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Characterization of microstates for confined systems and associated scale-dependent continuum fields via Fourier coefficients

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Abstract
The phase space description of a system of N point masses confined to a rectangular box is shown to be equivalent to knowledge of a minimal set of $6N$ complex Fourier coefficients associated with the discrete distributions of matter and momentum. The corresponding real-valued truncated Fourier series yield continuum densities of particle number and momentum at a specific length scale, ϵ_{min}. Continuum descriptions at any scale $\epsilon > \epsilon_{\text{min}}$ correspond to further truncation of these series. Attention is drawn to the relevance of the results to recent investigations of reproducible macroscopic behaviour, at a given pair ϵ and Δ of length time scales, using projection operator methodology.

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1. Preamble

Projection operator methodology [1], first advocated by Zwanzig [2], provides a formal procedure for arriving at equations which describe (scale-dependent) macroscopic behaviour starting from a phase space model of interacting particles [3–5]. There are, however, two fundamental problems:

F.P.1 Selection of an appropriate projection operator P, and

F.P.2 Justification of an operator identity (which involves combinations of P with the Liouville operator) central to the establishment of the relevant master equation.

F.P.2 is a major unproved result in the semigroup theory of operators for a general projection P on the space of functions of points ('microstates') X in phase space [6]. Furthermore, F.P.1

is of central importance, since all physical interpretations of macroscopic quantities depend explicitly upon P, as does the physical range of validity of the theory (via P-related hypotheses of local equilibrium and dynamic ergodicity). The choice of P may also bear crucially upon F.P.2.

In [4, 5] the development centred upon selection of a so-called *reduction map* $a_\varepsilon(X)$ at scale ε which identifies with each microstate the corresponding *ε-scale macrostate*. For particles confined to a rectangular box, $a_\varepsilon(X)$ was defined in [4] to be an ordered list of Fourier coefficients corresponding to the corpuscular distributions of mass, momentum, and energy (including interaction and confinement potential energies). The coefficients in question are only those associated with wavelengths in excess of ε. Of course, for macroscopic phenomena, ε greatly exceeds nearest-neighbour separations, and $a_\varepsilon(X)$ constitutes only very limited information about microstate X.

It is here shown that the phase space description of a confined set of N particles is *equivalent* to a set of $6N$ Fourier coefficients (modulo a realistic and very weak assumption about corpuscular motions). Further, there is a distinguished scale (smallest wavelength) associated with these coefficients. The $6N$ coefficients define two analytic real-valued functions (one scalar-valued, giving mass distribution, and the other vector-valued, delivering momentum distribution) which incorporate *complete* information about the microscopic situation. This result shows that it might be better, in the context of the overall study outlined above, to work directly with Fourier coefficients rather than phase space variables. For example, in holding on to only those coefficients with associated wavelengths greater than ε it is clear just what information is being neglected. This is not the case with the choice $a_\varepsilon(X)$ of reduction map discussed above. While there are still central questions about the role of energy considerations in such a change, there are significant simplifications in the mathematical representation of the corresponding projection operator. The existing development involves formal use of Dirac delta distributions, which are defined via piecewise changes of variable of a somewhat complicated nature. In working directly with Fourier coefficients there is a single change of variable from phase space as here delineated, after which the projection operator is defined in terms of multiple integration without any need to appeal to Dirac formalism. Such simplification may aid progress in F.P.2. (In this context the authors have been collaborating with Wilson Lamb and John Stewart (Strathclyde) and Aldo Belleni-Morante (Florence), investigating the relevance of B-bounded semigroups.)

While the foregoing motivates what follows, to workers in continuum mechanics there is intrinsic interest in displaying scale-dependent analytic functions which represent volumetric densities of extensive quantities. What is somewhat surprising is that there are such functions which incorporate complete information about the (classical) microscopic situation.

2. Introduction

Given a system of N point masses confined to the interior of a rectangular box, coefficients in the (multiple) Fourier series representations of the discrete distributions of corpuscular locations and momenta can be computed. Adopting the complex formulation of such series enables $6N$ complex coefficients to be identified from which complete phase space information can be recovered. These coefficients correspond to terms with wavelengths no smaller than $\epsilon_{\min} = L/N$, where L denotes the minimum box dimension. Together with their complex conjugates, such coefficients yield truncated Fourier series which serve as continuum fields constituting number and momentum densities at length scale $\epsilon_{\min}$. Such densities at an *arbitrary* scale ϵ correspond to truncation of these series with a wavelength cut-off ϵ. (Choices $\epsilon < \epsilon_{\min}$ are of no physical interest since in such cases coefficients in terms with wavelengths less than $\epsilon_{\min}$ depend upon the remaining coefficients, and are hence redundant.) Changing from phase space variables to the equivalent $6N$ Fourier coefficients is thus advantageous in its introduction of a hierarchy of scales. If information about the system is available only at a scale $\epsilon > \epsilon_{\min}$ then there is a natural subdivision of the $6N$ coefficients into those which correspond to wavelengths not less than ϵ and those which do not.

In section 3 a system of N particles confined to a linear interval is considered. Knowledge of N coefficients in the complex Fourier series representation of particle locations is shown to be completely equivalent to knowledge of these locations, whether or not particles coincide. Regard is paid to the nature of these coefficients, which determine uniquely, and are uniquely determined by, a polynomial of degree N. Not all such polynomials, and hence coefficients, correspond to particle distributions. In particular, it is shown how the N complex polynomial coefficients incorporate at most N distinct items of real-valued information. A further set of N coefficients in the complex Fourier series representation of the momentum distribution is shown to deliver individual corpuscular momenta whenever no two particles coincide. The foregoing coefficients and their conjugates delineate truncated real-valued analytic functions which serve as continuum location and momentum densities: the smallest wavelengths involved are not less than L/N, where L is the interval length. Generalization to three dimensions is effected in section 4. Knowledge of a set of $3N$ coefficients in each of the (triple, complex) Fourier series representations of particle locations and momenta is shown to suffice to recover such locations and corresponding momenta, provided no two particles have the same x coordinate (where axes are chosen parallel to box edges). Continuous dependence of locations and momenta upon time allows this latter restriction to be lifted for so-called *regular* motions. These are motions for which, during any finite time interval, the time measure of all instants at which two or more particles have the same x coordinate is zero. Continuum location and momentum densities are exhibited which embody all information concerning corpuscular locations and momenta, and are minimal in this respect. These truncated real-valued triple Fourier series may be further truncated to yield continuum descriptions at any macroscopic scale. A remark on the utility of selecting a description with different scales in different directions is made in the context of a two-phase macroscopic system. Concluding remarks are made in section 5 on the relevance of the results to studies of the effect of microscopic behaviour upon macroscopic fields via projection operator methodology.

3. One-dimensional considerations

Consider a set of N point masses confined within a linear interval of length $2l$. The location of each point mass is determined by its signed distance $x_j (j = 1, 2, \ldots, N)$ from the interval mid-point, whence $-l < x_j < l$. The particle distribution is

$$D(x) := \sum_{j=1}^{N} \delta(x - x_j). \tag{3.1}$$

The formal Fourier[3] series for D is given by

$$D(x) \sim \sum_{n=-\infty}^{+\infty} c_n \, \mathrm{e}^{\mathrm{i}n\pi x/l} \tag{3.2}$$

where

$$c_n := \frac{1}{2l} \int_{-l}^{l} D(y) \mathrm{e}^{-\mathrm{i}n\pi y/l} \, \mathrm{d}y = \frac{1}{2l} \sum_{j=1}^{N} \mathrm{e}^{-\mathrm{i}n\pi x_j/l}. \tag{3.3}$$

[3] For a precise discussion of Fourier series of distributions see [7].

We now prove that knowledge of $c_1, c_2, \ldots, c_N$ determines the locations of the point masses. More precisely, for $-l < x_j < l$ $(j = 1, 2, \ldots, N)$ let

$$\beta : \{x_1, x_2, \ldots, x_n\} \longrightarrow (c_1, c_2, \ldots, c_N) \tag{3.4}$$

denote the map defined by (3.3).

Remark 1. In writing (3.4) we have noted that, in using (3.3) to calculate c_n, all permutations of $x_1, x_2, \ldots, x_N$ yield the same value. Accordingly β is a function of the (unordered) set $\{x_1, x_2, \ldots, x_N\}$. Said differently, if an ordered N-tuple $(c_1, c_2, \ldots, c_N)$ lies in the range of β then all that can be inferred about any particle distribution which gives rise to this N-tuple is the set of N locations of the particles. The location of any *specific* particle is known only to be one of N possibilities.

Proposition 1. *β is invertible on its range.*

Proof. Writing

$$c'_n := 2lc_n \qquad \text{and} \qquad a_j := \mathrm{e}^{-\mathrm{i}\pi x_j/l} \tag{3.5}$$

relations (3.3) become

$$c'_n = \sum_{j=1}^{N} a_j^n. \tag{3.6}$$

We wish to show that, if $c'_1, \ldots, c'_N$ derive from a set $\{x_1, \ldots, x_N : -l < x_j < l\}$, via (3.6) and $(3.5)_2$, then this set is unique. To this end it can be shown that the N symmetric homogeneous multinomials c'_n in $a_1, a_2, \ldots, a_N$ suffice to determine uniquely the symmetric homogeneous multinomials in $a_1, a_2, \ldots, a_N$ which appear as coefficients in the polynomial

$$P_N(z) := (z - a_1)(z - a_2) \cdots (z - a_N) \tag{3.7}$$

$$\equiv z^N - \Pi_1 z^{N-1} + \Pi_2 z^{N-2} - \cdots + (-1)^N \Pi_N. \tag{3.8}$$

Here

$$\Pi_1 := \sum_{j=1}^{N} a_j \qquad \Pi_2 := \sum\sum_{\substack{j,k=1 \\ j<k}}^{N} a_j a_k$$
$$\Pi_3 := \sum\sum\sum_{\substack{j,k,l=1 \\ j<k<l}}^{N} a_j a_k a_l \qquad \cdots \qquad \Pi_N := a_1 a_2 \ldots a_N. \tag{3.9}$$

Indeed one has the Newton identities [8] $(n = 1, 2, \ldots, N)$

$$c'_n - \Pi_1 c'_{n-1} + \Pi_2 c'_{n-2} - \cdots + (-1)^{n-1} \Pi_{n-1} c'_1 + (-1)^n n\Pi_n = 0 \tag{3.10}$$

which enable $\Pi_2, \Pi_3, \ldots, \Pi_N$ to be obtained in turn, using (3.10) with $n = 2, 3, \ldots, N$, and noting $\Pi_1 = c'_1$. Having obtained $P_N(z)$ given by (3.8) in this way, the fundamental theorem of algebra furnishes a unique set of N complex zeros of P_N (multiple zeros being counted according to multiplicity). Accordingly the set $\{\mathrm{e}^{-\mathrm{i}\pi x_j/l}\}_{j=1,2,\ldots,N}$ is unique. However, since we seek only numbers x_j in the interval $(-l, l)$, the set $\{x_1, x_2, \ldots, x_N\}$ is thus unique. □

Remark 2. Locations $x_1, x_2, \ldots, x_N$ need not be distinct. While coincidence is non-physical for interactions governed by, for example, Lennard-Jones potentials, such an observation turns out to be important in subsequent generalization to three dimensions, wherein particles may not coincide, yet can share one or two coordinates.

Given any ordered N-tuple $(c_1, \ldots, c_N)$ of complex numbers which lie in the range of β, consider the truncated Fourier series

$$D_N(x) := \sum_{n=-N}^{N} c_n\, e^{in\pi x/l}. \tag{3.11}$$

Here it has been noted that, from (3.3),

$$c_0 = N/2l \qquad \text{and} \qquad c_{-n} = \bar{c}_n. \tag{3.12}$$

Remark 3. The function D_N is of interest because it is *real-valued* and is the *minimal* truncated series which incorporates all information concerning the set of particle locations. This follows from knowledge of $c_1, c_2, \ldots, c_N$ requiring that of $x_1, x_2, \ldots, x_N$ (via (3.5) and (3.6)), together with recovery of $\{x_1, x_2, \ldots, x_N\}$ from knowledge of $(c_1, c_2, \ldots, c_N)$ (via proposition 1). All higher-order Fourier coefficients require only the values of $a_1, a_2, \ldots, a_N$, which are yielded by $\{x_1, x_2, \ldots, x_N\}$ or, equivalently, $(c_1, c_2, \ldots, c_N)$. We note that D_N involves only terms with wavelengths $2l, l, 2l/3, \ldots, 2l/(N-1)$ and $2l/N$. Clearly, D_N constitutes a *continuum* description of particle distribution which is information-equivalent to the actual (discrete) distribution. Further truncation of the series, say to include terms generated by $c_1, c_2, \ldots, c_{N'}$ $(N' < N)$, yields a *reduced* (that is, 'coarser') continuum description involving only terms with wavelengths $2l, l, \ldots, 2l/N'$. Such a series can be regarded as a *continuum description at length scale* $2l/N'$. In this sense, the smallest length scale appropriate to such a continuum description of particle location is thus $2l/N$. Such considerations of scale distinguish the foregoing continuum description from, for example, that obtained in terms of polynomials which give least-squares fits of discrete information.

The coefficients of a truncated series of form (3.11) which satisfy (3.12) will not in general lie in the range of β. To see this we observe that the real and imaginary parts of N complex numbers $c_1, c_2, \ldots, c_N$ in general constitute $2N$ items of independent 'real' information, yet $\beta^{-1}(c_1, \ldots, c_N)$ yields only N such items if this expression is meaningful (that is, if $(c_1, \ldots, c_N)$ lies in the range of β). It is thus of interest to characterize those ordered complex N-tuples which *do* lie in the range of β. Since knowledge of $c_1, c_2, \ldots, c_N$ is equivalent to that of $\Pi_1, \Pi_2, \ldots, \Pi_N$ (given $\Pi_1 = c_1'$, $\Pi_2, \ldots, \Pi_N$, relations (3.10) can be used to obtain $c_2', c_3', \ldots, c_N'$ in turn), we can alternatively look at restrictions on P_N in this respect. Matters do not appear to be simple. However, a partial answer is provided by:

Proposition 2. *If $P_N(z)$, given by (3.8) and (3.9), is obtained from a particle distribution via $(3.5)_2$ then it is necessary that its coefficients satisfy*

$$\Pi_k = \Pi_N\, \bar{\Pi}_{N-k} \tag{3.13}$$

where $\Pi_0 := 1$ and $k = 1, 2, \ldots, N$.

Proof. Given a particle distribution $\{x_1, \ldots, x_N\}$, numbers $a_j (j = 1, 2, \ldots, N)$ and $c_{n'} (n' = 1, 2, \ldots, N)$ can be calculated from $(3.5)_2$ and (3.6). Identities (3.10) then yield in turn $\Pi_1, \Pi_2, \ldots, \Pi_N$ which, via (3.8), define $P_N(z)$, a polynomial of degree N whose zeros $a_1, \ldots, a_N$ all have modulus 1. That is, $a_j = e^{i\phi_j}$ and

$$P_N(z) \equiv (z - e^{i\phi_1})(z - e^{i\phi_2}) \cdots (z - e^{i\phi_N}) \tag{3.14}$$

where $-\pi < \phi_j < \pi$ (since $\phi_j = -\pi x_j/l$ and $-l < x_j < l$). Accordingly

$$\begin{aligned} z^N\, \overline{P_N\left(\frac{1}{\bar{z}}\right)} &\equiv z^N \left(\frac{1}{z} - e^{-i\phi_1}\right)\left(\frac{1}{z} - e^{-i\phi_2}\right) \cdots \left(\frac{1}{z} - e^{-i\phi_N}\right) \\ &\equiv e^{-i(\phi_1+\phi_2+\cdots+\phi_N)}(-1)^N (z - e^{i\phi_1}) \cdots (z - e^{i\phi_N}). \end{aligned}$$

That is,

$$z^N \overline{P_N\left(\frac{1}{\bar{z}}\right)} \equiv (-1)^N \,\bar{\Pi}_N\, P_N(z). \tag{3.15}$$

Thus, from (3.8)

$$1 - \bar{\Pi}_1 z + \bar{\Pi}_2 z^2 - \cdots + (-1)^N \bar{\Pi}_N z^N \equiv (-1)^N \bar{\Pi}_N \{z^N - \Pi_1 z^{N-1} + \cdots + (-1)^N \Pi_N\}. \tag{3.16}$$

Equating coefficients of $z^0, z^1, \ldots,$ and z^{N-1} yields

$$1 = \bar{\Pi}_N \Pi_N \qquad \bar{\Pi}_1 = \bar{\Pi}_N \Pi_{N-1} \qquad \cdots \qquad \bar{\Pi}_{N-1} = \bar{\Pi}_N \Pi_1$$

and hence (3.13) follows on taking conjugates. □

Corollary 2.1. *If $\rho e^{i\alpha}$ is a zero of polynomial P_N defined in (3.8), with coefficients which satisfy relations (3.13), then $\rho^{-1} e^{i\alpha}$ is also a zero of P_N.*

Proof. By hypothesis

$$\rho^N e^{iN\alpha} - \Pi_1 \rho^{N-1} e^{i(N-1)\alpha} + \cdots + (-1)^{N-1} \Pi_{N-1} \rho e^{i\alpha} + (-1)^N \Pi_N = 0. \tag{3.17}$$

Taking complex conjugates and multiplying by $(-1)^N \Pi_N e^{iN\alpha} \rho^{-N}$ yields (notice $\rho \neq 0$ since $|\Pi_N| = |a_1 a_2 \ldots a_N| = 1 \neq 0$)

$$(-1)^N \Pi_N + (-1)^{N-1} \Pi_N \bar{\Pi}_1 \rho^{-1} e^{i\alpha} + \cdots - \Pi_N \bar{\Pi}_{N-1} \rho^{-(N-1)} e^{i(N-1)\alpha} + \Pi_N \bar{\Pi}_N \rho^{-N} e^{iN\alpha} = 0. \tag{3.18}$$

Use of relations (3.13) yields the result. □

Corollary 2.2. *The N complex zeros of P_N in corollary 2.1 are characterized by no more than N distinct real numbers.*

Proof. Suppose P_N has zeros $a_1, a_2, \ldots, a_N$. Each zero of modulus 1 has form $e^{i\alpha}$($\alpha \in (-\pi, \pi)$ unique) characterized by the single real number α. The totality of (k say) such zeros is thus characterized by *at most* a collection of k distinct real numbers (since there may be multiple zeros of this type). Select any remaining zero, which must be of the form $\rho e^{i\alpha}$, with $\rho \neq 1$ and $\rho \neq 0$. Corollary 2.1 delivers $\rho^{-1} e^{i\alpha}$ as another zero. The zeros still unconsidered are such that none have moduli ρ or ρ^{-1}, or include at least one of the form $\rho e^{i\alpha}$, $\rho e^{i\beta}$, $\rho^{-1} e^{i\alpha}$, or $\rho^{-1} e^{i\beta}$ ($\beta \neq \alpha$). The latter case enables us to account for any zero of the form indicated at the expense of at most one real number (β). In the former case we may repeat the argument by inspecting any other zero, which must be of the form $\rho' e^{i\gamma}$ with $\rho' \neq \rho$ and $\rho' \neq \rho^{-1}$. In this procedure the number of distinct real numbers elicited clearly cannot exceed N. □

Remark 4. Corollary 2.2 indicates that relations (3.13) suffice to ensure that the zeros of P_N carry at most N distinct items of real-valued information. However, these relations fall short of characterizing P_N as deriving from a particle distribution, as will now be made evident.

Relations (3.13) are *necessary* if P_N is to derive from a particle distribution, but are not *sufficient*. Indeed, from definitions (3.9) one has the additional set of restrictions ($k = 1, 2, \ldots, N$)

$$|\Pi_k| \leqslant {}^N C_k. \tag{3.19}$$

(For example, noting that all zeros of P_N must have modulus 1,

$$|\Pi_2| \leqslant \sum_{\substack{j,k=1 \\ j<k}}^{N} |a_j\, a_k| = \sum_{\substack{j,k=1 \\ j<k}}^{N} |a_j|\,|a_k| = {}^N C_2).$$

Furthermore, the *totality* of restrictions (3.13) and (3.19) do not suffice to ensure the identification with P_N of a particle distribution[4]. A *sufficient* condition follows from:

Proposition 3. *If $\rho_1, \rho_2, \ldots, \rho_N$ are N positive numbers with product 1 then their sum is not less than N, and this sum equals N if and only if $\rho_j = 1$ $(j = 1, 2, \ldots, N)$.*

Proof. Let

$$S_N := \sum_{j=1}^{N} \rho_j = \rho_1 + \rho_2 + \cdots + \rho_{N-1} + \frac{1}{\rho_1\, \rho_2 \ldots \rho_{N-1}}. \tag{3.20}$$

Stationary values of S_N occur when $\partial S_N/\partial \rho_j = 0$. Thus

$$1 - \frac{1}{\rho_1^2\, \rho_2 \ldots \rho_{N-1}} = 1 - \frac{1}{\rho_1\, \rho_2^2 \ldots \rho_{N-1}} = \cdots = 1 - \frac{1}{\rho_1\, \rho_2 \ldots \rho_{N-1}^2} = 0.$$

Accordingly $\rho_1^2 \rho_2 \ldots \rho_{N-1} = \rho_1\, \rho_2^2 \ldots \rho_{N-1} = \cdots = \rho_1\, \rho_2 \ldots \rho_{N-1}^2$, whence $\rho_1 = \rho_2 = \cdots = \rho_{N-1}$ and thus $\rho_j^N = 1$ for each j. Hence $\rho_j = 1$, and the only stationary value occurs when each ρ_j equals 1. Writing $\rho_j = 1 + \varepsilon_j (j = 1, 2, \ldots, N-1)$, from (3.20)

$$S_N = N - 1 + \varepsilon_1 + \cdots + \varepsilon_{N-1} + \frac{1}{(1+\varepsilon_1)\cdots(1+\varepsilon_{N-1})}.$$

Noting $(1+\varepsilon)^{-1} = 1 - \varepsilon + \varepsilon^2 - \cdots$ if $|\varepsilon| < 1$,

$$S_N = N + \sum_{j=1}^{N-1} \varepsilon_j^2 + \sum_{\substack{j,k=1 \\ j<k}}^{N-1} \varepsilon_j\, \varepsilon_k + \text{ higher order terms}$$

$$= N + \sum_{\substack{j,k=1 \\ j<k}}^{N} \{(\varepsilon_j + \varepsilon_k/2)^2 + (\sqrt{3}\, \varepsilon_k/2)^2\} + \text{ higher order terms.}$$

It follows that the minimum value of S_N is N and this occurs only if each $\rho_j = 1$. □

Corollary 3.1. *If P_N satisfies relation (3.13) with $k = 0$, and the sum of the moduli of its zeros is N, then P_N corresponds to a particle distribution.*

Proof. If the zeros have moduli $\rho_1, \ldots, \rho_N$ then, since $k = 0$ in (3.13) yields $|\Pi_N| = 1$, $\rho_1\, \rho_2 \ldots \rho_N = 1$. If, in addition, $\sum_{j=1}^{N} \rho_j = N$ then proposition 3 implies all zeros have modulus 1, and hence P_N corresponds to a particle distribution. □

Remark 5. While the foregoing restrictions on a polynomial P_N of degree N concerning the product and sum of the moduli of its zeros are both necessary and sufficient to ensure it may be identified with a particle distribution, the restriction on the sum is not readily identified by inspection of its coefficients. Indeed, given the above two restrictions, the remaining restrictions (3.13) for $k \neq 0$ may be *deduced*, together with relations (3.19).

[4] Consider, for example, $P_3(z) := (z - \rho e^{i\theta})(z - \frac{1}{\rho} e^{i\theta})(z - e^{i\phi})$. If $\rho = 4/5$, $\cos(\phi - \theta) = -4/5$ and $\sin(\phi - \theta) = 3/5$, then restrictions (3.13) and (3.19) hold with $N = 3$.

Having discussed particle locations we now consider their physical attributes. Suppose that f_j denotes the value of a physical quantity associated with that particle located at x_j (for example, its mass, momentum or kinetic energy). The corresponding discrete distribution is

$$F(x) := \sum_{j=1}^{N} f_j\, \delta(x - x_j). \tag{3.21}$$

The formal Fourier series for F is given by

$$F(x) \sim \sum_{n=-\infty}^{\infty} \phi_n\, \mathrm{e}^{\mathrm{i}n\pi x/l} \tag{3.22}$$

where

$$\phi_n := \frac{1}{2l} \sum_{j=1}^{N} f_j\, a_j^n. \tag{3.23}$$

Proposition 4. *If no two point masses coincide then knowledge of $\phi_1, \ldots, \phi_N$ is equivalent to knowing that the particle whose location x_j is given by a_j has quantity value f_j ($j = 1, 2, \ldots, N$).*

Proof. Given $a_1, \ldots, a_N$, relations (3.23) with $n = 1, 2, \ldots, N$ constitute a set of N simultaneous linear equations for $\phi'_1, \ldots, \phi'_N$, where

$$\phi'_n := 2l\phi_n. \tag{3.24}$$

Indeed,

$$\phi'_n = \sum_{j=1}^{N} A_{nj}\, f_j \tag{3.25}$$

where

$$A_{nj} := a_j^n. \tag{3.26}$$

Relations (3.25) are invertible if and only if $\det[A_{nj}] \neq 0$. However

$$\det[A_{nj}] \equiv (-1)^{N(N-1)/2} a_1\, a_2 \cdots a_N \prod_{\substack{p,q=1 \\ p<q}}^{N} (a_p - a_q). \tag{3.27}$$

Since $|a_j| = 1$, invertibility is possible unless one or more factors $(a_p - a_q)$ vanish; equivalently, unless at least one pair of particles coincide. □

The main conclusion of this section follows from remark 3 and proposition 4, namely:

Theorem A. *If a set of N point masses are confined to the linear interval $(-l, l)$, and interact in such a way that no two coincide, then the appropriate phase space description is equivalent to the set of $2N$ complex-valued Fourier coefficients ($c_1, c_2, \ldots, c_N$, $\phi_1, \phi_2, \ldots, \phi_N$), where c_n is defined by (3.3) and ϕ_n by (3.23) with $f_j = p_j$ (the momentum of that particle located at x_j).*

Corollary A.1. *Equivalent to the phase space description of point masses, interacting as in theorem A, are the two real-valued analytic functions D_N and M_N, where D_N is defined by (3.11) and (3.3), and (via (3.23) with $f_j = p_j$)*

$$M_N(x) := \sum_{n=-N}^{N} \phi_n\, \mathrm{e}^{\mathrm{i}n\pi x/l}. \tag{3.28}$$

Remark 6. From (3.11) $c_0 = N/2l$. Further, from (3.23)

$$\phi_0 = \sum_{n=1}^{N} p_j/2l = \sum_{n=1}^{N} \sum_{k=1}^{N} (A^{-1})_{jk}\, \phi_k \tag{3.29}$$

where A denotes the matrix whose elements are given by (3.26). Accordingly c_0 and ϕ_0 are not independent variables. Writing coefficients in polar form as

$$c_n = r_n\, \mathrm{e}^{\mathrm{i}\theta_n} \qquad \phi_n = \rho_n\, \mathrm{e}^{\mathrm{i}\psi_n} \tag{3.30}$$

$(n = 1, 2, \ldots, N)$ and noting $c_{-n} = \bar{c}_n$, $\phi_{-n} = \bar{\phi}_n$, we have

$$D_N(x) = \frac{N}{2l} + 2\sum_{n=1}^{N} r_n \cos\left\{\frac{n\pi x}{l} + \theta_n\right\} \tag{3.31}$$

and

$$M_N(x) = \phi_0 + 2\sum_{n=1}^{N} \rho_n \cos\left\{\frac{n\pi x}{l} + \psi_n\right\} \tag{3.32}$$

with (from (3.29))

$$\phi_0 = \sum_{j=1}^{N} \sum_{k=1}^{N} (A^{-1})_{jk}\, \rho_k\, \mathrm{e}^{\mathrm{i}\psi_k}. \tag{3.33}$$

Recalling remark 3, D_N together with M_N constitutes a continuum description of particle locations and momenta which is minimal, in the sense of corresponding to a pair of truncated Fourier series which incorporate all corpuscular information, and such that any further truncation would result in loss of information. Truncation with last terms corresponding to $n = N' < N$ yields a ('coarser') description at scale $2l/N'$.

4. Three-dimensional considerations

Here we generalize the results of section 3 to three dimensions. The problem is thus to consider N point masses confined to the interior of a rectangular box (of dimensions $2l_1 \times 2l_2 \times 2l_3$, say) and to select a minimal set of Fourier coefficients associated with corpuscular locations and momenta which incorporate sufficient information to be able to recover these locations and momenta. Choosing Cartesian coordinates with origin at the centre of the box and axes parallel to its edges, let (x_j, y_j, z_j) denote the locations of the particles $(j = 1, 2, \ldots, N)$. The particle distribution

$$D(x, y, z) := \sum_{j=1}^{N} \delta(x - x_j)\, \delta(y - y_j)\, \delta(z - z_j) \tag{4.1}$$

has formal Fourier series

$$D(x, y, z) \sim \sum\sum_{k_1,k_2,k_3=-\infty}^{\infty}\sum c(\boldsymbol{k})\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}'} \tag{4.2}$$

where

$$c(\boldsymbol{k}) := \frac{1}{8l_1l_2l_3} \int_{-l_3}^{l_3} \int_{-l_2}^{l_2} \int_{-l_1}^{l_1} D(x, y, z)\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}'}\, \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}z \tag{4.3}$$

with

$$\boldsymbol{r}' := \left(\frac{\pi x}{l_1}, \frac{\pi y}{l_2}, \frac{\pi z}{l_3}\right) \qquad \text{and} \qquad \boldsymbol{k} := (k_1, k_2, k_3) \tag{4.4}$$

(k_1, k_2, k_3 integers).

Thus

$$c'(\boldsymbol{k}) := 8l_1l_2l_3\,c(\boldsymbol{k}) = \sum_{j=1}^{N} \alpha_j^{k_1}\,\beta_j^{k_2}\,\gamma_j^{k_3} \tag{4.5}$$

where

$$\alpha_j := \mathrm{e}^{-\mathrm{i}\pi x_j/l_1} \qquad \beta_j := \mathrm{e}^{-\mathrm{i}\pi y_j/l_2} \qquad \gamma_j := \mathrm{e}^{-\mathrm{i}\pi z_j/l_3}. \tag{4.6}$$

Consider $\{c'(n, 0, 0) : 1 \leqslant n \leqslant N\}$. From (4.5)

$$c'(n, 0, 0) = \sum_{j=1}^{N} \alpha_j^n. \tag{4.7}$$

This is precisely the situation addressed by proposition 1: see (3.6). Thus, given the set $\{c'(n, 0, 0)\}$ of N Fourier coefficients, there exists a unique set $\{\alpha_1, \ldots, \alpha_N\}$ of complex numbers which satisfy (4.7). Accordingly, since these derive from a particle distribution, $|\alpha_j| = 1$ by $(4.6)_1$, and there exists a unique $x_j \epsilon (-l_1, l_1)$ related to α_j by $(4.6)_1$.

Remark 7. The set $\{x_1, \ldots, x_N\}$ may involve repetitions. Even if particle interactions exclude coincidence, pairs of distinct particles are to be expected occasionally (and instantaneously) to share the same x coordinate as time evolves.

Remark 8. Naively, one might expect to consider the sets $\{c'(0, n, 0)\}$ and $\{c'(0, 0, n)\}$, $(n = 1, 2, \ldots, N)$, in order to locate all corpuscular locations. However, such sets yield only sets $\{y_1, \ldots, y_N)$ and $\{z_1, \ldots, z_N\}$ of y and z coordinates, with no indication of which z goes with which y (and which x). Said differently, knowledge of sets $\{c'(n, 0, 0)\}$, $\{c'(0, n, 0)\}$ and $\{c'(0, 0, n)\}$ yields a set of N^3 possible corpuscular locations (x, y, z), where $x \in \{x_1, \ldots, x_N\}$, $y \in \{y_1, \ldots, y_N\}$ and $z \in \{z_1, \ldots, z_N\}$.

Consider $\{c'(n, 1, 0) : 1 \leqslant n \leqslant N\}$. From (4.5)

$$c'(n, 1, 0) = \sum_{j=1}^{N} \alpha_j^n\,\beta_j = \sum_{j=1}^{N} A_{nj}\,\beta_j \tag{4.8}$$

where A_{nj} is given by (3.26) with $a_j = \alpha_j$ (with l replaced by l_1: cf $(3.5)_1$ and $(4.6)_1$). We may thus invoke proposition 4 (here $\phi'_n = c'(n, 1, 0)$) to deduce that there exists a unique solution $\beta_1, \ldots, \beta_N$ to the system (4.8) of N simultaneous linear equations, provided that $\alpha_1, \ldots, \alpha_N$ are all different. Similarly, under this latter condition, consideration of $\{c'(n, 0, 1) : 1 \leqslant n \leqslant N\}$ leads to the system

$$c'(n, 0, 1) = \sum_{j=1}^{N} A_{nj}\,\gamma_j \tag{4.9}$$

having a unique solution $\gamma_1, \ldots, \gamma_N$.

Remark 9. The foregoing shows that, provided the x coordinates of the N particles are all different (equivalent to $\alpha_1, \ldots, \alpha_N$ being all different), knowledge of the coefficients $c'(n, 1, 0)$ and $c'(n, 0, 1)$, where $1 \leqslant n \leqslant N$, enables a unique ordered pair (β_j, γ_j) to be associated with α_j for each $j = 1, \ldots, N$. Indeed we have established

Proposition 5. *If N particles, confined to a rectangular box, are distributed so that no two lie on any plane parallel to a box face, then (choosing coordinates so that x is constant on such a face) knowledge of the* $3N$ *Fourier coefficients* $c'(n, 0, 0)$, $c'(n, 1, 0)$ *and* $c'(n, 0, 1)$*, where* $n = 1, \ldots, N$*, suffices to determine the locations of all particles.*

Now, suppose that f_j denotes a scalar physical quantity associated with that particle located at (x_j, y_j, z_j). The corresponding distribution (cf (3.21)) is

$$F(x, y, z) := \sum_{j=1}^{N} f_j\, \delta(x - x_j)\, \delta(y - y_j)\, \delta(z - z_j). \tag{4.10}$$

Distribution F has formal Fourier series (cf (3.22) and (3.23))

$$F(x, y, z) \sim \frac{1}{8\, l_1\, l_2\, l_3} \sum\sum_{k_1,k_2,k_3=-\infty}^{\infty}\sum \phi'(\boldsymbol{k}) \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot \boldsymbol{r}'} \tag{4.11}$$

where

$$\phi'(\boldsymbol{k}) := \sum_{j=1}^{N} f_j\, \alpha_j^{k_1}\, \beta_j^{k_2}\, \gamma_j^{k_3} \tag{4.12}$$

and we have used the notation of (4.4) and (4.6). Knowledge of $\phi'(n, 0, 0)$ for $n = 1, \ldots, N$ enables, modulo the hypothesis of proposition 5, unique values $f_1, \ldots, f_N$ to be determined via invertibility of $[A_{nj}]$. It follows that knowledge of the $3N$ Fourier coefficients associated with the momentum components of the N particles (obtained in turn by choosing f_j first equal to the x component of the momentum of that particle located at (x_j, y_j, z_j), then equal to the y momentum component, and finally the z momentum component) is equivalent to knowledge of the corpuscular momenta. Suppose these momentum coefficients are denoted by $\phi'_x(n, 0, 0)$, $\phi'_n(n, 0, 0)$ and $\phi'_z(n, 0, 0)$, respectively $(n = 1, \ldots, N)$. We have thus established the three-dimensional analogue of theorem A, namely:

Theorem B. *The phase space description of a set of N point masses confined to a rectangular box is equivalent to the set of* $6N$ *Fourier coefficients* $(n = 1, \ldots, N)$ $c'(n, 0, 0)$, $c'(n, 1, 0)$, $c'(n, 0, 1)$, $\phi'_x(n, 0, 0)$, $\phi'_y(n, 0, 0)$ *and* $\phi'_z(n, 0, 0)$ *whenever no two particles share a common x coordinate.*

In motions of particles confined to a box there will naturally be many instants at which particle pairs lie on a plane parallel to one specific box face. However, in any finite time interval it may be highly unlikely that such a coincidence will be other than instantaneous. Said differently, it may be highly unlikely that such a coincidence will persist over a time interval (in which case the relevant particles would share a common velocity component over this interval). This motivates defining particle motions as *regular* if

R.M.1: particle locations are smooth functions of time, and

R.M.2: over any finite time interval the (Lebesgue) measure of all instants at which two or more particles lie on a plane parallel to a specific face is zero.

Immediately we have:

Corollary B.1. *In regular motions the conclusion of theorem B holds almost always.*

Indeed, we can say more:

Corollary B.2. *Knowledge of the Fourier coefficients in theorem B suffices, for regular motions, to recover the phase space description at all times.*

Proof. If τ is an instant in a regular motion at which theorem B is inapplicable then we can, via R.M.2, consider a sequence of instants $\{t_n\}_{n=1}^{\infty}$ which converges to τ and for each of which theorem B *is* appropriate. Consider the sequence $\{\beta_j(t_n)\}$ delivered by inversion of relations (4.8). Since $|\beta_j| = 1$ at any time, set $\{\beta_j(t_n)\}$ is bounded and thus has a limit point, $\hat{\beta}$ say, with $|\hat{\beta}| = 1$ (via the Bolzano–Weierstrass theorem and continuity of the modulus function). Since β_j is an analytic function of location, from R.M.1 β_j is a smooth (and hence, in particular, continuous) function of time and thus $\hat{\beta}$ is unique, and to be regarded as $\beta_j(\tau)$. Of course, this yields $y_j(\tau)$ via $(4.6)_2$. Identical reasoning establishes $z_j(\tau)$, and a similar argument delivers momentum components at instant τ (invoking continuity of such, guaranteed by R.M.1). □

Remark 9. Corollary B.2 continues to hold if R.M.2 is relaxed to:

R.M.2′: over any finite time interval, the set of all instants at which no particle pairs lie on a plane parallel to a specific face is dense in this interval.

Remark 10. While most physical interest might relate to particle interactions which preclude instantaneous coincidence, the foregoing holds for such coincidence: the only restriction is that motions be *regular*.

The analogue of corollary A.1. is:

Corollary B.3. *The phase space description of a set of N point masses, confined to a regular box and undergoing regular motions, is equivalent to the two real-valued analytic functions:*

$$D_N(\boldsymbol{x}) := \sum\sum_{k_1,k_2,k_3=-N}^{N}\sum c(\boldsymbol{k})\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}'} \tag{4.13}$$

and

$$\boldsymbol{M}_N(\boldsymbol{x}) := \sum\sum_{k_1,k_2,k_3=-N}^{N}\sum \phi'(\boldsymbol{k})\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}'}. \tag{4.14}$$

Here $c(\boldsymbol{k})$ is given by (4.5) and (4.6), while

$$\phi'(\boldsymbol{k}) := \sum_{j=1}^{N} \boldsymbol{p}_j\, \alpha_j^{k_1}\, \beta_j^{k_2}\, \gamma_j^{k_3} \tag{4.15}$$

where $\boldsymbol{p}_j$ is the momentum of a particle located at (x_j, y_j, z_j).

Remark 11. Recalling remark 6, D_N together with $\boldsymbol{M}_N$ furnishes a continuum description of particle locations and momenta which is minimal. The smallest wavelength involved is $\varepsilon_{\min} := \min\{2\mathrm{l}_1/\mathrm{N}, 2\mathrm{l}_2/\mathrm{N}, 2\mathrm{l}_3/\mathrm{N}\}$. Further truncation delivers a coarser description. A continuum description at scale $\epsilon > \epsilon_{\min}$ corresponds to truncation of (4.13) and (4.14) in which N is replaced by the integral part N' of the smallest of $2l_1/\varepsilon$, $2l_2/\varepsilon$ and $2l_3/\varepsilon$.

Remark 12. It may be desirable to truncate (4.13) and (4.14) at different wavelengths in different directions. For example, particles confined to a box by separation-dependent wall potentials, and interacting via Lennard-Jones potentials, may, under gravity parallel to a box edge, give rise to a liquid–vapour system. It would then be useful to adopt a fine scale in the gravitational direction (in order to 'resolve' the interfacial region) but use a much coarser description in 'lateral' directions.

5. Concluding remarks

The projection operator method is based upon a change of phase space variables to an equivalent set of variables which is the union of two sets, one of which is considered to furnish macroscopic information, and the other sub-macroscopic detail, about the system. If X is an element ('microstate') of phase space $\mathbb{P}$, let $S = \hat{S}(X)$ and $F = \hat{F}(X)$ denote the aforementioned macroscopic and sub-macroscopic variables, respectively. The general form of projection operator (see [5], section 3) is given, for any function f of microstate, by $P : f \to Pf$, where

$$(Pf)(X) := \int_{\mathbb{P}} f(Y)\, w(Y)\, \delta(\hat{S}(Y) - \hat{S}(X))\, \mathrm{d}Y \Big/ \int_{\mathbb{P}} w(Y)\, \delta(\hat{S}(Y) - \hat{S}(X))\, \mathrm{d}Y. \qquad (5.1)$$

Here w is a weighting function (usually an equilibrium probability density) and the 'δ' symbolism indicates integration is to be effected only over microstates which yield the same macrostate as X, namely $\hat{S}(X)$. Thus $(Pf)(X)$ is an ensemble average, where the ensemble consists of the set of those microstates which correspond to macrostate $\hat{S}(X)$, furnished with probability density w. The time evolution of f in any microprocess is delivered in terms of the action of the Liouville operator upon f, and an operator identity yields the evolution of Pf. The latter evolution has identifiable reversible and irreversible contributions, and leads (with $f = \rho$, the probability density function on $\mathbb{P}$) to the appropriate master equation.

The foregoing is formal in the sense that *any* variable change from $\mathbb{P}$ allows the new variables to be divided into two arbitrary complementary subsets, and the projection operator procedure implemented. *However, the physical content of the resulting master equation depends crucially upon the selection of macroscopic variables.* In this work the change to certain Fourier coefficients as variables lends itself in a natural way to such selection via length scale considerations[5]. Specifically, in order to study macroscopic behaviour at length scale ε, the relevant variables are those Fourier coefficients which correspond to wavelengths not less than ϵ.

In recent work [4, 5] a modified version of the procedure indicated above was adopted. Addressing reproducible macroscopic behaviour at scales ϵ and Δ of length and time, the variable change involves *local* replacement of a certain number of phase space variables by coefficients in the Fourier series representations of corpuscular mass, momentum and energy distributions. Such coefficients correspond to a wavelength cut-off ϵ. Hypotheses of local equilibrium at scales ε, Δ (equivalent to $w = 1$ in (5.1)) and dynamic ergodicity (relating ensemble averages delivered by the projection operator to ε, Δ local corpuscular averages) provide the link with observations made at these scales.

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