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Phase Space Density Representations in Fluid Dynamics

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Phase space density representations of inviscid fluid dynamics were recently discussed by Abarbanel and Rouhi. Here it is shown that such representations may be simply derived and interpreted by means of the Liouville equation corresponding to the dynamical system of ordinary differential equations that describes fluid particle trajectories. The Hamiltonian and Poisson bracket for the phase space density then emerge as immediate consequences of the corresponding structure of the dynamics. For barotropic fluids, this approach leads by direct construction to the formulation presented by Abarbanel and Rouhi. Extensions of this formulation to inhomogeneous incompressible fluids and to fluids in which the state equation involves an additional transported scalar variable are constructed by augmenting the single-particle dynamics and phase space to include the relevant additional variable.

KEY WORDS: Phase space; Liouville equation; fluid dynamics; Hamiltonian; Poisson bracket.

1. INTRODUCTION

The purpose of this paper is to show that phase space density representations for inviscid fluid dynamics, of the type recently discussed by Abarbanel and Rouhi(1) (AR), may be derived and interpreted by an alternative approach which seems somewhat simpler. This approach leads to the desired Hamiltonian form of the phase space density evolution by direct construction, and it permits an immediate extension to a wider class of fluid flows.

The development is based upon the Liouville equation corresponding to the dynamical system of ordinary differential equations which describes

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the trajectories of the individual Lagrangian fluid particles.(2) The phase density function defined by AR is shown to be a special solution of this Liouville equation, corresponding to the case in which there is no dispersion of velocities in the initial distribution. The Hamiltonian function and Poisson bracket for the evolution of the phase space density then emerge as immediate consequences of the corresponding structure of the dynamics.

For the case of barotropic fluids, the present approach provides a straightforward and purely constructive route to the formulation presented by AR. This case is particularly simple because the pressure gradient divided by density is itself the gradient of a scalar quantity. This quantity is formally equivalent to an external potential, which then appears as an additive term in the single-particle Hamiltonian.

A similar treatment of more general inviscid fluid flows is less straightforward, as the pressure gradient divided by density is in general no longer a gradient. However, this complication can be circumvented by including the appropriate additional scalar variable in the single-particle dynamics and corresponding phase space. In the case of inhomogeneous incompressible fluids, the appropriate additional variable is the specific volume of the fluid particle, which is conserved in the motion. The constraint that the fluid velocity field be solenoidal is then automatically contained in the time evolution of the phase-space density. Compressible fluids in which the state equation involves an additional transported scalar variable may be dealt with in a similar way. We thereby obtain phase space density representations of these more general fluid flows, including explicit expressions for the Hamiltonians and Poisson brackets therein.

2. GENERAL PRELIMINARIES

Consider a deterministic dynamical system of the general form

$$\dot{\mathbf{x}} = \mathbf{U}(\mathbf{x}, t) \tag{1}$$

where $\mathbf{x} = (x_1, x_2, \ldots)$ is a vector of dependent variables which specifies the state of the system. The Liouville equation corresponding to Eq. (1) is just the continuity equation in state space,(2)

$$\frac{\partial F}{\partial t} + \frac{\partial}{\partial \mathbf{x}} \cdot (F\mathbf{U}) = 0 \tag{2}$$

Here $F(\mathbf{x}, t)$ is the probability distribution function for an ensemble of similar systems, each of which is governed by Eq. (1) but which differ in their initial conditions according to an arbitrary initial distribution $F(\mathbf{x}, 0)$.

The distribution function is defined so that $F(\mathbf{x}, t)\,d\mathbf{x}$ is the fraction of the ensemble with states in the interval $(\mathbf{x}, \mathbf{x}+d\mathbf{x})$ at time t.

In this paper we are concerned with Hamiltonian systems, for which $\mathbf{U}(\mathbf{x}, t)$ takes the form[(3)]

$$\mathbf{U}=\mathbf{A}\cdot(\partial H/\partial\mathbf{x}) \tag{3}$$

where $H(\mathbf{x}, t)$ is the Hamiltonian function and $\mathbf{A}(\mathbf{x})$ is an antisymmetric matrix satisfying the condition

$$(\partial/\partial\mathbf{x})\cdot\mathbf{A}(\mathbf{x})=0 \tag{4}$$

The antisymmetry of $\mathbf{A}$ implies at once that if H has no explicit time dependence, then it is a constant of the motion. Equation (4), together with the antisymmetry of $\mathbf{A}$, implies that $(\partial/\partial\mathbf{x})\cdot[\mathbf{A}\cdot(\partial H/\partial\mathbf{x})]=0$. Equation (4) therefore ensures that the dynamics generates a volume-preserving flow in the phase space; Hamiltonian systems of physical origin always seem to satisfy this condition. [Here we assume that the variables $\mathbf{x}$ constitute a "natural representation" of the state of the system.[(3,4)] Otherwise, Eq. (4) must be replaced by its covariant analog, namely $(\partial/\partial\mathbf{x})\cdot(g^{-1/2}\mathbf{A})=0$, where $g(\mathbf{x})$ is the determinant of a metric tensor in state space.[(2-5)]]

The Poisson bracket for the system is defined by

$$\{f, g\}=(\partial f/\partial\mathbf{x})\cdot\mathbf{A}\cdot(\partial g/\partial\mathbf{x}) \tag{5}$$

in terms of which the equations of motion take the form

$$\dot{\mathbf{x}}=\{\mathbf{x}, H\} \tag{6}$$

The time evolution of an arbitrary observable quantity $Q(\mathbf{x}, t)$ obeys

$$\dot{Q}=\partial Q/\partial t+\{Q, H\} \tag{7}$$

The corresponding Hamiltonian form of the Liouville equation is obtained by substituting Eq. (3) into Eq. (2) and making use of Eq. (4). The result is

$$\partial F/\partial t+\{F, H\}=0 \tag{8}$$

Thus, the Hamiltonian structure of the Liouville equation is a direct consequence and reflection of the corresponding structure of the underlying dynamics.

Of course, there are other properties that are commonly associated with Hamiltonian behavior,[(6)] but they do not interact with the present development, so we need not assume them. Of these, the most fundamental and important is that the Poisson bracket of Eq. (5) satisfy the Jacobi identity. If in addition the matrix **A** is nonsingular (which requires that the number of variables be even), Darboux' theorem guarantees that the system can be reduced to canonical form by a transformation of variables,(6) and this in turn implies incompressibility of the phase flow. In the present context, however, the incompressibility condition itself is the relevant property, and this condition is satisfied for a wider class of systems than are encompassed by Darboux' theorem. In particular, it can be satisfied for systems of an odd number of variables.(3)

3. BAROTROPIC FLUID DYNAMICS

We consider a barotropic fluid governed by the equations of motion(1)

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{9}$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla \Psi + \mathbf{u} \times \mathbf{\Omega}(\mathbf{r}) - \nabla \Phi \tag{10}$$

where $\rho(\mathbf{r}, t)$ is the mass density, $\mathbf{u}(\mathbf{r}, t)$ is the fluid velocity, $\mathbf{\Omega}/2$ is a rotation rate, $\Phi(\mathbf{r}, t)$ is an external potential field, and $\Psi(\mathbf{r}, t) = \psi(\rho(\mathbf{r}, t))$, where

$$\psi(\rho) = \int^{\rho} d\rho' \, \frac{1}{\rho'} \frac{dp(\rho')}{d\rho'} \tag{11}$$

and $p(\rho)$ is the barotropic state function. Barotropic behavior is usually a consequence of assuming that either the specific entropy or the temperature is constant and uniform, in which case ψ respectively represents either the specific enthalpy or the chemical potential.

The first step is to write down ordinary differential equations corresponding to Eqs. (9) and (10) which describe the fluid particle trajectories. Since a convective derivative is simply a total time derivative following a fluid particle, these equations take the form

$$\dot{\mathbf{r}} = \mathbf{v} \tag{12}$$

$$\dot{\mathbf{v}} = -(\partial/\partial \mathbf{r})(\Psi + \Phi) + \mathbf{v} \times \mathbf{\Omega}(\mathbf{r}) \tag{13}$$

where $\mathbf{r}$ and $\mathbf{v}$ are now to be interpreted as *dependent* variables which respectively represent the position and velocity of a fluid particle. This system can be put into our standard Hamiltonian form by letting $\mathbf{x} = (\mathbf{r}, \mathbf{v})$,

$$H(\mathbf{r}, \mathbf{v}, t) = \tfrac{1}{2} |\mathbf{v}|^2 + \Psi(\mathbf{r}, t) + \Phi(\mathbf{r}, t) \tag{14}$$

and

$$\mathsf{A}=\begin{pmatrix} \mathbf{0} & \mathsf{U} \\ -\mathsf{U} & \mathbf{\Omega}\cdot\boldsymbol{\epsilon} \end{pmatrix} \tag{15}$$

where $\mathbf{0}$ is the 3×3 zero tensor, U is the 3×3 unit tensor, and $\boldsymbol{\epsilon}$ is the Levi-Civita antisymmetric third-order tensor. Notice that Eq. (4) is in fact satisfied. According to Eq. (5), the Poisson bracket of two arbitrary functions $f(\mathbf{r}, \mathbf{v})$ and $g(\mathbf{r}, \mathbf{v})$ is then given by

$$\{f, g\}=\frac{\partial f}{\partial \mathbf{r}}\cdot\frac{\partial g}{\partial \mathbf{v}}-\frac{\partial f}{\partial \mathbf{v}}\cdot\frac{\partial g}{\partial \mathbf{r}}+\left(\frac{\partial f}{\partial \mathbf{v}}\times\frac{\partial g}{\partial \mathbf{v}}\right)\cdot\mathbf{\Omega} \tag{16}$$

from which one readily verifies that the fundamental brackets of $\mathbf{r}$ and $\mathbf{v}$ with each other agree with those given by AR. Equation (2) for the time evolution of the phase space density F takes the AR form

$$\frac{\partial F}{\partial t}+\mathbf{v}\cdot\frac{\partial F}{\partial \mathbf{r}}+\left[-\frac{\partial}{\partial \mathbf{r}}(\Psi+\Phi)+\mathbf{v}\times\mathbf{\Omega}\right]\cdot\frac{\partial F}{\partial \mathbf{v}}=0 \tag{17}$$

According to the general development of Section 2, the equivalent Hamiltonian form of Eq. (17) is simply Eq. (8) with the Poisson bracket given by Eq. (16).

Equation (17) admits a much broader class of solutions than those considered by AR. However, it is only for the AR subclass of solutions that the moments of F satisfy the closed fluid dynamical equations of motion (9) and (10). The reason is that the Liouville equation admits solutions in which there is a distribution in particle velocities at each point in space, whereas the fluid dynamical description attributes a unique fluid particle velocity to each point in space. To make contact with fluid dynamics, it is therefore necessary to restrict attention to phase space densities proportional to a delta function in velocity space; i.e., to density functions F of the form

$$F(\mathbf{r}, \mathbf{v}, t)=\rho(\mathbf{r}, t)\,\delta(\mathbf{v}-\mathbf{u}(\mathbf{r}, t)) \tag{18}$$

In order to verify that solutions of this form in fact exist, one combines Eqs. (17) and (18) to obtain

$$J(\mathbf{r}, t)\,\delta(\mathbf{v}-\mathbf{u}(\mathbf{r}, t))-\rho(\mathbf{r}, t)\,\mathbf{K}(\mathbf{r}, t)\cdot\boldsymbol{\delta}'(\mathbf{v}-\mathbf{u}(\mathbf{r}, t))=0 \tag{19}$$

where $J(\mathbf{r}, t)$ stands for the left member of Eq. (9), $\mathbf{K}(\mathbf{r}, t)=\partial\mathbf{u}/\partial t+\mathbf{u}\cdot\nabla\mathbf{u}+\nabla(\Psi+\Phi)-\mathbf{u}\times\mathbf{\Omega}$, $\boldsymbol{\delta}'(\mathbf{v})=\partial\delta(\mathbf{v})/\partial\mathbf{v}$, and use has been made of the identity $\mathbf{v}\boldsymbol{\delta}'(\mathbf{v}-\mathbf{u})=\mathbf{u}\boldsymbol{\delta}'(\mathbf{v}-\mathbf{u})-\delta(\mathbf{v}-\mathbf{u})\,\mathsf{U}$. In order for Eq. (19) to be satisfied, the coefficients of $\delta(\mathbf{v}-\mathbf{u})$ and $\delta'(\mathbf{v}-\mathbf{u})$ therein must separately vanish, and this requires that the functions $\rho(\mathbf{r}, t)$ and $\mathbf{u}(\mathbf{r}, t)$ appearing in Eq. (18) satisfy Eqs. (9) and (10). Thus, phase space densities of the form (18) are indeed solutions of Eq. (17) if the fluid dynamical equations (9) and (10) are satisfied. We have therefore arrived at the AR formulation for barotropic fluids by an alternative and purely constructive route.

It should be noted that the restriction to solutions of the form (18) is in reality only a restriction on the initial density function $F_0(\mathbf{r}, \mathbf{v}) = F(\mathbf{r}, \mathbf{v}, 0)$. The Liouville equation (17) constitutes an initial value problem for F, so that $F(\mathbf{r}, \mathbf{v}, t)$ is uniquely determined by $F_0(\mathbf{r}, \mathbf{v})$. It follows that solutions of the form (18) uniquely evolve from initial conditions of the same form; i.e., if F has the form (18) at $t = 0$, then this form is preserved at all future times.

4. COMPRESSIBLE FLUIDS WITH ARBITRARY STATE EQUATIONS

We now generalize the preceding development to compressible fluids in which the state equation includes a dependence on an additional transported scalar variable. The fluid dynamical equations for this case may be written as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{20}$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p + \mathbf{u} \times \mathbf{\Omega} - \nabla \Phi \tag{21}$$

$$\frac{\partial \chi}{\partial t} + \mathbf{u} \cdot \nabla \chi = 0 \tag{22}$$

where p, ρ, and χ are related by an equation of state which may be written as $\rho = \rho(p, \chi)$. Equation (22) states that the specific quantity χ is conserved along a fluid particle trajectory, and we are therefore led to consider the value of χ for the fluid particle as an additional variable in the single-particle dynamical description. The single-particle dynamics corresponding to Eqs. (20)–(22) is therefore taken to be

$$\dot{\mathbf{r}} = \mathbf{v} \tag{23}$$

$$\dot{\mathbf{v}} = -(\partial/\partial \mathbf{r})(\Psi + \Phi) + \mathbf{v} \times \mathbf{\Omega}(\mathbf{r}) \tag{24}$$

$$\dot{z} = 0 \tag{25}$$

where z is the value of χ for the fluid particle, and $\Psi(\mathbf{r}, z, t) = \psi(p(\mathbf{r}, t), z)$, where

$$\psi(p, \chi) = \int^{p} \frac{dp'}{\rho(p', \chi)} \tag{26}$$

and the integral is to be performed at constant χ. As in the barotropic case, if χ is the specific entropy, ψ is the specific enthalpy, while if χ is the temperature, ψ is the chemical potential. Here, however, χ has different values for different fluid particles.

The system of Eqs. (23)–(25) can be put into our standard Hamiltonian form by letting $\mathbf{x} = (\mathbf{r}, \mathbf{v}, z)$,

$$H(\mathbf{r}, \mathbf{v}, z, t) = \tfrac{1}{2}|\mathbf{v}|^2 + \Psi(\mathbf{r}, z, t) + \Phi(\mathbf{r}, t) \tag{27}$$

and

$$\mathsf{A} = \begin{pmatrix} \mathbf{0} & \mathsf{U} & \mathbf{0} \\ -\mathsf{U} & \boldsymbol{\Omega}\cdot\boldsymbol{\epsilon} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & 0 \end{pmatrix} \tag{28}$$

where $\mathbf{0}$ is the three-dimensional zero vector. We observe that Eq. (4) is again satisfied. According to Eq. (5), the Poisson bracket of two arbitrary functions $f(\mathbf{r}, \mathbf{v}, z)$ and $g(\mathbf{r}, \mathbf{v}, z)$ is then given by

$$\{f, g\} = \frac{\partial f}{\partial \mathbf{r}}\cdot\frac{\partial g}{\partial \mathbf{v}} - \frac{\partial f}{\partial \mathbf{v}}\cdot\frac{\partial g}{\partial \mathbf{r}} + \left(\frac{\partial f}{\partial \mathbf{v}}\times\frac{\partial g}{\partial \mathbf{v}}\right)\cdot\boldsymbol{\Omega} \tag{29}$$

which looks formally the same as Eq. (16), but is different because it acts on a different class of phase functions defined on the enlarged phase space $(\mathbf{r}, \mathbf{v}, z)$. Equation (2) for the time evolution of the phase space density $F(\mathbf{r}, \mathbf{v}, z, t)$ takes the form

$$\frac{\partial F}{\partial t} + \mathbf{v}\cdot\frac{\partial F}{\partial \mathbf{r}} + \left[-\frac{\partial}{\partial \mathbf{r}}(\Psi + \Phi) + \mathbf{v}\times\boldsymbol{\Omega}\right]\cdot\frac{\partial F}{\partial \mathbf{v}} = 0 \tag{30}$$

The corresponding Hamiltonian form is again simply given by Eq. (8), with the Poisson bracket defined by Eq. (29). In order to make contact with fluid dynamics, it is again necessary to restrict attention to density functions proportional to the appropriate delta functions. The appropriate form for present purposes is

$$F(\mathbf{r}, \mathbf{v}, z, t) = \rho(\mathbf{r}, t)\,\delta(\mathbf{v} - \mathbf{u}(\mathbf{r}, t))\,\delta(z - \chi(\mathbf{r}, t)) \tag{31}$$

In order to verify that solutions of this form in fact exist, one combines Eqs. (30) and (31) to obtain

$$J\delta(\mathbf{v}-\mathbf{u})\,\delta(z-\chi)-\rho\mathbf{K}\cdot\boldsymbol{\delta}'(\mathbf{v}-\mathbf{u})\,\delta(z-\chi)-\rho L\delta(\mathbf{v}-\mathbf{u})\,\delta'(z-\chi)=0 \qquad (32)$$

where $J(\mathbf{r}, t)$ and $\mathbf{K}(\mathbf{r}, t)$ are defined as before, and $L(\mathbf{r}, t)=\partial\chi/\partial t+\mathbf{u}\cdot\nabla\chi$. In order for Eq. (32) to be satisfied, the coefficients J, $\mathbf{K}$, and L must separately vanish, and this yields precisely Eqs. (20)–(22).

This development provides a complete solution to the problem posed by AR of representing this class of fluid flows by means of a phase space density whose time evolution is Hamiltonian in character. Explicit forms have been given for the Hamiltonian and Poisson brackets in this representation. This has been accomplished by augmenting the single-particle dynamics and phase space to include the additional variable z. In addition to its mathematical convenience, this augmentation is physically sensible, as the extra variable is needed to completely specify the state of the fluid particle. A description in terms of $\mathbf{r}$ and $\mathbf{v}$ alone is manifestly incomplete and should not be expected. Even if such a description could be found, it would evidently be of the nature of a contraction of the present description lacking any intrinsic significance.

5. INHOMOGENEOUS INCOMPRESSIBLE FLUIDS

In addition to the barotropic fluid description of Section 3, AR also presented a phase space density representation of homogeneous incompressible flow. In this case, however, the formulation seems unsatisfactory in two respects. First, the solenoidal condition on the velocity field is not a consequence of the phase space density dynamics but must be externally imposed. Second, the restriction to homogeneous flow seems essential to the AR development, whereas a generic treatment of incompressible flow should properly include the case of an inhomogeneous fluid, in which density continues to be transported and the solenoidal condition is a separate constraint. The homogeneous case is merely a special case in which the initial density field happens to be uniform.

A more satisfactory treatment of incompressible flow, in which both of the above difficulties are eliminated, is obtained by observing that inhomogeneous incompressible flow is merely a special case of the development in Section 4. This case is realized by letting χ be the specific volume $1/\rho$. Equation (22) then combines with Eq. (20) to yield the solenoidal incompressibility condition

$$\nabla\cdot\mathbf{u}=0 \qquad (33)$$

on the velocity field. The state equation now becomes simply $\rho = 1/\chi$, independent of pressure, so that the pressure is no longer given by a state equation but is implicitly determined by the solenoidal constraint of Eq. (33). Equation (26) now reduces to $\psi(p, \chi) = \chi p$, so that $\Psi(\mathbf{r}, z, t) = zp(\mathbf{r}, t)$ and $\partial\Psi/\partial\mathbf{r} = z\,\partial p/\partial\mathbf{r}$. With these identifications the entire formalism of Section 4 now applies to inhomogeneous incompressible flow. We have therefore constructed a complete Hamiltonian phase space density representation of inhomogeneous incompressible flow, in which the solenoidal condition of Eq. (33) is properly carried along during the time evolution.

6. CONCLUDING REMARKS

Phase space density representations in fluid dynamics have been approached from the point of view of the Liouville equation corresponding to the system of ordinary differential equations representing the motion of individual Lagrangian fluid particles. This approach establishes a direct connection between the Hamiltonian structure of the phase space density evolution and that of the corresponding single-particle dynamics. This equivalence is useful because the latter structure is usually easier to construct than the former.

Explicit phase-space density representations, including the form of the Hamiltonians and Poisson brackets, have been constructed for barotropic fluids, inhomogeneous incompressible fluids, and compressible fluids with arbitrary state equations. The results for the barotropic case duplicated those of AR. The formulations for the other two cases are new, and were based upon an augmentation of the single-particle dynamics and phase space to include the relevant additional variable.

One naturally inquires as to whether such phase space density representations are of any fundamental significance. The answer would seem to be in the negative. A fluid in motion is actually a system of *interacting* fluid particles, whereas the present representations are based upon finding an equivalent single-particle description, and this seems rather artificial. Perhaps in consequence, the Hamiltonians that appear in such formulations also seem artificial. Nevertheless, such representations may be useful for technical purposes, as the paper of AR illustrates. There may also be circumstances in which the corresponding systems of ordinary differential equations, such as Eqs. (23)–(25), are useful. In particular, such systems might serve as a basis for the construction of numerical methods in which the underlying Hamiltonian structure is preserved.(7)

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