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Hamiltonian formulation of the evolution of moments over clusters of non-interacting particles

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Abstract. The study of the evolution of the moments over a cluster of identical classical particles without mutual interactions is extended to the case where the motion of each particle is described by an arbitrary Hamiltonian. In the case of moments of the second and third order and ignoring contributions from moments higher than the third, differential equations are derived for the moments as well as explicit expansions. A distinction is made between the evolution of moments relative to the centroid and that of moments relative to a particle with initial position and velocity equal to those of the centroid. Although the former moments are more directly applicable and are independent of the choice of initial time, the latter have formal advantages. It is shown that these two types of moments differ in terms of order not less than four.

1. Introduction

If a cluster of classical particles is subject to a force field, the cluster will change with time both in its spatial distribution and in the distribution of velocities. One approach to studying these effects is to examine the moments of the cluster.

Moments are usually referred to the centroid $\bar{\boldsymbol{x}} = N^{-1}\sum_A \boldsymbol{x}^{(A)}$, where $\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \ldots, \boldsymbol{x}^{(N)}$ are the locations of the particles, but for most of this paper, they will be referred to another point $\boldsymbol{\xi}$. Thus the second-order moments are

$$\begin{aligned}
\chi_{ij} &= N^{-1}\sum_A (x_i^{(A)} - \xi_i)(x_j^{(A)} - \xi_j) \\
\zeta_{ij} &= N^{-1}\sum_A (x_i^{(A)} - \xi_i)(\dot{x}_j^{(A)} - \dot{\xi}_j) \qquad (1.1) \\
\omega_{ij} &= N^{-1}\sum_A (\dot{x}_i^{(A)} - \dot{\xi}_i)(\dot{x}_j^{(A)} - \dot{\xi}_j).
\end{aligned}$$

These have a direct physical interpretation; for example, the diagonal elements χ_{ii} measure the mean-square deviation from $\boldsymbol{\xi}$ in the ith direction while the off-diagonal elements χ_{ij} measure the correlation between deviations in the ith direction with deviations in the jth. The elements of ζ_{ij} measure the extent to which deviations in velocity are correlated with deviations in position. To provide greater detail of the cluster, one could then examine the third-order moments and so on.

For the case of a cluster of identical classical particles moving without mutual interaction under forces describable by a potential $V(\boldsymbol{x})$, the equations of motion for the second-order moments were reduced in an earlier paper (Andrews 1981b) to an approximate set which determine the moments for all times from the moments at some initial time. This was achieved by expanding the potential about the position of a particle with the same initial position and momentum as the centroid. The trajectory of this particle will be referred to as the *basal trajectory*, $\boldsymbol{\xi}(t)$. Unless otherwise stated, all moments will be referred to the basal trajectory. The set of differential equations so found was approximate to the extent that all terms of the third order or higher in the deviations from $\boldsymbol{\xi}$ were ignored. It was further shown how these equations could be solved in terms of a complete set u_i^m, v_j^n of solutions of the time-dependent oscillator equation

$$\ddot{u}_i + \phi_{ij}(t) u_j = 0 \tag{1.2}$$

where $\phi_{ij}(t) = m^{-1} V_{ij}(\boldsymbol{\xi})$. The required complete set of solutions can be found by differentiating the trajectories under the potential V with respect to initial position and velocity. This approach was extended in the case of one spatial dimension to third-order and higher moments by Reid and Ray (1983). These two discussions focused attention on particular mathematical aspects, the first on invariants of the time-dependent oscillator equation and the second on a certain hierarchy of self-adjoint equations that arise.

The purpose of the present paper is to illuminate the earlier work and to extend it to the case of a cluster of identical particles whose motion is described by a Hamiltonian, still excluding mutual interactions. At the same time third-order moments will be included and a more compact notation will be adopted: by collecting the n generalised coordinates q_i and the n momenta p_i into one $2n$-dimensional vector x^α significant formal simplification is achieved. For example, the three second-order moment matrices χ_{ij}, ζ_{ij}, ω_{ij} are contained in one symmetric $2n$-dimensional matrix, $\chi^{\alpha\beta}$. The formal advantages are enhanced by the fact that the transformation between the x^α and their initial values (described by the matrices u_i^m, v_j^n and their time derivatives) is symplectic.

In the earlier work, the moment expansion for the moments in terms of their initial values was obtained by solving their differential equations. In the quantum context, where this work had its origins (Andrews 1981a), there are no trajectories and solving the differential equations appears to be the only method available. But in the case of a cluster of classical particles one can sum directly over the trajectories to obtain the moment expansion and this is carried out in § 3.

In the earlier work it has not been completely clear whether one should expand the potential about the centroid or about the basal trajectory. Both are possible but the view is taken here that there are great formal advantages in expanding about the basal trajectory and evaluating all moments about the basal trajectory. It is shown that moments referred to the basal trajectory differ from moments referred to the centroid only in terms of the fourth order. In applications one normally requires the moments about the centroid; indeed the moments about the basal trajectory suffer from the great disadvantage that they depend on the choice of initial time. It is, however, a straightforward matter to transform between these two types of moments and this is dealt with in § 6.

2. The symplectic notation and the symplectic transformation

The particle trajectories will satisfy Hamilton's equations

$$\dot{q}_i = \partial H/\partial p_i \qquad \dot{p}_i = -\partial H/\partial q_i \tag{2.1}$$

where $H(\boldsymbol{q}, \boldsymbol{p}, t)$ is the Hamiltonian and the index i runs from 1 to n, where n is the number of generalised coordinates q required (normally three). Using the symplectic notation (see e.g. Goldstein 1980, p 347 and § 9-3), let Greek indices run from 1 to $2n$ and introduce x^α with $x^i = q_i$ and $x^{n+i} = p_i$ for $i = 1, 2, \ldots, n$. Also introduce $\varepsilon^{\alpha\beta}$ such that $\varepsilon^{i,n+i} = 1$, $\varepsilon^{n+i,i} = -1$ for $1 \leqslant i \leqslant n$ and all other elements are zero. Written as a block matrix, with $n \times n$ blocks and (α, β) element equal to $\varepsilon^{\alpha\beta}$,

$$\varepsilon = \left(\begin{array}{c|c} 0 & 1 \\ \hline -1 & 0 \end{array}\right). \tag{2.2}$$

Now Hamilton's equations can be written

$$\dot{x}^\alpha = \varepsilon^{\alpha\beta} H_\beta \tag{2.3}$$

where, as usual, a subscript β on H denotes partial differentiation with respect to x^β.

A particular trajectory $x^\alpha(\boldsymbol{a}, t)$ can be characterised by its initial values $\boldsymbol{a}$; thus $x^\alpha(\boldsymbol{a}, 0) = a^\alpha$. Consider now a cluster of identical non-interacting particles specified by $a^\alpha{}_A$, $A = 1, \ldots, N$. The basal trajectory ξ^α is defined to be the trajectory with initial value $\bar{a}^\alpha = N^{-1} \Sigma_A a^\alpha{}_A$.

The analogues of the functions u_i^j, v_i^j and their time derivatives are

$$u^\alpha{}_\beta(t) = \partial x^\alpha / \partial a^\beta |_{\boldsymbol{a} = \bar{\boldsymbol{a}}} \tag{2.4}$$

and differentiating Hamilton's equations (2.3) yields

$$\dot{u}^\alpha{}_\beta = \varepsilon^{\alpha\gamma} h_{\gamma\delta} u^\delta{}_\beta \tag{2.5}$$

where $h_{\gamma\delta}(t)$ is $H_{\gamma\delta}$ evaluated on the basal trajectory. This equation is the Hamiltonian generalisation of the time-dependent oscillator equation (1.2).

Since the transformation from a^α to x^α will be canonical, one would expect $u^\alpha{}_\beta$ to be symplectic, i.e.

$$U^{-1} = \varepsilon \tilde{U} \varepsilon \tag{2.6}$$

and this can be verified directly as follows. In matrix form, (2.5) reads $\dot{U} = \varepsilon h U$ and, since $\tilde{\varepsilon} = -\varepsilon$ and $\tilde{h} = h$, the transpose of this is $\dot{\tilde{U}} = -\tilde{U} h \varepsilon$. Therefore, using $\varepsilon^2 = 1$,

$$\mathrm{d}(\tilde{U} \varepsilon U)/\mathrm{d}t = \dot{\tilde{U}} \varepsilon U + \tilde{U} \varepsilon \dot{U} = 0.$$

Since the initial value of $u^\alpha{}_\beta$ is $\delta^\alpha{}_\beta$, equation (2.6) follows.

3. Evolution of the moments to third order

In this section, no use will be made of Hamilton's equations. All that will be assumed is that we are dealing with a family of trajectories that can be expanded about the basal one in powers of the deviations of the initial position and velocity from those of the basal trajectory. It then emerges that the moments at any later time can be expressed as an expansion involving only the initial moments and the coefficients in the expansion of the trajectories.

Expanding the trajectories about the basal one yields

$$x^\alpha(\boldsymbol{a}, t) = \xi^\alpha + (a^\beta - \bar{a}^\beta) u^\alpha{}_\beta + \tfrac{1}{2}(a^\beta - \bar{a}^\beta)(a^\gamma - \bar{a}^\gamma) p^\alpha{}_{\beta\gamma} + \mathrm{O}(3) \tag{3.1}$$

where $O(m)$ is used to represent quantities of order m in the deviations from the basal trajectory and

$$p^{\alpha}{}_{\beta\gamma}(t) = \partial^2 x^{\alpha}/\partial a^{\beta}\,\partial a^{\gamma}|_{a=\bar{a}}. \tag{3.2}$$

Writing $X^{\alpha} = x^{\alpha} - \xi^{\alpha}$, the second-order moments are

$$\chi^{\alpha\beta} = N^{-1}\sum_{A} X^{\alpha}{}_{A} X^{\beta}{}_{A} \tag{3.3}$$

and the third-order moments will be written as

$$\kappa^{\alpha\beta\gamma} = N^{-1}\sum_{A} X^{\alpha}{}_{A} X^{\beta}{}_{A} X^{\gamma}{}_{A}. \tag{3.4}$$

Inserting (3.1) for X^{α} into these sums and retaining terms up to the third order yields

$$\chi^{\alpha\beta} = \chi_0{}^{\delta\sigma} u^{\alpha}{}_{\delta} u^{\beta}{}_{\sigma} + \tfrac{1}{2}\kappa_0{}^{\delta\sigma\rho}(u^{\alpha}{}_{\delta} p^{\beta}{}_{\sigma\rho} + u^{\beta}{}_{\delta} p^{\alpha}{}_{\sigma\rho}) + O(4) \tag{3.5}$$

$$\kappa^{\alpha\beta\gamma} = \kappa_0{}^{\delta\sigma\rho} u^{\alpha}{}_{\delta} u^{\beta}{}_{\sigma} u^{\gamma}{}_{\rho} + O(4). \tag{3.6}$$

The evolution of the centroid is simply obtained by summing (3.1) over the cluster:

$$\bar{x}^{\alpha} = \xi^{\alpha} + \tfrac{1}{2}\chi_0{}^{\beta\gamma} p^{\alpha}{}_{\beta\gamma} + O(3). \tag{3.7}$$

In comparing these results with earlier work, one must recognise that $\kappa^{\alpha\beta\gamma}$ contains four third-rank tensors in the n-dimensional formalism. These were labelled η, σ, κ, τ by Reid and Ray (1983), who dealt only with one dimension. When the Hamiltonian is just the sum of the kinetic and potential energies and equation (3.6) is reduced to one dimension ($n = 1$) and is written out in terms of these four quantities, the result agrees with equations (3.9) of Reid and Ray. These authors did not give the result corresponding to (3.5), for which it would have been necessary to solve their differential equations (3.7). These differential equations can be solved by the method to be given in § 5.

It is clear that the procedure that led to (3.6) can be extended to any order to show that for the moments of order m,

$$\chi^{\alpha_1\alpha_2\cdots\alpha_m} = \chi_0{}^{\beta_1\beta_2\cdots\beta_m} u^{\alpha_1}{}_{\beta_1} u^{\alpha_2}{}_{\beta_2} \ldots u^{\alpha_m}{}_{\beta_m} + O(m+1), \tag{3.8}$$

here using χ to denote moments of any order. This result generalises the corresponding result of Reid and Ray.

4. Differential equations

Expanding the Hamiltonian about the basal trajectory gives

$$H_{\beta}(\boldsymbol{x}, t) = H_{\beta}(\boldsymbol{\xi} + \boldsymbol{X}, t) = h_{\beta} + X^{\gamma} h_{\beta\gamma} + \tfrac{1}{2} X^{\gamma} X^{\delta} h_{\beta\gamma\delta} + O(3).$$

Inserting this into (2.3) leads to

$$\dot{X}^{\alpha} = \varepsilon^{\alpha\beta} h_{\beta\gamma} X^{\gamma} + \tfrac{1}{2}\varepsilon^{\alpha\beta} h_{\beta\gamma\delta} X^{\gamma} X^{\delta} + O(3) \tag{4.1}$$

where we have used $\dot{\xi}^{\alpha} = \varepsilon^{\alpha\beta} h_{\beta}$. Now differentiating the second-order moment (3.3) and inserting (4.1) yields

$$\dot{\chi}^{\alpha\rho} = \varepsilon^{\alpha\beta} h_{\beta\gamma} \chi^{\gamma\rho} + \varepsilon^{\rho\beta} h_{\beta\gamma} \chi^{\gamma\alpha} + \tfrac{1}{2}\varepsilon^{\alpha\beta} h_{\beta\gamma\delta} \kappa^{\gamma\delta\rho} + \tfrac{1}{2}\varepsilon^{\rho\beta} h_{\beta\gamma\delta} \kappa^{\gamma\delta\alpha} + O(4). \tag{4.2}$$

Similarly, for the derivative of the third-order moment κ, evaluated only to the third order,

$$\dot{\kappa}^{\alpha\beta\gamma} = \varepsilon^{\alpha\delta} h_{\delta\sigma} \kappa^{\sigma\beta\gamma} + \varepsilon^{\beta\delta} h_{\delta\sigma} \kappa^{\sigma\gamma\alpha} + \varepsilon^{\gamma\delta} h_{\delta\sigma} \kappa^{\sigma\alpha\beta} + \mathrm{O}(4). \tag{4.3}$$

Of course the expressions for the moments given in (3.5) and (3.6) must satisfy these differential equations. Verification of this requires $\dot{u}^{\alpha}{}_{\beta}$, given in (2.5), and also $\dot{p}^{\alpha}{}_{\beta\gamma}$ which can be found by differentiating (2.3) twice:

$$\dot{p}^{\alpha}{}_{\beta\gamma} = \varepsilon^{\alpha\sigma} h_{\sigma\delta} p^{\delta}{}_{\beta\gamma} + \varepsilon^{\alpha\sigma} h_{\sigma\delta\lambda} u^{\delta}{}_{\beta} u^{\lambda}{}_{\gamma}. \tag{4.4}$$

Equations (4.2) generalise my earlier results (Andrews 1981b, equation 11) to the third order and to arbitrary Hamiltonian systems, while (4.2) and (4.3) generalise the corresponding equations (3.4) and (3.7) of Reid and Ray (1983) to arbitrary dimensions and Hamiltonians.

5. Solution of certain inhomogeneous equations

Inhomogeneous equations of the form

$$\dot{\rho}^{\alpha} = \varepsilon^{\alpha\gamma} h_{\gamma\delta} \rho^{\delta} + f^{\alpha} \tag{5.1}$$

can be solved by the standard procedure (for example, Coddington and Levinson 1955, theorem 3.1) to give

$$\rho^{\alpha}(t) = u^{\alpha}{}_{\beta}(t) \rho^{\beta}(0) + \int_0^t G^{\alpha}{}_{\beta}(t, t') f^{\beta}(t')\, \mathrm{d}t' \tag{5.2}$$

where

$$G^{\alpha}{}_{\beta}(t, t') = u^{\alpha}{}_{\gamma}(t) \varepsilon^{\gamma\delta} u^{\sigma}{}_{\delta}(t') \varepsilon_{\sigma\beta}. \tag{5.3}$$

The symplectic property implies $G^{\alpha}{}_{\beta}(t, t) = \delta^{\alpha}{}_{\beta}$ and from (2.5) it follows that

$$\mathrm{d}G^{\alpha}{}_{\beta}(t, t')/\mathrm{d}t = \varepsilon^{\alpha\gamma} h_{\gamma\delta}(t) G^{\delta}{}_{\beta}(t, t'). \tag{5.4}$$

These properties ensure that (5.2) satisfies (5.1).

Since equation (4.4) for $p^{\alpha}{}_{\beta\gamma}$ is of the form (5.1) it follows that the $p^{\alpha}{}_{\beta\gamma}$ can be expressed as an integral over products of the $u^{\mu}{}_{\nu}$ and the third derivative of the Hamiltonian:

$$p^{\alpha}{}_{\beta\gamma}(t) = \int_0^t G^{\alpha}{}_{\mu}(t, t') \varepsilon^{\mu\sigma} h^{\sigma}_{\sigma\delta\lambda}(t') u^{\delta'}{}_{\beta}(t') u^{\lambda}{}_{\gamma}(t')\, \mathrm{d}t. \tag{5.5}$$

It is also possible to solve inhomogeneous equations of the form of (4.2),

$$\dot{\rho}^{\alpha\beta} = \varepsilon^{\alpha\gamma} h_{\gamma\delta} \rho^{\delta\beta} + \varepsilon^{\beta\gamma} h_{\gamma\delta} \rho^{\delta\alpha} + f^{\alpha\beta} \tag{5.6}$$

where $f^{\alpha\beta}$ and $\rho^{\alpha\beta}$ are symmetric. By inspection, the solution is

$$\rho^{\alpha\beta}(t) = u^{\alpha}{}_{\gamma} u^{\beta}{}_{\delta} \rho^{\gamma\delta}(0) + \int_0^t G^{\alpha}{}_{\gamma}(t, t') G^{\beta}{}_{\delta}(t, t') f^{\gamma\delta}(t')\, \mathrm{d}t. \tag{5.7}$$

6. Moments relative to the centroid

It is straightforward to transform the moments to a different point of reference. Here we need to transform the moments relative to the basal trajectory to those relative to the centroid. Writing $\underset{\sim}{\chi}^{\alpha\beta}$, $\underset{\sim}{\kappa}^{\alpha\beta\gamma}$ for the moments relative to the centroid, let $\Delta^\alpha = \bar{x}^\alpha - \xi^\alpha$ and expand the moments in powers of Δ. Thus

$$\chi^{\alpha\beta} = N^{-1} \sum_A (x^\alpha_A - \bar{x}^\alpha + \Delta^\alpha)(x^\beta_A - \bar{x}^\beta + \Delta^\beta) = \underset{\sim}{\chi}^{\alpha\beta} + \Delta^\alpha \Delta^\beta. \tag{6.1}$$

Similarly,

$$\kappa^{\alpha\beta\gamma} = \underset{\sim}{\kappa}^{\alpha\beta\gamma} + \Delta^\alpha \underset{\sim}{\chi}^{\beta\gamma} + \Delta^\beta \underset{\sim}{\chi}^{\gamma\alpha} + \Delta^\gamma \underset{\sim}{\chi}^{\alpha\beta} + \Delta^\alpha \Delta^\beta \Delta^\gamma \tag{6.2}$$

and the inverse of this is

$$\underset{\sim}{\kappa}^{\alpha\beta\gamma} = \kappa^{\alpha\beta\gamma} - \Delta^\alpha \chi^{\beta\gamma} - \Delta^\beta \chi^{\gamma\alpha} - \Delta^\gamma \chi^{\alpha\beta} + 2\Delta^\alpha \Delta^\beta \Delta^\gamma. \tag{6.3}$$

Equation (3.7) reads $\Delta^\alpha = \frac{1}{2}\chi_0{}^{\beta\gamma} p^\alpha{}_{\beta\gamma} + O(3)$, and hence the difference between the moments relative to the centroid and the moments relative to the basal trajectory is of the fourth order.

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