;\, \dots;\, z_n;\, t)$$

$$-f_j^{(n+1)}(z_1;\, g_1^-, v_{n+1};\, z_2;\, \dots;\, z_n;\, t)\} \qquad (2.2)$$

where $n = 1, 2, \dots$; j is an integer; $K_j^{(n)}$ is the n-particle Liouville operator which includes only interactions between particle j and the unlabelled particles; $g_1^- = g_1 - \varepsilon\,\mathrm{sgn}\,(v_{n+1}-v_1)$ and $(j) = j + \mathrm{sgn}\,(v_{n+1}-v_1)$ (see Anstis *et al.* [1]).

3. The non-periodic initial value problem

3.1. Derivation of governing equations

We set up an initial value problem as follows. For $j = 0$, set

$$f_0^{(1)}(z_1;\, 0) = \delta(g_1)\,\delta(v_1 - v').$$

For $j \neq 0$, let $f_j^{(1)}(z_1;0)$ be a regular function (in the "distribution" sense) with the following properties. Define $f_j^g(g_1;\, 0) = \int_{-\infty}^{+\infty} dv_1 f_j^{(1)}(g_1, v_1;\, 0)$ and demand that $\int_{-\infty}^{+\infty} dg_1 f_j^g(g_1;\, 0) = 1$ and support $f_j^g \subseteq [0,\infty)$ for $j > 0$, support $f_j^g \subseteq (-\infty, 0]$ for $j < 0$. We shall assume that

$$\sum_{j=1}^{+\infty} f_j^g(g_1;\, 0) \quad \left(\text{resp.}\ \sum_{j=-1}^{-\infty} f_j^g(g_1;\, 0)\right)$$

is bounded and continuous on $g_1 \in [0,\infty)$ (resp. $(-\infty, 0]$). The ordering of the particles in coordinate space is reflected in the constraint that

$$\int dg\, g f_{j_1}^{(g)}(g;\, 0) \geqslant \int dg\, g f_{j_2}^{(g)}(g;\, 0) \quad \text{for } j_1 > j_2$$

(see Appendix B). The requirements that there should be finite particle number, energy and momentum in each finite region of coordinate space are also considered in this Appendix. A further property will be required, namely that the average density of particles be equal to a finite quantity ρ. The most natural way to express this condition is in terms of $(C-1)$ summability (Hille [9]). The condition becomes

$$\lim_{\mathscr{L}\to+\infty}\frac{1}{\mathscr{L}}\int_0^{\mathscr{L}} dg \sum_{j=1}^{+\infty} f_j^g(g) = \rho$$

and (3.1.1)

$$\lim_{\mathscr{L}\to+\infty}\frac{1}{\mathscr{L}}\int_{-\mathscr{L}}^{0} dg \sum_{j=-1}^{-\infty} f_j^g(g) = \rho.$$

The $(C-1)$ summability condition is a natural choice to make (see the work of Doplicher *et al.* [4] for a higher dimensional analogue) and will be useful for the asymptotic analysis.

Our analysis shall depend crucially on a partial factorization property of the reduced distribution functions at the initial time. Consider the n-particle distribution function for $j=0$. From (2.1) we have

$$f_0^{(n)}(z^1; z^2; \ldots; z^n; 0) = f_0^{(1)}(z^1; 0) \sum_{\substack{j_2, j_3, \ldots, j_n=-\infty \\ j_\alpha\neq j_\beta, \alpha\neq\beta, j_\alpha\neq 0}}^{+\infty} f_{j_2 j_3\ldots j_n}^{(n-1)}(z^2; z^3; \ldots; z^n; 0). \tag{3.1.2}$$

Since the particle $j=0$ acts as a wall at $t=0$, we choose initial conditions such that there are no correlations between particles to the left of the origin and those to the right of the origin at the initial time. The second factor in (3.1.2) may be decomposed as

$$\sum_{\substack{\Gamma^+,\Gamma^- \\ \Gamma^+\cup\Gamma^-=(2,3,\ldots,n) \\ |\Gamma^\pm|=\gamma^\pm}} \left(\sum_{\substack{j_{m_i}=-\infty, m_i\in\Gamma^- \\ i\in\{1,2,\ldots,\gamma^-\} \\ j_\alpha\neq j_\beta, \alpha\neq\beta}}^{-1} f_{j_{m_1} j_{m_2}\ldots j_{m_{\gamma^-}}}^{(\gamma^-)}(z^{m_1}; z^{m_2}; \ldots; z^{m_{\gamma^-}}; 0) \right)$$
$$\times \left(\sum_{\substack{j_{m_i'}=1, m_i'\in\Gamma^+ \\ 1\in\{1,2,\ldots,\gamma^+\} \\ j_\alpha\neq j_\beta, \alpha\neq\beta}}^{+\infty} f_{j_{m_1'} j_{m_2'}\ldots j_{m_{\gamma^+}'}}^{(\gamma^+)}(z^{m_1'}; z^{m_2'}; \ldots; z^{m_{\gamma^+}'}; 0) \right) \tag{3.1.3}$$

($\cup$ represents disjoint union and $|-|$ represents the cardinality of a set).

The factors in this expression are distributed functions associated with the particles confined to either $g<0$ or $g>0$ at the initial time by a hard wall at the origin. These expressions are symmetrized distribution functions and consequently describe the behaviour of a system of unlabelled particles. An unlabelled gas of point particles with "hard-core" interaction in one dimension is precisely equivalent to the corresponding ideal gas (see Jepsen [10] or Lebowitz and Percus [11]). Consequently it is natural to restrict one's attention to the case where the above higher order symmetrized distribution functions for $g<0$ (resp. $g>0$) factorize

as a product of single particle distribution functions $\sum_{j=-1}^{-\infty} f_j^{(1)}$ (resp. $\sum_{j=+1}^{+\infty} f_j^{(1)}$).†
For this case, we may deduce from (3.1.2) and (3.1.3) that

$$f_0^{(n)}(z^1; z^2; \ldots; z^n; 0) = f_0^{(1)}(z^1; 0) \times \prod_{i=2}^{n} \left(\sum_{j=-\infty, j\neq 0}^{+\infty} f_j^{(1)}(z^i; 0) \right). \tag{3.1.4}$$

This choice of course includes the case where the background of particles is in equilibrium at the initial time. Transport coefficients are determined by the correlation functions associated with this quasi-equilibrium choice of initial conditions.

Consider now the factorization properties of the corresponding distribution function for $j \neq 0$. The function is clearly regular in the variable z^1. In fact we may write except for $g^i = g^n = 0$ $(i = 2, 3, \ldots, n-1)$

$$\begin{aligned} f_j^{(n)}(z^1; z^2; \ldots; z^n; 0) = f_j^{(n-1)}&(z^1; z^2; \ldots; z^{n-1}; 0) \\ &\times \left(\sum_{k=-\infty, k\neq 0}^{+\infty} f_k^{(1)}(z^n; 0) + \delta(g^n)\, \delta(v^n - v') \right) \\ &+ g_j^{(n)}(z^1; z^2; \ldots; z^n; 0), \end{aligned} \tag{3.1.5}$$

where $g_j^{(n)}$ is regular in the variables z^1 and z^n. In fact (3.1.5) may be used for all j provided we exclude the case $g^i = g^n = 0$ $(i \neq n)$.

We extend the definition of $g_j^{(n)}$ to arbitrary times $t \geqslant 0$ by the following formula: for $n \geqslant 2$,

$$\begin{aligned} f_j^{(n)}(z^1; z^2; \ldots; z^n; t) = f_j^{(n-1)}&(z^1; z^2; \ldots; z^{n-1}; t) \\ &\times \left(\sum_{k=-\infty, k\neq 0}^{+\infty} f_k^{(1)}(g^n - v^n t, v^n; 0) + \delta(g^n - v^n t)\, \delta(v^n - v') \right) \\ &+ g_j^{(n)}(z^1; z^2; \ldots; z^n; t) \\ &\text{except for } g^i = g^n = v't \quad (i \neq n). \end{aligned} \tag{3.1.6}$$

Now we confine our attention to pre-collision regions of the n-particle phase space in which $g_j^{(n)}$ is defined. These are regions in which particle j has not suffered a collision in its past history under n-particle motion. Denote these regions (excluding points such that $g^i - v^i(t-s) = g^n - v^n(t-s) = v's$: $0 \leqslant s \leqslant t$) by R_p^t. For such a

† Such states may be obtained from the equilibrium state of the corresponding semi-infinite system by perturbation with an external potential.

region, the operator $((\partial/\partial t)+K_j^{(n)})$ appearing in (2.2) may be replaced by

$$\left(\frac{\partial}{\partial t}+\sum_{k=1}^{n} v_k \frac{\partial}{\partial g_k}\right)$$

and the equations can be integrated from $t=0$ to a time $t>0$ to obtain a solution for any point in R_p^t. Note that it is always possible to choose $z_2, z_3, \ldots, z_n$ so that $(z_1; g_1^- v_{n+1}; z_2; \ldots; z_n; t)$ lies in R_p^t. If we use also the fact that

$$\left(\frac{\partial}{\partial t}+\sum_{k=2}^{n} v_k \frac{\partial}{\partial g_k}\right)\left(\sum_{r=-\infty\, r\neq 0}^{+\infty} f_r^{(1)}(g_n - v_n t, v_n; 0)+\delta(g_n - v_n t)\,\delta(v_n - v')\right)=0, \quad (3.1.7)$$

it is possible to show that $g_j^{(n)}$ $(n\geqslant 2)$ satisfy the same set of equations (2.2) as $f_j^{(n)}$, if we consider only points in R_p^t.

Consider now the regularity of the function $g_j^{(n)}(z_1; z_2; \ldots; z_n; t)$ with respect to the variables z_1 and z_n in R_p^t. The most general form that the function $g_j^{(n)}$ can take is as follows:

$$g_j^{(n)}(z_1; z_2; \ldots; z_n; t) = g_j^{(n)\delta}(v'; z_2; \ldots; z_n; t)\,\delta(g_1 - v_1 t)\,\delta(v_1 - v')$$
$$+ g_j^{(n)\,\mathrm{reg}}(z_1; z_2; \ldots; z_n; t), \quad (3.1.8)$$

where $g_j^{(n)\delta}, g_j^{(n)\,\mathrm{reg}}$ are regular in the variable z_1. By substitution into the $g_j^{(n)}$ hierarchy and equating the coefficients of terms with a $\delta(g_1 - v_1 t)\,\delta(v_1 - v')$ factor, we obtain the following equations for $g_j^{(n)\delta}$ $(n\leqslant 2)$ in R_p^t:

$$\left(\frac{\partial}{\partial t}+\sum_{k=2}^{n} v_k \frac{\partial}{\partial g_k}\right) g_j^{(n)\delta}(v'; z_2; \ldots; z_n; t)$$
$$= \lim_{\varepsilon\to 0}\int_{-\infty}^{+\infty} dv_{n+1}\,|v_{n+1}-v_1|\,(g_{(j)}^{(n+1)\delta}(v'; (v't)^- v_{n+1}; z_2; \ldots; z_n; t)$$
$$- g_j^{(n+1)\delta}(v'; (v't)^-, v_{n+1}; z_2; \ldots; z_n; t)). \quad (3.1.9)$$

Using the uniqueness of solutions of (3.1.9) together with the initial condition $g_j^{(n)\delta}(v'; z_2; \ldots; z_n; 0) = 0$ for $n\geqslant 2$ in R_p^0, it follows that $g_j^{(n)\delta}(v'; z_2; \ldots; z_n; t) = 0$ for all points in R_p^t $(n\geqslant 2)$. Consequently $g_j^{(n)}(z_1; z_2; \ldots; z_n; t)$ is regular in z_1 for all points in R_p^t and a similar analysis shows that the same result holds with respect to z_n. In particular, we may conclude that $g_j^{(2)}(z_1; g_1^-, v_2; t)$ is a regular function for all $\varepsilon>0$ and $t\geqslant 0$.

This result may now be used in the analysis of the first hierarchy equation for $f_j^{(n)}$ (with $n = 1$). Upon substitution of the factorized form for $f_j^{(2)}$, we obtain:

$$\begin{aligned}
&\left(\frac{\partial}{\partial t}+v_1\frac{\partial}{\partial g_1}\right)f_j^{(1)}(z_1;\, t)\\
&\quad = \gamma(g_1, v_1;\, t)\cdot\{f_{j-1}^{(1)}(z_1;\, t)-f_j^{(1)}(z_1;\, t)\}+\beta(g_1, v_1;\, t)\cdot\{f_{j+1}^{(1)}(z_1;\, t)-f_j^{(1)}(z_1;\, t)\}\\
&\qquad +\lim_{\xi\to 0}\delta(g_1^{\mp}-v't)\\
&\qquad\quad \times(H(v'-v_1)(v'-v_1)\cdot[f_{j+1}^{(1)}(z_1;\, t)-f_j^{(1)}(z_1;\, t)]\\
&\qquad\qquad +H(v_1-v')(v_1-v')\cdot[f_{j-1}^{(1)}(z_1;\, t)-f_j^{(1)}(z_1;\, t)])\\
&\qquad +\lim_{\varepsilon\to 0}\int_{-\infty}^{+\infty}dv_2|v_2-v_1|\cdot\{g_j^{(2)}(z_1;\, g_1^{-}, v_2;\, t)-g_j^{(2)}(z_1;\, g_1^{-}, v_2;\, t)\},
\end{aligned} \tag{3.1.10}$$

where $H(\,)$ is the Heaviside step function, $g_1^{\mp} = g_1-\xi\operatorname{sgn}(v'-v_1)$ and we have set

$$\gamma(g_1, v_1;\, t) = \int_{-\infty}^{v_1}dv_2(v_1-v_2)\sum_{k=-\infty,k\neq 0}^{+\infty}f_k^{(1)}(g_1-v_2t, v_2;\, 0)$$

and (3.1.11)

$$\beta(g_1, v_1;\, t) = \int_{v_1}^{+\infty}dv_2(v_2-v_1)\sum_{k=-\infty,k\neq 0}^{+\infty}f_k^{(1)}(g_1-v_2t, v_2;\, 0).$$

Our previous analysis shows that the last term in (3.1.10) is regular in g_1 and v_1. From this we conclude that the term exhibiting explicitly the delta-function may be replaced by the jump condition:

$$\lim_{\xi\to 0}f_j^{(1)}(v't-\xi, v_1;\, t) = \lim_{\xi\to 0}f_{j+1}^{(1)}(v't+\xi, v_1;\, t). \tag{3.1.12}$$

The resulting equation is satisfied everywhere except the line $g_1 = v't$ where $f_j^{(1)}$ has a simple discontinuity given by (3.1.12) (*cf.* Anstis *et al.* [1]).

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

$$f_j^{(1)}(z_1;\, t) = f_j^{(1)\delta}(t)\,\delta(g_1-v_1t)\,\delta(v_1-v')+f_j^{(1)\,\mathrm{reg}}(z_1;\, t), \tag{3.1.13}$$

where $f_j^{(1)\delta}$ and $f_j^{(1)\,\mathrm{reg}}$ are regular functions. Substituting (3.1.13) into (3.1.10) gives us uncoupled equations for both $f_j^{(1)\delta}$ and $f_j^{(1)\,\mathrm{reg}}$. In particular for $f_j^{(1)\delta}$, (3.1.10) yields:

$$\frac{d}{dt}f_j^{(1)\delta}(t) = \gamma(v';\, t)\cdot\{f_{j-1}^{(1)\delta}(t)-f_j^{(1)\delta}(t)\}+\beta(v';\, t)\cdot\{f_{j+1}^{(1)\delta}(t)-f_j^{(1)\delta}(t)\}, \tag{3.1.14}$$

where

$$\gamma(v';\, t) = \gamma(v't, v';\, t)$$

and

$$\beta(v';\, t) = \beta(v't, v';\, t).$$

The initial conditions associated with the problem described are simply

$$f_j^{(1)\delta}(0) = \delta_{j,0} \quad \text{(Kronecker delta).} \tag{3.1.15}$$

Consider a class of initial value problems (labelled by N) where the distribution function for particle j is given by $f_{j-N}^{(1)}(z_1;\, 0)$ at $t = 0$. If we take an arbitrary convex linear combination of these initial conditions, it follows that the associated single particle distribution functions will still satisfy (3.1.14). However, we will have the more general initial conditions: $f_j^{(1)\delta}(0) \geqslant 0$ for all j and

$$\sum_{j=-\infty}^{+\infty} f_j^{(1)\delta}(0) = 1. \tag{3.1.16}$$

A conservative result is easily derived from (3.1.14) by summing over the index j. It follows that:

$$\sum_{j=-\infty}^{+\infty} f_j^{(1)\delta}(t) = \sum_{j=-\infty}^{+\infty} f_j^{(1)\delta}(0) = 1 \tag{3.1.17}$$

from (3.1.16) for all $t \geqslant 0$, that is, there is always a probability of unity of finding a particle on the trajectory $g_1 = v't$, given that there is a probability of unity of finding a particle at $g_1 = 0$ with velocity v' at the initial time.

3.2. The initial value problem with specialized initial conditions

Initial conditions shall be assumed here to take the form

$$f_0^{(1)}(z_1;\, 0) = \delta(g_1)\,\delta(v_1 - v')$$

and for $j \neq 0$

$$f_j^{(1)}(z_1;\, 0) = f_j^{(g)}(g_1)\, h(v_1). \tag{3.2.1}$$

The $f_j^{(1)}$ satisfy all conditions previously asserted together with the constraints

$$\int_{-\infty}^{+\infty} dv_1\, h(v_1) = 1 \quad \text{and} \quad \sum_{k=-\infty,\, k\neq 0}^{+\infty} f_k^{g}(g_1) = \rho \quad \text{(constant).} \tag{3.2.2}$$

This is the case for the quasi-equilibrium initial conditions (see Anstis *et al.* [1]). The equations (3.1.14) can be solved by Fourier transform techniques (see [1]). However, the methods developed below will exhibit more clearly the structure of

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the equations. Using (3.2.2), we find

$$\gamma(v';t) = \gamma(v') = \gamma = \rho \int_{-\infty}^{v'} dv(v'-v)\,h(v)$$

and

$$\beta(v',t) = \beta(v') = \beta = \rho \int_{v'}^{+\infty} dv(v-v')\,h(v).$$

Equations (3.1.14) may be written abstractly as

$$\frac{d}{dt}\mathbf{f}^{(1)\delta}(t) = \mathbf{C}\cdot\mathbf{f}^{(1)\delta}(t) \tag{3.2.3}$$

where $\mathbf{f}^{(1)\delta}$ is regarded as a column vector in the sequence space ι^1 (see Taylor [13]) with components $f_j^{(1)\delta}$, and $\mathbf{C}$ is a linear operator on ι^1. In the usual matrix representation $\mathbf{C} = (C_{ij})$, we have

$$C_{ij} = \beta\delta_{j-1,i} + \gamma\delta_{j+1,i} - (\gamma+\beta)\,\delta_{i,j}.$$

The ι^1 norm is defined as $\|\mathbf{f}\|_1 = \sum_{j=-\infty}^{+\infty}|f_j|$. In fact $\mathbf{C}$: $\iota^1 \to \iota^1$ and is a bounded, non-compact, linear operator (*cf.* Taylor [13]).

We shall next determine the spectrum of $\mathbf{C}$. Let $\sigma(\ )$ denote the spectrum of an operator. Then $\sigma(\ ) = P\sigma(\ ) \cup C\sigma(\ ) \cup R\sigma(\ )$ where $P\sigma(\ )$, $C\sigma(\ )$ and $R\sigma(\ )$ denote the point, continuous and residual spectra (respectively). Define a bounded linear operator $\mathbf{C}^0$ on ι^1 by

$$\mathbf{C} = \mathbf{C}^0 - (\alpha+\beta)\,\mathbf{I} \tag{3.2.4}$$

where $\mathbf{I}$ is the identity on ι^1. Because of the obvious relations

$$P\sigma(\mathbf{C}) = P\sigma(\mathbf{C}^0) - (\gamma+\beta), \quad C\sigma(\mathbf{C}) = C\sigma(\mathbf{C}^0) - (\gamma+\beta)$$

and

$$R\sigma(\mathbf{C}) = R\sigma(\mathbf{C}^0) - (\gamma+\beta),$$

it will suffice to determine the spectrum of $\mathbf{C}^0$.

Firstly we prove that $P\sigma(\mathbf{C}^0)$ is empty. The eigenvalue equation in component form for $\mathbf{C}^0$ becomes

$$\lambda f_j = \gamma f_{j-1} + \beta f_{j+1} \quad \text{for all } j, \quad \mathbf{f} \in \iota^1 \quad (\mathbf{f} \neq \mathbf{0}). \tag{3.2.5}$$

Define the (continuous) function

$$\eta(\theta) = \sum_{j=-\infty}^{+\infty} \exp(i\theta j f_j),$$

where $\eta(\theta)$ is not identically zero by Parseval's formula. Transforming (3.2.5) gives $\lambda = \gamma \exp(+\hat{\imath}\theta) + \beta \exp(-\hat{\imath}\theta)$ for θ such that $\eta(\theta) \neq 0$. This is a contradiction since $\gamma > 0$, $\beta > 0$ and λ is independent of θ. So $P\sigma(\mathbf{C}^0)$ is empty.

To determine the other components of $\sigma(\mathbf{C}^0)$, we shall work with $\mathbf{C}^{0'}$, the Banach space adjoint of $\mathbf{C}^0$. Now $\mathbf{C}^{0'}$ is a bounded linear operator on the dual space ι^∞ of ι^1 (ι^∞ is the space of bounded sequences). In the usual matrix representation $\mathbf{C}^{0'} = (C_{ij}^{0'})$, we have

$$C_{ij}^{0'} = \gamma \delta_{j-1,i} + \beta \delta_{j+1,i}. \tag{3.2.6}$$

To proceed further an alternative characterization of the spectrum is used. For a bounded linear operator on a sequence space ι, define the compression spectrum to be

$$\Gamma(\mathbf{G}) = \{\lambda \in \mathbf{C} : \mathscr{R}(\lambda \mathbf{I} - \mathbf{G}) \neq \iota\} \quad (\mathscr{R} = \text{range})$$

and the approximate point spectrum as

$$\Pi(\mathbf{G}) = \{\lambda \in \mathbf{C}: \text{for all } \varepsilon > 0, \text{ there exists } \mathbf{x} \in \iota \text{ with } \|\mathbf{x}\| = 1$$

such that

$$\|\lambda \mathbf{x} - \mathbf{G}\mathbf{x}\| < \varepsilon\}.$$

Then $P\sigma \subseteq \Pi$, $C\sigma = \Pi \setminus (\Gamma \cup P\sigma)$ and $R\sigma = \Gamma \setminus P\sigma$ (see Halmos [8]). We shall need also the following results:

$$\sigma(\mathbf{C}^0) = \sigma(\mathbf{C}^{0'}),\ P\sigma(\mathbf{C}^{0'}) = \Gamma(\mathbf{C}^0) \tag{3.2.7}$$

First we shall prove that $C\sigma(\mathbf{C}^0)$ is contained in the ellipse

$$E = \{\lambda \in \mathbf{C}: \lambda = \gamma \exp(\hat{\imath}\theta) + \beta \exp(-\hat{\imath}\theta): \theta \in [0, 2\pi)\}.$$

The result is derived easily from the corresponding analysis for the Hilbert space $\iota^2 \supseteq \iota^1$ (Appendix C) and using the norm inequality $\|-\|_2 \leqslant \|-\|_1$ together with the definition of $C\sigma(\ )$. This leads to the simplified characterization of $\sigma(\mathbf{C}^0) = \sigma(\mathbf{C}^{0'})$. From above

$$\sigma(\mathbf{C}^0) = \{C\sigma(\mathbf{C}^0) \subseteq E\} \cup \{P\sigma(\mathbf{C}^{0'}) = \Gamma(\mathbf{C}^0) = R\sigma(\mathbf{C}^0)\}.$$

To complete the analysis, we shall determine $P\sigma(\mathbf{C}^{0'})$. Let $\mathbf{x}^\lambda \in \iota^\infty$ be an eigenvector of $\mathbf{C}^{0'}$ corresponding to the eigenvalue $\lambda \in \mathbf{C}$. The jth component of the eigenvalue equation becomes $\lambda x_j^\lambda = \gamma x_{j+1}^\lambda + \beta x_{j-1}^\lambda$ where $x_j^\lambda \neq 0$ for all j. We transform this equation to one in a generalized function space Q' (for a suitable class of test functions Q). Define

$$\eta(\theta) = \sum_{j=-\infty}^{+\infty} \exp(\hat{\imath}\theta j)\, x_j^\lambda \in Q'. \tag{3.2.8}$$

For example in the space of tempered distributions, the above series converges to a generalized function if and only if $x_j^\lambda = O(|j|^N)$ for some N as $|j| \to \infty$ (see Lighthill [12]). Furthermore, $\mathbf{x}^\lambda \neq \mathbf{0}$ in ι^∞ implies that $\eta \neq 0$ in Q'. Transforming (3.2.8) results in the equation (in Q')

$$(\lambda - \gamma \exp(-\hat{\imath}\theta) - \beta \exp(+\hat{\imath}\theta))\,\eta(\theta) = 0.$$

Choosing $\lambda \in E$, it follows that this equation has no non-zero solutions $\eta \in Q'$ (a contradiction). Therefore $P\sigma(\mathbf{C}^{0'}) \subseteq E$. Suppose

$$\lambda = \gamma \exp(-i\theta^*) + \beta \exp(+i\theta^*), \quad \theta^* \in [0, 2\pi) \quad (\text{so } \lambda \in E).$$

A corresponding ι^∞ eigenvector is given in component form by

$$x_j^\lambda = (1/2\pi)\exp(-\hat{\imath}\theta^* j) \quad (j \text{ an integer.})$$

Consequently $P\sigma(\mathbf{C}^{0'}) = E$ and finally we conclude that

$$\sigma(\mathbf{C}) = R\sigma(\mathbf{C}) = \{\lambda \in \mathbf{C}\colon \lambda = (\gamma+\beta)(\cos\theta - 1) + (\gamma - \beta)\,\hat{\imath}\sin\theta\colon \ \theta \in [0, 2\pi)\}. \tag{3.2.9}$$

3.3. Properties of the governing equation for general initial conditions

Returning to the general case, we rewrite (3.1.14) in the form of an ι^1 equation:

$$\frac{d}{dt}\mathbf{f}^{(1)\delta}(t) = \mathbf{C}(t)\cdot\mathbf{f}^{(1)\delta}(t), \tag{3.3.1}$$

where in the matrix representation $\mathbf{C}(t) = (C_{ij}(t))$ we have

$$C_{ij}(t) = \beta(v', t)\,\delta_{j-1,i} + \gamma(v', t)\,\delta_{j+1,i} - (\gamma(v', t) + \beta(v', t))\,\delta_{i,j}.$$

(Again these equations could be solved by Fourier transform methods.) The matrices $\mathbf{C}(t)$ satisfy the commutation relations

$$[\mathbf{C}(t), \mathbf{C}(t')]_- = \mathbf{C}(t)\cdot\mathbf{C}(t') - \mathbf{C}(t')\cdot\mathbf{C}(t) = 0 \quad \text{for all } t, t' \geqslant 0.$$

It may then be shown that

$$\left[\int_\alpha^\beta dt\,\mathbf{C}(t), \int_\gamma^\delta dt\,\mathbf{C}(t)\right]_- = 0 \quad \text{for arbitrary } \alpha, \beta, \gamma, \delta \geqslant 0$$

(see Dunford and Schwartz [5]). Using this result, together with the Baker–Campbell–Hausdorff theorem, it follows that the solution of (3.3.1) may be expressed as

$$\mathbf{f}^{(1)\delta}(t) = \exp\left(\left[\frac{1}{t}\int_0^t dt'\,\mathbf{C}(t')\right]\cdot t\right)\mathbf{f}^{(1)\delta}(0). \tag{3.3.2}$$

The behaviour of $f_j^{(1)s}(t)$ in time is determined by the spectrum of the operator $(1/t)\int_0^t dt'\,\mathbf{C}(t')$ which from (3.2) is given by

$$\sigma\left(\frac{1}{t}\int_0^t dt'\,\mathbf{C}(t')\right) = R\sigma\left(\frac{1}{t}\int_0^t dt'\,\mathbf{C}(t')\right)$$

$$= \left\{\lambda\in\mathbf{C}\colon \lambda = \left\{\frac{1}{t}\int_0^t dt'(\gamma(v',t')+\beta(v',t'))\right\}(\cos\theta-1)\right.$$

$$\left. + \left\{\frac{1}{t}\int_0^t dt'(\gamma(v',t')-\beta(v',t'))\right\} \hat{\imath}\sin\theta\colon\ \theta\in[0,2\pi)\right\}. \qquad (3.3.3)$$

We shall consider the asymptotic behaviour of the spectrum for $t\to\infty$. Make the special choice of initial conditions $f_0^{(1)}(z_1;0) = \delta(g_1)\,\delta(v_1-v')$ and for $j\neq 0$, $f_j^{(1)}(z_1;0) = f_j^s(g_1)\,h(v_1)$. Then $f_j^{(1)}$ must satisfy the constraints described in (3.1) and $\int_{-\infty}^{+\infty} dv_1\,h(v_1) = 1$. In this case

$$\gamma(v',t) = \int_{-\infty}^{v'} dv_2(v'-v_2)\,h(v_2)\cdot \sum_{k=-\infty,k\neq 0}^{+\infty} f_k^s((v'-v_2)\,t)$$

and

$$\beta(v',t) = \int_{v'}^{+\infty} dv_2(v_2-v')\,h(v_2) \sum_{k=-\infty,k\neq 0}^{+\infty} f_k^s((v'-v_2)\,t). \qquad (3.3.4)$$

In this expression $\beta(v',t)$ may be written in the form

$$\beta(v',t) = \frac{1}{t}\int_0^{+\infty} dy\,G\left(\frac{y}{t}\right)\cdot f(y), \qquad (3.3.5)$$

where $G(x) = xh(x+v')\in L^1(-\infty,+\infty)$ (Lebesgue integrable functions) and $f(y) = \sum_{k=-\infty,k\neq 0}^{+\infty} f_k^{(1)s}(y)$ is bounded and continuous on $(0,\infty)$.

Define a class of functions $G_1(\tau)\in W(0,\infty)\subseteq L^1(0,\infty)$ by the requirement that $\int_0^{+\infty}\tau^{\lambda\hat{\imath}}G_1(\tau)\,d\tau\neq 0$ for all real λ. In particular $G_1(\tau) = H(1-\tau)\in W(0,\infty)$. The asymptotic analysis of $\beta(v',t)$ shall be achieved using a Tauberian theorem stated by E. Hille (and N. Wiener) [9]. If $G_1(y)\in W(0,\infty)$, $G(y)\in L^1(0,\infty)$ and $f(y)$ is bounded and continuous and if

$$\lim_{t\to\infty}\frac{1}{t}\int_0^{+\infty} G_1\left(\frac{y}{t}\right) f(y)\,dy = a\int_0^{+\infty} G_1(y)\,dy$$

then

$$\lim_{t\to\infty}\frac{1}{t}\int_0^{+\infty} G\left(\frac{y}{t}\right) f(y)\,dy = a\int_0^{+\infty} G(y)\,dy.$$

The theorem may be proved by noting that the dilations about the origin of any $G_1 \in W(0,\infty)$ are dense in $L^1(0,\infty)$. Making the choice of functions indicated, it follows from (3.1.1) that $\lim_{t\to\infty}\beta(v',t) = \beta(v')$. A similar analysis shows that $\lim_{t\to\infty}\gamma(v',t) = \gamma(v')$. Consequently $\beta(v',t)$ and $\gamma(v',t)$ are $(C-1)$ summable to $\beta(v')$ and $\gamma(v')$ (resp.). Hence, as $t\to\infty$, the set $\sigma((1/t)\int_0^t dt'\,\mathbf{C}(t'))$ approaches $\sigma(\mathbf{C})$ as in (3.2.9).

4. The periodic initial value problem

4.1. Derivation of the governing equations

We set up the initial value problem as follows. Set $f_0^{(1)}(z_1;\,0) = \delta(g_1)\,\delta(v_1-v')$ and for $j\in\{1,2,\dots,P-1\}$, let $f_j^{(1)}(z_1;\,0)$ be a regular function with the following properties. Define

$$f_j^g(g_1;\,0) = \int_{-\infty}^{+\infty} dv_1 f_j^{(1)}(g_1,v_1;\,0).$$

Then we require support $f_j^g(g_1;\,0)\subseteq[0,L]$ for $j\in\{1,2,\dots,P-1\}$. We shall assume that

$$\sum_{j=1}^{P-1} f_j^g(g_1;\,0)$$

is continuous and hence bounded on $[0,L]$. There is a normalization condition $\int_0^L dg f_j^g(g;0) = 1;\ j\in\{1,2,\dots,P-1\}$. A periodicity condition is imposed on the reduced distribution functions of the form:

$$f^{(m)}_{j_1j_2\dots j_m}(g_1,v_1;\,g_2,v_2;\,\dots;\,g_m,v_m;\,0)$$
$$= f^{(m)}_{j_1+\kappa Pj_2+\kappa P\dots j_m+\kappa P}(g_1+\kappa L,v_1;\,g_2+\kappa L,v_2;\,\dots;\,g_m+\kappa L,v_m;\,0) \tag{4.1.1}$$

for all integers $m,\kappa;\ m\geqslant 1$. In particular (4.1.1) defines $f_j^{(1)}$ for $j\in\{0,1,\dots,P-1\}$. The ordering of particles again imposes the constraint proved in Appendix A. In this section we shall make use of the periodized distribution functions defined by

$$\bar{f}_j^{(n)}(z_1;\,z_2;\,\dots;\,z_n;\,t) = \sum_{j'\equiv j(\mathrm{mod}\,P)} f_{j'}^{(n)}(z_1;\,z_2;\,\dots;\,z_n;\,t). \tag{4.1.2}$$

Here j should now be regarded as an index modulo P. As in (3.1), a partial factorization result for the initial conditions is of crucial importance for the following analysis. Since the particles in different cells $[\kappa L,(\kappa+1)L]$, κ an integer, do not interact with each other at the initial time, it is natural to impose a factorization condition (*cf.* (3.1.3)). For any set of non-equal integers $\{j_1,j_2,\dots,j_m\}$, make the decomposition

$$\{1,2,\ldots,m\} = \bigcup_{\kappa=-\infty}^{+\infty} \Gamma_\kappa \cup \Gamma_j$$

where $\Gamma_\kappa = \{n_1{}^\kappa, n_2{}^\kappa, \ldots, n_{\gamma\kappa}{}^\kappa\}$ and $j_{n_i{}^\kappa} \in \{\kappa P+1, \kappa P+2, \ldots, kP+(P-1)\}$ and $n' \in \Gamma$ implies $j_{n'} \equiv 0 \pmod P$. The factorization condition then takes the form:

$$f^{(m)}_{j_1 j_2 \ldots j_m}(z_1;\, z_2;\, \ldots;\, z_m;\, 0)$$
$$= \prod_{\kappa=-\infty}^{+\infty} f^{(\gamma\kappa)}_{j_{n_1}{}^\kappa j_{n_2}{}^\kappa \ldots j_{n_{\gamma\kappa}}{}^\kappa}(z_{n_1{}^\kappa};\, \ldots;\, z_{n_{\gamma\kappa}{}^\kappa};\, 0) \prod_{n' \in \Gamma} f^{(1)}_{j_{n'}}(z_{n'};\, 0) \qquad (4.1.3)$$

(we have set $f^{(0)} \equiv 1$). If we make the natural restriction to states where the symmetrized distribution functions for each cell $(\kappa L, (\kappa+1)L)$ factorize as a product of sums $\sum_{j=1}^{P-1} \bar{f}^{(1)}_j(\cdot\,;\, 0)$ at the initial time, then the following holds: suppose n_κ of the g_i $(i = 1,2,\ldots,n)$ lie in $(\kappa L, (\kappa+1)L)$, then

$$\bar{f}^{(n)}_0(z_1;\, z_2;\, \ldots;\, z_n;\, 0) = \bar{f}^{(1)}_0(z_1;\, 0) \prod_{\tilde{\kappa}=-\infty,\, n_{\tilde{\kappa}} \neq 0}^{+\infty} \left(\prod_{i=1}^{n_{\tilde{\kappa}}} \frac{P-i+1}{P} \right)$$
$$\times \prod_{i=2}^{n} \left(\sum_{k=1}^{P-1} \bar{f}^{(1)}_k(z_i;\, 0) + \sum_{\kappa=-\infty}^{+\infty} \delta(g_i - \kappa L)\, \delta(v_i - v') \right)$$
$$(4.1.4)$$

excluding points such that $g_\alpha = g_\beta = mL$ for some α, β, m. The numerical factor appears as a result of normalization. The above result is of course true for the special case where the particles in each cell $(\kappa L, (\kappa+1)L)$ are in equilibrium at the initial time. Then (4.1.4) may be rewritten as

$$\bar{f}^{(n)}_0(z_1;\, z_2;\, \ldots;\, z_n;\, 0) = \bar{f}^{(n-1)}_0(z_1;\, z_2;\, \ldots;\, z_{n-1};\, 0)\, C(g_2, g_3, \ldots, g_n;\, P)$$
$$\times \left(\sum_{k=1}^{P-1} \bar{f}^{(1)}_k(z_n;\, 0) + \sum_{\kappa=-\infty}^{+\infty} \delta(g_n - \kappa L)\, \delta(v_n - v') \right) \qquad (4.1.5)$$

where

$$C(g_2, g_3, \ldots, g_n;\, P) = \begin{cases} 1 & \text{if } g_n = mL \text{ for some integer } m, \\ \dfrac{P-m+1}{P} & \text{if } g_n \in (kL, (k+1)L) \text{ for some integer } k \text{ and so are } m-1 \text{ other } g_i;\ i = 2,3,\ldots,n-1 \text{ again excluding points } g_\alpha = g_\beta = mL \text{ for some } \alpha, \beta, m. \end{cases}$$

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Let us now define another hierarchy of functions $\bar{g}_j^{(n)}$ ($n \geqslant 2$) by

$$
\begin{aligned}
&\bar{f}_j^{(n)}(z_1;\, z_2;\, \dots;\, z_n;\, t) \\
&\quad = \bar{f}_j^{(n-1)}(z_1;\, z_2;\, \dots;\, z_{n-1};\, t) \\
&\qquad \times \left(\sum_{k=1}^{P-1} \bar{f}_k^{(1)}(g_n - v_n t, v_n;\, 0) + \sum_{\kappa=-\infty}^{+\infty} \delta(g_n - v_n t - \kappa L)\, \delta(v_n - v') \right) \\
&\qquad + \bar{g}_j^{(n)}(z_1;\, z_2;\, \dots;\, z_n;\, t) \qquad (4.1.6)
\end{aligned}
$$

excluding points $g_\alpha - v' t = g_\beta - v' t = mL$ for some α, β, m. The functions $\bar{g}_j^{(n)}$ satisfy the same set of hierarchy equations as $\bar{f}_j^{(n)}$ in pre-collision regions of phase space and excluding the same points mentioned above. From these equations, we may show $\bar{g}_j^{(n)}$ are regular with respect to z_n in appropriate regions. At the initial time, the coefficient of the delta-function part of $\bar{g}_j^{(n)}$ with respect to z_1 has the order of magnitude (if $\delta_{j,0}^P$ denotes the Kronecker delta mod P)

$$
\delta_{j,0}^P \bar{f}^{(n-2)}(z_2;\, z_3;\, \dots;\, z_{n-1};\, 0) \left(\sum_{j=1}^{P-1} \bar{f}_j^{(1)}(z_n;\, 0) \right) \min (O(1), O(n\varepsilon)) \qquad (4.1.7)
$$

where $\bar{f}^{(n-2)}$ is the symmetrized distribution function and $\varepsilon = 1/P$ is small in the high density regime. It is not difficult to show that in the regions under consideration, the functions $\bar{g}_j^{(n)}$ at arbitrary times are bounded by exponential growth from their initial values. Banach space techniques may be employed here to provide a rigorous analysis of the linear differential operator (hierarchy) equations. In particular these considerations may be applied to analyse $\bar{g}_j^{(2)}(z_1;\, g_1^-, v_2;\, t)$.

This result is used in the analysis of the first hierarchy equation for $\bar{f}_j^{(n)}$ ($n = 1$). Upon substitution of the factorized form for $\bar{f}_j^{(2)}$, we obtain

$$
\begin{aligned}
&\left(\frac{\partial}{\partial t} + v_1 \frac{\partial}{\partial g_1} \right) \bar{f}_j^{(1)}(z_1;\, t) \\
&\quad = \gamma^P(g_1, v_1;\, t) \cdot \{ \bar{f}_{j-1}^{(1)}(z_1;\, t) - \bar{f}_j^{(1)}(z_1;\, t) \} + \beta^P(g_1, v_1;\, t) \\
&\qquad \times \{ \bar{f}_{j+1}^{(1)}(z_1;\, t) - \bar{f}_j^{(1)}(z_1;\, t) \} + \lim_{\xi \to 0} \sum_{\kappa=-\infty}^{+\infty} \delta(g_1^= - v' t - \kappa L) \\
&\qquad \times (H(v' - v_1)(v' - v_1) [\bar{f}_{j+1}^{(1)}(z_1;\, t) - \bar{f}_j^{(1)}(z_1;\, t)] \\
&\qquad + H(v_1 - v')(v_1 - v') [\bar{f}_{j-1}^{(1)}(z_1;\, t) - \bar{f}_j^{(1)}(z_1;\, t)]) \\
&\qquad + \lim_{\varepsilon \to 0} \int_{-\infty}^{+\infty} dv_2 |v_2 - v_1| \cdot \{ \bar{g}_{(j)}^{(2)}(z_1;\, g_1^-, v_2;\, t) - \bar{g}_j^{(2)}(z_1;\, g_1^-, v_2;\, t) \}, \qquad (4.1.8)
\end{aligned}
$$

with $j \in \{0, 1, \ldots, P-1\}$ interpreted modulo P. The functions $H(\ )$ and g_1^- have been defined in (3.1), and in (4.1.8) we have set

$$\gamma^P(g_1, v_1;\ t) = \int_{-\infty}^{v_1} dv_2(v_1 - v_2) \sum_{k=1}^{P-1} \bar{f}_k^{(1)}(g_1 - v_2 t, v_2;\ 0)$$

and

$$\beta^P(g_1, v_1;\ t) = \int_{v_1}^{+\infty} dv_2(v_2 - v_1) \sum_{k=1}^{P-1} \bar{f}_k^{(1)}(g_1 - v_2 t, v_2;\ 0). \tag{4.1.9}$$

Our previous analysis shows that the last term in (4.1.8) is regular in g_1^-. From this we conclude that the term exhibiting explicitly the delta-function may be replaced by the jump conditions:

$$\lim_{\xi \to 0} \bar{f}_j^{(1)}(v't + \kappa L - \xi, v_1;\ t) = \lim_{\xi \to 0} \bar{f}_{j+1}^{(1)}(v't + \kappa L + \xi, v_1;\ t) \tag{4.1.10}$$

for all integral κ. The resulting equation is satisfied everywhere except on the lines $g_1 = \kappa L + v't$ where $\bar{f}_j^{(1)}$ has a simple discontinuity given by (4.1.10).

For $g_1 \in [v't, v't + L)$, make the decomposition

$$\bar{f}_j^{(1)}(z_1;\ t) = \bar{f}_j^{(1)\delta}(t)\, \delta(g_1 - v_1 t)\, \delta(v_1 - v') + \bar{f}_j^{(1)\,\mathrm{reg}}(z_1;\ t), \tag{4.1.11}$$

where $\bar{f}_j^{(1)\delta}$ and $\bar{f}_j^{(1)\,\mathrm{reg}}$ are regular functions. The function $\bar{f}_j^{(1)}$ is determined outside this interval by periodic extension. Henceforth we shall restrict our attention to the high density regime and the range of time for which the delta-function part of $\bar{g}_j^{(2)}$ with respect to z_1 makes a negligible contribution to (4.1.8) ($t \ll t_{mf} |\ln \varepsilon|$; $t_{mf} = (\beta m)^{\frac{1}{2}} \rho^{-1}$). For $\bar{f}_j^{(1)\delta}$ we obtain

$$\frac{d}{dt} \bar{f}_j^{(1)\delta}(t) \simeq \gamma^P(v', t) \cdot \{\bar{f}_{j-1}^{(1)\delta}(t) - \bar{f}_j^{(1)\delta}(t)\} + \beta^P(v', t) \cdot \{\bar{f}_{j+1}^{(1)\delta}(t) - \bar{f}_j^{(1)\delta}(t)\} \tag{4.1.12}$$

where j is interpreted modulo P and where

$$\gamma^P(v', t) = \gamma^P(v' t, v';\ t) \quad \text{and} \quad \beta^P(v', t) = \beta^P(v't, v';\ t).$$

Define the Kronecker delta function (modulo P) to be $\delta_{j,k}^P = 1$ if $j \equiv k \pmod P$ and $\delta_{j,k}^P = 0$ if $j \not\equiv k \pmod P$. The initial conditions associated with the problem described above are simply $\bar{f}_j^{(1)\delta}(0) = \delta_{j,0}^P$. However, the more general conditions $\bar{f}_j^{(1)\delta}(0) \geqslant 0$ and

$$\sum_{k=0}^{P-1} \bar{f}_k^{(1)\delta}(0) = 1$$

may be associated with a physical initial value problem where (4.1.12) are again the appropriate evolution equations (*cf.* (3.1.16)).

A conservation result is derived from (4.1.12) by summing over the index j. It follows that

$$\sum_{k=0}^{P-1} \bar{f}_k^{(1)\delta}(t) = \sum_{k=0}^{P-1} \bar{f}_k^{(1)\delta}(0) = 1 \quad \text{for all } t \geqslant 0.$$

Again this result may be interpreted physically (*cf.* 3.1) and is in fact exact.

4.2. The initial value problem with specialized initial conditions

The initial conditions are specified by analogy with (3.2).

$$\bar{f}_0^{(1)}(z_1;\, 0) = \sum_{\kappa=-\infty}^{+\infty} \delta(g_1 + \kappa L)\, \delta(v_1 - v')$$

and for $j \not\equiv 0 \pmod{P}$,

$$\bar{f}_j^{(1)}(z_1;\, 0) = \bar{f}_j^g(g_1)\, h(v_1)$$

where $\bar{f}_j^{(1)}$ satisfies all conditions previously asserted together with the constraints $h\,()$ as in (3.2.1) and (3.2.2) and

$$\sum_{k=1}^{P-1} \bar{f}_k^{(1)}(z_1;\, 0) = \frac{P-1}{L} = \rho \quad \text{(constant)}.$$

An example of such a situation is where the particles in the cell $[0, L]$ are in equilibrium at the initial time. In this case

$$h(v_1) = \left(\frac{m\beta}{2\pi}\right)^{\frac{1}{2}} \exp\left(-\tfrac{1}{2} m\beta v_1^2\right),$$

where $\beta = 1/kT$ is the statistical temperature and

$$\bar{f}_j^g(g_1) = \left\{\frac{(L-g)^{P-1-j}}{(P-1-j)!}\, \frac{g^{j-1}}{(j-1)!}\right\} \Big/ \frac{L^{P-1}}{(P-1)!}, \tag{4.2.1}$$

where $g_1 \in (0, \mathrm{L})$ and $j \in \{1, 2, \ldots, P-1\}$. Equation (4.2.1) follows from a simple generalization of the calculation of the partition function for a Tonks gas (*cf.* Thompson [14]). The delta-function part of the distribution functions, $\bar{f}_j^{(1)\delta}$, satisfy the equations:

$$\frac{d}{dt} \bar{f}_j^{(1)\delta}(t) \simeq \gamma(v') \{\bar{f}_{j-1}^{(1)\delta}(t) - \bar{f}_j^{(1)\delta}(t)\} + \beta(v') \{\bar{f}_{j+1}^{(1)\delta}(t) - \bar{f}_j^{(1)\delta}(t)\}, \tag{4.2.2}$$

where $\gamma = \gamma(v')$ and $\beta = \beta(v')$ have been defined in (3.2). The initial conditions are again $\bar{f}_j^{(1)\delta}(0) = \delta_{j,0}^P$. (These may be generalized.) Equation (4.2.2) will be

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solved using methods of spectral theory; however, first we describe briefly a Fourier-"type" transform method of solution (*cf.* Anstis *et al.* [1] for the non-periodic case). Define a set of functions

$$\Phi_k(j) = \exp\left(\hat{\imath}\frac{2\pi kj}{P}\right) \tag{4.2.3}$$

The functions $\Phi_k(j)$ satisfy the orthogonality conditions

$$\sum_{k=0}^{P-1} \overline{\Phi_k(j)}\,\Phi_k(j') = P\delta^P_{j\,j'}. \tag{4.2.4}$$

Next define

$$\eta_k(t) = \sum_{j=0}^{P-1} \Phi_k(j) \tilde{f}_j^{(1)\delta}(t).$$

Then (4.2.2) may be transformed to

$$\frac{d}{dt}\eta_k(t) \simeq \left\{\gamma(v')\left(\exp\left(\frac{2\pi\hat{\imath}k}{P}\right)-1\right)+\beta(v')\left(\exp\left(-\frac{2\pi\hat{\imath}k}{P}\right)-1\right)\right\}\eta_k(t) \tag{4.2.5}$$

which has the solution

$$\eta_k(t) \simeq \exp\left\{\gamma(v')\left(\exp\left(\frac{2\pi\hat{\imath}k}{P}\right)-1\right)t+\beta(v')\left(\exp\left(-\frac{2\pi\hat{\imath}k}{P}\right)-1\right)t\right\}\eta_k(0). \tag{4.2.6}$$

The $\tilde{f}_j^{(1)\delta}(t)$ may be obtained by applying the inverse transform:

$$\tilde{f}_j^{(1)\delta}(t) = \frac{1}{P}\sum_{k=0}^{P-1} \overline{\Phi_k(j)}\,\eta_k(t).$$

To implement the methods of spectral theory, write (4.2.2) in matrix form

$$\frac{d}{dt}\tilde{\mathbf{f}}^{(1)\delta}(t) \simeq \mathbf{C}^P \cdot \tilde{\mathbf{f}}^{(1)\delta}(t), \tag{4.2.7}$$

where $\tilde{\mathbf{f}}^{(1)\delta}$ is a P-dimensional vector with components $\tilde{f}_j^{(1)\delta}$ and $\mathbf{C}^P = (C^P_{ij})$ is a $P \times P$ matrix, where

$$C^P_{ij} = \beta\delta^P_{j-1,i} + \gamma\delta^P_{j+1,i} - (\gamma+\beta)\,\delta^P_{i,j}. \tag{4.2.8}$$

All indices are interpreted modulo P and may be taken to lie in the set $\{0, 1, \ldots, P-1\}$. Define the $P \times P$ matrix $\mathbf{C}^{0P}$ by

$$\mathbf{C}^P = \mathbf{C}^{0P} - (\gamma+\beta)\,\mathbf{I} \tag{4.2.9}$$

where $\mathbf{I}$ is the $P \times P$ identity matrix (*cf.* (3.2.4)). Then

$$\sigma(\mathbf{C}^P) = \sigma(\mathbf{C}^{0P}) - (\gamma+\beta)$$

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(and of course, $\sigma(\,) = P\sigma(\,)$ here). Thus to find $\sigma(\mathbf{C}^P)$ it will suffice to determine $\sigma(\mathbf{C}^{0P})$. The spectrum of $\mathbf{C}^{0P}$ may be calculated by applying the above-mentioned Fourier-"type" transformation to the eigenvalue equation. This in effect diagonalizes $\mathbf{C}^{0P}$. More directly, the spectrum of $\mathbf{C}^{0P}$ may be evaluated by writing $\mathbf{C}^{0P}$ as a sum of two commuting cyclic matrices $\mathbf{C}^{0P} = \boldsymbol{\beta}^P + \boldsymbol{\gamma}^P$ where $\boldsymbol{\beta}^P = (\beta^P_{i,j})$ and $\beta^P_{i,j} = \beta\delta^P_{j-1,i}$ and $\boldsymbol{\gamma}^P = (\gamma^P_{i,j})$, where $\gamma^P_{i,j} = \gamma\delta^P_{j+1,i}$. Since the eigenvalues of $\boldsymbol{\gamma}^P$ and $\boldsymbol{\beta}^P$ are non-degenerate, a set of simultaneous eigenvectors can be constructed for these matrices (see Ziock [15]). In fact we may choose these to be the complete orthonormal set $\{\mathbf{e}^n : n = 0, 1, 2, \ldots, P-1\}$ where

$$e^n_j = P^{-\frac{1}{2}} \exp\left(\frac{2\pi \hat{\imath} n j}{P}\right).$$

The corresponding eigenvalues are given by

$$\lambda n = \gamma \exp\left(-\frac{2\pi \hat{\imath} n}{P}\right) + \beta \exp\left(+\frac{2\pi \hat{\imath} n}{P}\right), \quad n = 0, 1, \ldots, P-1.$$

Consequently

$$\sigma(\mathbf{C}^P) = P\sigma(\mathbf{C}^P) = \left\{\lambda \in \mathbf{C} : \lambda = (\gamma+\beta)\left(\cos\left(\frac{2\pi n}{P}\right) - 1\right) + (\gamma-\beta)\,\hat{\imath}\sin\left(\frac{2\pi n}{P}\right),\right.$$
$$\left. n = 0, 1, \ldots, P-1\right\}. \tag{4.2.10}$$

4.3. Properties of the governing equation for general initial conditions

The general equations (4.1.2) could be solved using the Fourier-"type" transformation methods developed in (4.2). We develop instead spectral theoretic methods for comparison with (3.3). In matrix form, (4.1.12) become

$$\frac{d}{dt}\mathbf{f}^{(1)\delta}(t) \simeq \mathbf{C}^P(t)\cdot\mathbf{f}^{(1)\delta}(t), \tag{4.3.1}$$

where the $P \times P$ matrix

$$\mathbf{C}^P(t) = (C^P_{ij}(t))$$

and

$$C^P_{ij}(t) = \beta(v', t)\,\delta^P_{j-1,i} + \gamma(v', t)\,\delta^P_{j+1,i} - (\gamma(v', t) + \beta(v', t))\,\delta^P_{i,j}\cdot\mathbf{C}^P(t)$$

satisfy the commutation relations $[\mathbf{C}^P(t), \mathbf{C}^P(t')]_- = 0$ for all $t, t' \geqslant 0$. Consequently, the solution of (4.3.1) may be written as (*cf.* (3.3.2)):

$$\mathbf{f}^{(1)\delta}(t) \simeq \exp\left(\left[\frac{1}{t}\int_0^t dt'\, \mathbf{C}^P(t')\right] t\right) \mathbf{f}^{(1)\delta}(0). \tag{4.3.2}$$

The behaviour of $\hat{f}_j^{(1)\delta}(t)$ in time is determined by the spectrum of the operator $(1/t)\int_0^t dt'\, \mathbf{C}^P(t')$ which, by comparison with (4.2), is given by

$$\begin{aligned} &\sigma\left(\frac{1}{t}\int_0^t dt'\, \mathbf{C}^P(t')\right) \\ &= P\sigma\left(\frac{1}{t}\int_0^t dt'\, \mathbf{C}^P(t')\right) \\ &= \left\{\lambda \in \mathbf{C} : \lambda = \left\{\frac{1}{t}\int_0^t dt'(\gamma^P(v', t') + \beta^P(v', t'))\right\}\left(\cos\left(\frac{2\pi n}{P}\right) - 1\right)\right. \\ &\qquad + \left\{\frac{1}{t}\int_0^t dt'(\gamma^P(v', t') - \beta^P(v', t'))\right\} \hat{\imath}\sin\left(\frac{2\pi n}{P}\right), \\ &\qquad \left. n \in \{0, 1, 2, \ldots, P-1\}\right\}. \end{aligned} \tag{4.3.3}$$

Since we are working in a finite dimensional space, we may give a more expiicit representation of the evolution operator $\exp(\int_0^t dt'\, \mathbf{C}^P(t'))$. It is clear from a decomposition of $\int_0^t dt'\, \mathbf{C}^P(t')$ into a sum of cyclic matrices that this operator has the same eigenvectors as $\mathbf{C}^P$. These may be chosen as the complete orthonormal set $\{\mathbf{e}^n : n = 0, 1, \ldots, P-1\}$ previously defined. The corresponding eigenvalues are:

$$\begin{aligned} \lambda n(t) = &\int_0^t dt'(\gamma^P(v', t') + \beta^P(v', t'))\left(\cos\left(\frac{2\pi n}{P}\right) - 1\right) \\ &+ \int_0^t dt'(\gamma^P(v', t') - \beta^P(v', t'))\, \hat{\imath}\sin\left(\frac{2\pi n}{P}\right), \quad n \in \{0, 1, \ldots, P-1\} \end{aligned} \tag{4.3.4}$$

The projection operator corresponding to the nth eigenspace is given by $\mathbf{E}_n = (\mathbf{e}_j^n)(\mathbf{e}_j^n)^H$ where H is the Hermitian transpose. The (r, s) component of $\mathbf{E}_n$ is given by

$$(\mathbf{E}_n)_{r,s} = \frac{1}{P}\exp\left(\frac{2\pi \hat{\imath} n(r-s)}{P}\right). \tag{4.3.5}$$

Since all eigenvalues are non-degenerate, the following spectral representation

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applies (Dunford and Schwartz [14])

$$\exp\left(\int_0^t dt'\,\mathbf{C}^P(t')\right) = \sum_{n=0}^{P-1} \exp\left(\int_0^t dt'\,\lambda n(t')\right)\mathbf{E}_n. \tag{4.3.6}$$

Consequently

$$\bar{f}_j^{(1)\delta}(t) \simeq \sum_{n=0}^{P-1}\sum_{k=0}^{P-1}\frac{1}{P}\exp\left(\int_0^t dt'\,\lambda n(t')\right)\exp\left(\frac{2\pi i n(j-k)}{P}\right)\bar{f}_k^{(1)\delta}(0). \tag{4.3.7}$$

To consider the asymptotic behaviour of the spectrum (4.3.3) as $t\to\infty$, make the special choice of initial conditions

$$\bar{f}_0^{(1)}(z_1;\,0) = \sum_{\kappa=-\infty}^{+\infty} \delta(g_1+\kappa L)\,\delta(v_1-v')$$

and for $j\not\equiv 0 \pmod P$ let $\bar{f}_j^{(1)}(z_1;\,0)$ satisfy the constraints specified in (4.1) together with the condition that $\bar{f}_j^{(1)}(z_1;\,0) = \bar{f}_j^{s}(g_1)\cdot h(v_1)$, $h(\,)$ as in (3.2.1) and (3.2.2). In this case

$$\gamma^P(v',t) = \int_{-\infty}^{v'} dv_2(v'-v_2)\,h(v_2)\cdot\sum_{k=1}^{P-1}\bar{f}_k^{s}((v'-v_2)\,t)$$

and

$$\beta^P(v',t) = \int_{v'}^{\infty} dv_2(v_2-v')\,h(v_2)\cdot\sum_{k=1}^{P-1}\bar{f}_k^{s}((v'-v_2)\,t). \tag{4.3.8}$$

As $t\to\infty$, $\sum_{k=1}^{P-1}\bar{f}_k^{s}((v'-v_2)\,t)$ becomes highly oscillatory as a function of v_2. This suggests that the asymptotic behaviour of $\gamma^P(v',t)$ and $\beta^P(v',t)$ may be determined by a suitable generalization of the Riemann–Lebesque lemma. Define

$$\bar{f}^{s}(x) = \sum_{k=1}^{P-1}\bar{f}_k^{s}(x), \quad F(x) = \bar{f}^{s}(x)-\rho$$

and finally

$$\mathscr{F}(v'-v_2;\,t) = \int_{v'}^{v_2} dw\,F((v'-w)\,t).$$

Since $\rho=(P-1)/L$ and the $\bar{f}_k^{s}$ are normalized, we may show that $\mathscr{F}(L\kappa/t;\,t)=0$ for all integers κ, hence $\mathscr{F}(w,t)$ is periodic in w of period L/t. We must examine expressions of the form $\int_{v'}^{\infty} dv\,\phi(v)\bar{f}^{s}((v'-v)\,t)$, where $\phi(v)$, $(d/dv)\,\phi(v)\to 0$ as $|v|\to\infty$ "sufficiently fast". Now

$$\int_{v'}^{\infty} dv\,\phi(v)\bar{f}^{s}((v'-v)\,t) = \rho\int_{v'}^{\infty} dv\,\phi(v) + \int_{v'}^{\infty} dv\,\frac{d}{dv}\phi(v)\,\mathscr{F}(v'-v;\,t)$$

and

$$|\mathscr{F}(v'-v;\, t)| \leqslant \frac{1}{t}\int_0^L dw\,|F(w)|.$$

Consequently

$$\int_{v'}^{\infty} dv\, \phi(v) \bar{f}^{s}(v'-v)\, t) = \rho \int_{v'}^{\infty} dv\, \phi(v) + O\left(\frac{1}{t}\right) \quad \text{as } t \to \infty.$$

Therefore

$$\beta^P(v', t) = \beta(v') + O\left(\frac{1}{t}\right) \quad \text{as } t \to \infty.$$

A similar analysis shows that

$$\gamma^P(v', t) = \gamma(v') + O\left(\frac{1}{t}\right) \quad \text{as } t \to \infty.$$

Here $\beta(v')$ and $\gamma(v')$ are the same quantities as defined in (3.2). Consequently $\beta^P(v', t)$ and $\gamma^P(v', t)$ are $(C-1)$ summable to $\beta(v')$ and $\gamma(v')$ (resp.). Hence, as $t \to \infty$, the set $((1/t)\int_0^t dt'\, \mathbf{C}^P(t'))$ approaches $\sigma(\mathbf{C}^P)$ as in (4.2.10).

5. Summary

In Sections 3 and 4, we have set up the non-periodic and periodic problems so that in each case the average background particle density is the same (ρ). This has resulted in an interesting relationship between the spectra of the operators $\mathbf{C}(t)$ and $\mathbf{C}^P(t)$ associated with the time evolution of $\mathbf{f}^{(1)\delta}$ and $\bar{\mathbf{f}}^{(1)\delta}$ (resp.). This relationship is particularly clear in the cases where we have chosen specialized initial conditions (so the spectra are independent of time). In the non-periodic case, the (residue) spectrum is an ellipse in the complex plane. For the periodic case, the (point) spectrum consists of P points situated on this ellipse. In both cases $\lambda = 0$ is a point of the spectrum (representing the existence of an equilibrium state). All other points of the spectrum have negative real part (representing a decay to equilibrium).

Let us now consider the "thermodynamic limit" of the periodic case in the sense that we let $L \to \infty$, $P \to \infty$ so that $\rho = (P-1)/L$ is constant. As P increases, the number of eigenvalues (of $\mathbf{C}^P$) increases. However, they remain on the ellipse (which is invariant since ρ is constant) and as $P \to \infty$, they coalesce to form the whole ellipse. If we take the high density limit $P \to \infty$, $L = \text{constant}$ (so $\rho \to \infty$), the number of eigenvalues (of $\mathbf{C}^P$) on the ellipse again increases in proportion to P. However, since the size of the ellipse also increases in proportion to P, they do not coalesce. It it also valuable to note qualitatively that the nature of the time evolution is insensitive to the particular choice of inhomogeneous initial conditions. Indeed the asymptotic form of the evolution equations depends only on the mean background density ρ rather than on the details of the initial distribution of background particles.

For the non-periodic case, we may determine the nature of the asymptotic approach to equilibrium of the delta-function part of the distribution functions. We shall make use of the solutions for $f_j^{(1)\delta}(t)$ obtained from the Fourier analysis. For the initial condition $f_j^{(1)\delta}(0) = \delta_{j,0}$, these assume the form

$$f_j^{(1)\delta}(t) = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta \exp(i[(\beta-\gamma)(\sin\theta)\,t - j\theta])\exp((\gamma+\beta)(\cos\theta - 1)\,t). \qquad (5.1)$$

The asymptotic analysis of this expression as $t\to\infty$ is suited to Laplace's method (see Carrier *et al.* [3]). We obtain as $t\to\infty$,

$$\begin{aligned} f_j^{(1)\delta}(t) &\sim \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\theta \exp(i[(\beta-\gamma)\,t - j]\,\theta)\exp(-\tfrac{1}{2}(\gamma+\beta)\,\theta^2 t) \\ &= \frac{1}{(2\pi)^{\frac{1}{2}}}\frac{1}{[(\gamma+\beta)\,t]^{\frac{1}{2}}}\exp\left(-\frac{(\beta-\gamma)^2 t}{2(\beta+\gamma)} + \frac{(\beta-\gamma)_j}{(\beta+\gamma)} - \frac{j^2}{2(\gamma+\beta)\,t}\right) \\ &\approx \left(\frac{1}{O(t/t_{mf})}\right)^{\frac{1}{2}}\exp(-O(t/t_{mf})). \end{aligned} \qquad (5.2)$$

This modified exponential decay is associated with a time scale $O(t_{mf})$ as expected. As mentioned above, this type of decay gives an accurate description of the behaviour of the periodic system for sufficiently small times.

Usually correlation functions associated with the delta-function part of the distribution functions are derived from expressions of the form

$$\int_{-\infty}^{+\infty} dv'\, C(v') f_j^{(1)\delta}(t) \qquad (5.3)$$

for suitable functions $C(v')$. Note that $f_j^{(1)\delta}(t)$ depends implicitly on v' through the dependence of γ and β on v'. The nature of (5.3) as a function of time will depend on the nature of $\beta-\gamma$ and $\beta+\gamma$ as functions of v'. From the definitions of these functions

$$\beta(v') - \gamma(v') = -\rho v'$$

and (5.4)

$$\beta(v') + \gamma(v') \geq \int_{-\infty}^{+\infty} dv\,|v - v^h|\,h(v) > 0,$$

where

$$\int_{-\infty}^{v^h} dv\, h(v) = \int_{v^h}^{\infty} dv\, h(v).$$

It follows from (5.2) that the major contribution to $\int_{-\infty}^{+\infty} dv'\, C(v') f_j^{(1)\delta}(t)$ for large t comes from the neighbourhood of $v' = 0$. This corresponds to the degenerate case where the elliptical spectrum of **C** lies along the negative real axis. If we suppose that $C(v') \sim Cv'^n$ as $v' \to 0$, then as $t \to \infty$

$$\int_{-\infty}^{+\infty} dv'\, C(v') f_j^{(1)\delta}(t) \sim O\left(\left(\frac{t}{t_{mf}}\right)^{-(n/2+1)}\right)$$

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Appendix A

In this appendix, we give a meaning to expressions of the form

$$\text{“lim”} \langle \delta(z^1 - z_{j_1}(t)) \ldots \delta(z^n - z_{j_n}(t)) \rangle_V$$

for both canonical and grand canonical ensemble averages. A difficulty arises because we wish to work ultimately with a system occupying an infinite region of coordinate space. For such a system we cannot define a complete distribution function (containing all the information about the system). However, we would still like to think of the reduced distribution functions as related in some sense to a complete distribution function. Such a relationship guarantees that the reduced distribution functions satisfy certain consistency relations. Consequently we shall introduce certain complete distribution functions associated with finite regions of coordinate space and regard the infinite system as being described by a suitable infinite volume limit of these.

First we develop this programme via the canonical ensemble. Let

$$F_{\text{c.e.}}^{M,N}(V | z_{-M};\, z_{-M+1};\, \ldots;\, z_N;\, t)$$

be a complete normalized $(M+N+1)$-particle distribution function in the canonical ensemble associated with a system of $M+N+1$ particles confined to a region V of

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coordinate space. The particles are labelled with an index $j \in \{-M, -M+1, \ldots, N\}$ and are ordered from left to right with j increasing (see previous discussion). Here z_j denotes the position in phase space of particle j (at a time t). In terms of this function, the above average is given by

$$\langle \delta(z^1 - z_{j_1}(t)) \ldots \delta(z^n - z_{j_n}(t)) \rangle_V$$
$$= \left(\prod_{i=-M}^{N} \int_V dg_i \int_{-\infty}^{+\infty} dv_i \right) \delta(z^1 - z_{j_1})\, \delta(z^2 - z_{j_2}) \ldots \delta(z^n - z_{j_n})$$
$$\times F_{\text{c.e.}}^{M,N}(V | z_{-M};\, z_{-M+1};\, \ldots;\, z_N;\, t),$$

where we have chosen M and N sufficiently large that

$$\{j_1, j_2, \ldots, j_n\} \subseteq \{-M, -M+1, \ldots, N\}.$$

In this case "lim" is taken to be a suitable thermodynamic limit. For the non-periodic case, we may choose $V = [-M\rho, N\rho]$ and then let $M, N \to \infty$ with ρ fixed. For the periodic case, we may choose

$$\left[-M\left(1 - \frac{1}{P}\right)\rho, N\left(1 - \frac{1}{P}\right)\rho \right]$$

and again let $M, N \to \infty$ with ρ fixed.

Next consider the corresponding analysis for the grand canonical ensemble. For $\kappa \in \mathbf{R}$ let $[\kappa]$ denote the largest integer not greater than κ. The proportion of systems of the grand canonical ensemble which are represented by a point

$$(z_{-[N/2]}, z_{-[N/2]+1}, \ldots, z_{-[N/2]+N-1})$$

in the N-particle phase space at a time t is determined by

$$F_{\text{g.c.e.}}^{N}(V | z_{-[N/2]};\, \ldots;\, z_{-[N/2]+N-1};\, t).$$

Again the particles are labelled with an index

$$j \in \left\{ -\left[\frac{N}{2}\right], -\left[\frac{N}{2}\right] + 1, \ldots, -\left[\frac{N}{2}\right] + N - 1 \right\}$$

and are ordered from left to right with j increasing (see previous discussion). Again z_j denotes the position of particle j (at a time t). These functions are normalized by the condition

$$\sum_{N=0}^{\infty} \left(\prod_{i=-[N/2]}^{-[N/2]+N-1} \int_V dg_i \int_{-\infty}^{+\infty} dv_i \right) F_{\text{g.c.e.}}^{N}(V | z_{-[N/2]};\, \ldots;\, z_{-[N/2]+N-1};\, t) = 1$$

(with a suitable interpretation for the $N = 0$ term). In terms of these functions, the above average is given by

$$\langle \delta(z^1 - z_{j_1}(t)) \ldots \delta(z^n - z_{j_n}(t)) \rangle_V$$

$$= \sum_{N=N^*}^{\infty} \left(\prod_{i=-[N/2]}^{-[N/2]+(N-1)} \int_V dg_i \int_{-\infty}^{+\infty} dv_i \right) \delta(z^1 - z_j)(z^2 - z_{j_2}) \ldots \delta(z^n - z_{j_n})$$

$$\times F^N_{\text{g.c.e.}}(V | z_{-[N/2]}; \ldots; z_{-[N/2]+N-1}; t)$$

where N^* is the minimum value of N such that

$$\{j_1, j_2, \ldots, j_n\} \subseteq \left\{ -\left[\frac{N}{2}\right], -\left[\frac{N}{2}\right] + 1, \ldots, -\left[\frac{N}{2}\right] + N - 1 \right\}.$$

We should point out that the inclusion or omission of any particular N-particle phase space component of the grand canonical ensemble is of no consequence when we consider the $V \to \infty$ limit. Secondly, the inclusion of a $1/N!$ weight in the sum above does not appear here (see also Anstis *et al.* [1]). We may think of this as a result of the fact that $F^N_{\text{g.c.e.}}$ pertain to an ordered system of particles thus restricting their support to a fraction $1/N!$ of total coordinate space, that is, the $1/N!$ weighting is implicit in the definition. Finally, we remark that in this case "lim" is simply taken as an infinite volume limit. More explicitly, if $V = [-L', +L']$, we require $L' \to +\infty$.

Appendix B

(i) Ordering of particles in coordinate space

We shall prove that the inequality

$$\int_{-\infty}^{+\infty} dg\, g f^s_{j_1}(g; t) \geqslant \int_{-\infty}^{+\infty} dg\, g f^s_{j_2}(g; t) \quad \text{for } j_1 \geqslant j_2$$

holds as a consequence of the ordering of the particles. To prove this inequality, we shall need a result concerning the single particle distribution function. Firstly, a finite system V of N particles is considered. For such a system

$$f^{(1)}_{j_1}(z_1; t) = \frac{1}{(N-1)!} \left(\prod_{i=2}^{N} \int_{V \times \mathbf{R}} dz_i \right) \sum_{\substack{j_2 j_3 \ldots j_N \neq j_1 \\ j_\alpha \neq j_\beta, \alpha \neq \beta}} f^{(N)}_{j_1 j_2 \ldots j_N}(z_1; \ldots; z_N; t)$$

$$= \frac{1}{(N-1)!} \left(\prod_{i=2}^{N} \int_{V \times \mathbf{R}} dz_i \right) f^{(N)}_j(z_1; \ldots; z_N; t).$$

However,

$$f^{(N)}_{j_1 j_2 \dots j_N}(z_1;\, z_2;\, \dots;\, z_N;\, t) = f^{(N)}_{j_{p_1} j_{p_2} \dots j_{p_N}}(z_{p_1};\, z_{p_2};\, \dots;\, z_{p_N};\, t)$$

where $p\colon (1,2,3,\dots,N) \to (1,2,3,\dots,N)$ is a permutation of these N elements. Consequently $f^{(1)}_j(z_1;\, t)$ is also given by the expression:

$$f^{(1)}_j(z_j;\, t) = \prod_{i=1, i\neq j}^{N} \int_{V\times\mathbf{R}} dz_i\, f^{(N)}_{1\,2 \dots j \dots N}(z_1;\, z_2;\, \dots;\, z_{j_1};\, \dots;\, z_N;\, t).$$

Therefore

$$\begin{aligned}
&\int dg\, g\{f^{g}_{j_1}(g;\, t) - f^{g}_{j_2}(g;\, t)\}\\
&\qquad = \prod_{i=1}^{N} \int_{V\times\mathbf{R}} dz_i (g_{j_1} - g_{j_2})\, f^{(N)}_{1\,2\dots j_2 \dots j_1 \dots N}(z_1;\, \dots;\, z_{j_2};\, \dots;\, z_{j_1};\, \dots;\, z_N;\, t)\\
&\qquad \geqslant 0 \quad \text{since } f^{(N)}_{1\,2\dots j_2\dots j_1\dots N}(z_1;\, \dots;\, z_{j_2};\, \dots;\, z_{j_1};\, \dots;\, z_N;\, t)\\
&\qquad = 0 \quad \text{if } g_{j_1} < g_{j_2}.
\end{aligned}$$

The result for an infinite system follows by taking the thermodynamic limit.

(ii) Constraints on particle number, momentum and energy

For our choice of initial conditions $f^{(1)}_j(z;\, 0)$ to represent a physical system, we must demand that (i) associated with any finite region of coordinate space there is a finite particle number, momentum and energy. Furthermore, we shall require that (ii) for regions of a given size, there is a uniform bound on each of these quantities. To see the nature of the constraint that these conditions impose on the distribution functions, consider first the case where we have the factorization property $f^{(1)}_j(z;\, 0) = f^{g}_j(g)\, h(v)$ for $j \neq 0$. For normalization, we choose that

$$\int_{-\infty}^{+\infty} dv\, h(v) = 1.$$

In order that each particle have finite (kinetic) energy, we require that

$$\int_{-\infty}^{+\infty} dv\, v^2\, h(v) < \infty.$$

Using this constraint together with the normalization condition we note that

$$\int_{-\infty}^{+\infty} dv\, |v|\, h(v) < \int_{-\infty}^{+\infty} dv\, h(v) + \int_{|v|>1} v^2\, h(v) < \infty$$

so $\int_{-\infty}^{+\infty} dv\, vh(v) < \infty$. This is necessary for each particle to have finite momentum. For (i), it is sufficient that

$$\sum_{j=-\infty}^{+\infty} f_j^s(g)$$

be locally integrable. For (ii), we could divide the real line up into intervals of equal length and demand that there be a uniform bound on the particle numbers associated with these intervals. A necessary condition for (ii) is that

$$\frac{1}{\mathscr{L}} \int_0^{\mathscr{L}} dg \sum_{j=-\infty}^{+\infty} f_j^s(g)$$

and

$$\frac{1}{\mathscr{L}} \int_{-\mathscr{L}}^{0} dg \sum_{j=-\infty}^{+\infty} f_j^s(g)$$

be bounded. Furthermore, if we require that there should exist an average particle density for the infinite system, then the limits of these expressions as $\mathscr{L} \to \infty$ should exist, that is

$$\sum_{j=-1}^{-\infty} f_j^s(g) \quad \text{and} \quad \sum_{j=1}^{+\infty} f_j^s(g)$$

should be $(C-1)$ summable. However, $(C-1)$ summability is not sufficient for (ii). If we want the asymptotic analysis of (3.3) to be valid, then we require that

$$\sum_{j=-\infty}^{+\infty} f_j^s$$

be bounded and strongly measurable. In particular, the choice that on $(0, \infty)$ and $(-\infty, 0)$ separately that $\sum_{j=-\infty}^{+\infty} f_j^s$ be bounded and continuous guarantees all the above properties. If we do not have the factorization property, then the various quantities must be examined separately. In order that the particle number be well behaved, we must impose constraints on

$$\sum_{j=-\infty}^{+\infty} \int_{-\infty}^{+\infty} dv\, f_j^{(1)}(g, v;\, 0)$$

analogous to the above. The behaviour of the (kinetic) energy is determined by the quantity

$$\sum_{j=-\infty}^{+\infty} \int_{-\infty}^{+\infty} dv\, v^2 f_j^{(1)}(g, v;\, 0)$$

and separate constraints must be imposed on this quantity to guarantee (i) and (ii) and the existence of a mean energy density. That (i) and (ii) are valid for the momentum is a consequence of the corresponding properties for particle number and energy.

Finally, we mention that there should be sufficient conditions on $f_j^{(1)}$ to guarantee that $\gamma(v'; t)$ and $\beta(v'; t)$ are suitably well behaved for fixed v' as a function of t. In particular we must be able to integrate the governing equations to obtain a solution.

Appendix C

Spectral analysis of $\mathbf{C}^0$ in ι^2

A sequence space analysis (*cf.* 3.2) may be employed noting that ι^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 $L^2(0, 2\pi)$ be the (Hilbert) space of Lebesgue square integrable functions on $[0, 2\pi]$. This space is congruent to ι^2, that is, there exists an isometric isomorphism $J: \iota^2 \to L^2(0, 2\pi)$. If $\mathbf{y} \in \iota^2$, then it may be represented by a function $Y = J\mathbf{y}$ in $L^2(0, 2\pi)$ and a bounded linear operator $\mathbf{G}$ on ι^2 is represented by $G = J\mathbf{G}J^{-1}$ on $L^2(0, 2\pi)$. Using the isometric and isomorphic properties of J, it is easy to show that $\sigma(G) = \sigma(\mathbf{G})$, or more specifically that $P\sigma(G) = P\sigma(\mathbf{G})$, $C\sigma(G) = C\sigma(\mathbf{G})$ and $R\sigma(G) = R\sigma(\mathbf{G})$.

Next let us determine the operator C^0 on $L^2(0, 2\pi)$ corresponding to the matrix operator $\mathbf{C}^0$ on ι^2. To do this, we note that J may be realized in the following way. For any $\mathbf{y} \in \iota^2$, $Y = J\mathbf{y} \in L^2(0, 2\pi)$ is given by

$$Y(\eta) = \sum_{j=-\infty}^{+\infty} \exp(\hat{\imath} j\eta)\, y_j, \quad \eta \in [0, 2\pi].$$

Let $\mathbf{y} = \mathbf{C}^0\mathbf{x}$, then in component form this equation becomes

$$y_j = \gamma x_{j-1} + \beta x_{j+1}.$$

Apply the transform

$$\sum_{j=-\infty}^{+\infty} \exp(\hat{\imath} j\eta)$$

to this equation, giving

$$\sum_{j=-\infty}^{+\infty} \exp(\hat{\imath} j\eta)\, y_j = (\gamma \exp(\hat{\imath}\eta) + \beta \exp(-\hat{\imath}\eta) \sum_{j=-\infty}^{+\infty} \exp(\hat{\imath} j\eta)\, x_j, \quad \eta \in [0, 2\pi].$$

Writing $Y = J\mathbf{y}$ and $X = J\mathbf{x}$, this equation becomes

$$Y(\eta) = (\gamma \exp(\hat{\imath}\eta) + \beta \exp(-\hat{\imath}\eta))\, X(\eta), \quad \eta \in [0, 2\pi].$$

We conclude that C^0 is given by the normal, multiplicative operator

$$\mathrm{C}^0 = \gamma \exp(\hat{\imath}\eta) + \beta \exp(-\hat{\imath}\eta), \quad \eta \in [0, 2\pi].$$

Such operators are called factor transforms and a sufficient condition that they represent bounded linear operators on $L^2(0, 2\pi)$ is that they be essentially bounded and measurable (as a function of η) on $[0, 2\pi]$ (*cf.* Hille [9] for the $L^2(-\infty, +\infty)$ case). Thus C^0 above satisfies the required condition.

Consider the behaviour of the operator $\lambda - C$. Suppose

$$\lambda \notin E = \{\lambda \in \mathbf{C}\colon \lambda = \gamma \exp(\hat{\imath}\theta) + \beta \exp(-\hat{\imath}\theta)\colon \theta \in [0, 2\pi)\}.$$

Then $\lambda - C^0$ is continuous, bounded (in modulus) and bounded away from zero for $\eta \in [0, 2\pi]$. Consequently, $\lambda - C^0$ is invertible and therefore $\lambda \notin \sigma(C^0)$. So $\sigma(C^0) \subseteq E$. From the general theory of normal operators (see Dunford and Schwartz [14]), $R\sigma(C^0) = \emptyset$. Thus it remains to determine $P\sigma(C^0)$ and $C\sigma(C^0)$.

Suppose $\lambda \in E$ and $(\lambda - C^0)X(\eta) = 0$ in $L^2[0, 2\pi]$. Since $\lambda - C^0$ is a continuous function of η and equal to zero at only one point of $(0, 2\pi)$, it follows that $X(\eta) = 0$ is the only $L^2(0, 2\pi)$ solution of the above equation. Consequently $P\sigma(C) = \emptyset$.

Again choose $\lambda \in E$, that is, $\lambda = \gamma \exp(\hat{\imath}\eta^*) + \beta \exp(-\hat{\imath}\eta^*)$, where $\eta^* \in (0, 2\pi)$, and let $Y(\eta) \in L^2(0, 2\pi)$ be continuous and non-zero at $\eta = \eta^*$. Suppose

$$Y(\eta) = \{\lambda - (\gamma \exp(\hat{\imath}\eta) + \beta \exp(-\hat{\imath}\eta))\}\, X(\eta),$$

where $\eta \in (0, 2\pi)$. Then

$$X(\eta) = Y(\eta)/\{\lambda - (\gamma \exp(\hat{\imath}\eta) + \beta \exp(-\hat{\imath}\eta))\} \notin L^2(0, 2\pi).$$

Consequently $\lambda - C^0$ is not invertible, so $\lambda \in \sigma(C^0)$. In conclusion

$$P\sigma(C^0) = P\sigma(\mathbf{C}^0) = \emptyset = R\sigma(\mathbf{C}^0) = P\sigma(C^0)$$

and

$$C\sigma(C^0) = E = C\sigma(\mathbf{C}^0).$$

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