

Hamiltonian Dynamics

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Synopsis

Hamiltonian dynamics describes the evolution of conservative physical systems. Originally developed as a generalization of Newtonian mechanics, it represents a core component of any undergraduate physics curriculum. What is not so widely recognized is that the ideal (i.e. conservative) form of the governing equations used in dynamical meteorology are also Hamiltonian dynamical systems. This chapter explains how this is so, and some of the consequences that follow from this fact. It is important to be able to connect theoretical results across the hierarchy of various models used in dynamical meteorology, from the simplest to the most complex. Hamiltonian dynamics is what allows one to do precisely that.

Keywords

available potential energy, Casimir invariant, conservation laws, Eliassen-Palm wave activity, momentum flux, potential vorticity, pseudoenergy, pseudomomentum, stability, wave activity

Key points

- The governing equations of dynamical meteorology are examples of Hamiltonian dynamical systems
- Hamiltonian dynamical structure provides a unifying framework which connects specific theories across a hierarchy of models
- Wave-activity conservation laws and stability theorems are notable examples

1. Introduction

Hamiltonian dynamics describes the evolution of conservative physical systems. Originally developed as a generalization of Newtonian mechanics, describing gravitationally driven motion from the simple pendulum to celestial mechanics, it also applies to such diverse areas of physics as quantum mechanics, quantum field theory, statistical mechanics, electromagnetism, and optics — in short, to any physical system for which dissipation is negligible. Dynamical meteorology consists of the fundamental laws of physics, including Newton's second law. For many purposes, diabatic and viscous processes can be neglected and the equations are then conservative. (For example, in idealized modeling studies, dissipation is often only present for numerical reasons and is kept as small as possible.) In such cases dynamical meteorology obeys Hamiltonian dynamics. Even when nonconservative processes are not negligible, it often turns out that separate analysis of the conservative dynamics, which fully describes the nonlinear interactions, is essential for an understanding of the complete system, and the Hamiltonian description can play a useful role in this respect. Energy budgets and momentum transfer by waves are but two examples.

Hamiltonian dynamics is often associated with conservation of energy, but it is in fact much more than that. Hamiltonian dynamical systems possess a mathematical structure that ensures some remarkable properties. Perhaps the most important is the connection between symmetries and conservation laws known as Noether's theorem. Well-known examples are the fact that conservation of energy is linked to symmetry in time, and conservation of momentum to symmetry in space. Less well-known is the fact that material conservation of potential vorticity, so crucial to the theory of dynamical meteorology, is also connected to a symmetry by Noether's theorem, but to a symmetry that is invisible in the Eulerian formulation of the governing equations. It turns out that one can exploit the underlying Hamiltonian structure of a system through the relevant conservation laws even if the explicit form of that structure is not known, which is useful for applications. As is shown in detail below, symmetry-based conservation laws provide a general theory of available potential energy, and show why it is that Rossby waves carry negative zonal momentum, thereby explaining both the maintenance of the westerlies and the stratospheric Brewer–Dobson circulation. Such laws also provide a powerful way of deriving stability criteria.

Dynamical meteorologists use a variety of theoretical models, ranging from the fully compressible equations through the hydrostatic primitive, Boussinesq, and quasi-geostrophic equations to the barotropic equations. With such a zoo of models, it is crucial to know the extent to which theories developed for one model carry over to another. Hamiltonian dynamics provides this unifying framework. All the models just mentioned are in fact Hamiltonian, and models can be grouped into families according to their Hamiltonian structure. In this way it becomes immediately apparent, for example, that the Charney–Stern stability theorem for baroclinic quasi-geostrophic flow is the counterpart to Rayleigh's inflection-point theorem for barotropic

flow, and that an analogous stability theorem will exist for any balanced model having a similar Hamiltonian structure, no matter what the definition is of the potential vorticity. Thus, it is precisely through its abstract character that Hamiltonian dynamics has many powerful applications in theoretical dynamical meteorology. The main applications discussed here are presented in Table 1.

The exposition in this Chapter is intended to be self-contained, but is necessarily kept succinct. In addition to the specific references provided, readers may wish to consult Salmon (1988), Shepherd (1990) or Morrison (1998) for general treatments of Hamiltonian fluid dynamics. Note that there are different ways to represent Hamiltonian dynamics: Hamilton's principle, Poisson brackets, or the symplectic formulation. In this chapter we follow the symplectic formulation as being most readily linked to the traditional governing equations.

Table 1: The main applications in theoretical dynamical meteorology discussed in this chapter, grouped according to their pedigree within Hamiltonian dynamics (pseudoenergy or pseudomomentum) and their nature (conservation law or stability theorem).

	Pseudoenergy	Pseudomomentum
Conservation law	Available potential energy	Eliassen-Palm wave activity
Stability theorem	Static stability Centrifugal stability Symmetric stability	Rayleigh-Kuo Charney-Stern

2. Canonical and Noncanonical Dynamics

In classical mechanics (Landau and Lifshitz, 1976), canonical Hamiltonian dynamical systems are those described by Hamilton's equations (eqns [1]).

$$\frac{dq_i}{dt} = \frac{\partial \mathcal{H}}{\partial p_i}, \quad \frac{dp_i}{dt} = -\frac{\partial \mathcal{H}}{\partial q_i} \quad [i = 1, \dots, N] \quad [1]$$

Here $\mathcal{H}(\mathbf{q}, \mathbf{p})$ is the Hamiltonian function, $\mathbf{q} \equiv (q_1, \dots, q_N)$ are the generalized coordinates, and $\mathbf{p} \equiv (p_1, \dots, p_N)$ the generalized momenta. For so-called natural systems with $\mathcal{H} = (|\mathbf{p}|^2/2m) + U(\mathbf{q})$, where m is the mass and U the potential energy, eqns [1] immediately lead to eqn [2], which is Newton's second law for a conservative system.

$$m \frac{d^2 q_i}{dt^2} = -\frac{\partial U}{\partial q_i} \quad [i = 1, \dots, N] \quad [2]$$

Conservation of energy follows directly from eqns [1], for any \mathcal{H} , by the chain rule (repeated indices are summed).

$$\frac{d\mathcal{H}}{dt} = \frac{\partial \mathcal{H}}{\partial q_i} \frac{dq_i}{dt} + \frac{\partial \mathcal{H}}{\partial p_i} \frac{dp_i}{dt} = \frac{\partial \mathcal{H}}{\partial q_i} \frac{\partial \mathcal{H}}{\partial p_i} - \frac{\partial \mathcal{H}}{\partial p_i} \frac{\partial \mathcal{H}}{\partial q_i} = 0 \quad [3]$$

2.1 Symplectic Formulation

The theory of canonical transformations suggests that there is nothing special about the q s and p s, and Hamilton's equations [1] can be written in the so-called symplectic form, eqn [4].

$$\frac{du_i}{dt} = J_{ij} \frac{\partial \mathcal{H}}{\partial u_j} \quad [i = 1, \dots, 2N] \quad [4]$$

In eqn [4], $\mathbf{u} = (q_1, \dots, q_N, p_1, \dots, p_N)$ and J is given by eqn [5], where I is the $N \times N$ identity matrix.

$$J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \quad [5]$$

J has certain mathematical properties, including skew-symmetry. More generally, one can take those properties to be the definition of Hamiltonian structure, with J not necessarily of the form of eqn [5]. The skew-symmetry of J nevertheless guarantees energy conservation (eqn [6]).

$$\frac{d\mathcal{H}}{dt} = \frac{\partial\mathcal{H}}{\partial u_i} \frac{du_i}{dt} = \frac{\partial\mathcal{H}}{\partial u_i} J_{ij} \frac{\partial\mathcal{H}}{\partial u_j} = 0 \quad [6]$$

There is an important distinction between systems with a nonsingular (or invertible) J , which can always be transformed into the canonical form of eqn [5], and those with a singular (or noninvertible) J . The latter, known as noncanonical systems, possess a special class of invariant functions known as Casimir invariants (Sudarshan and Mukunda, 1973). These are the solutions of eqn [7] (for canonical systems the solutions are just constants).

$$J_{ij} \frac{\partial\mathcal{C}}{\partial u_j} = 0 \quad [i = 1, \dots, 2N] \quad [7]$$

That they are necessarily conserved in time then follows from the skew-symmetry of J (eqn [8]).

$$\frac{d\mathcal{C}}{dt} = \frac{\partial\mathcal{C}}{\partial u_i} \frac{du_i}{dt} = \frac{\partial\mathcal{C}}{\partial u_i} J_{ij} \frac{\partial\mathcal{H}}{\partial u_j} = -\frac{\partial\mathcal{H}}{\partial u_i} J_{ij} \frac{\partial\mathcal{C}}{\partial u_j} = 0 \quad [8]$$

The best-known example of a noncanonical Hamiltonian system is Euler's equations for rigid-body dynamics (Arnold, 1989). Having an odd number of evolution equations (three in this case), the system is necessarily noncanonical because any skew-symmetric matrix of odd dimension must be singular. There is one Casimir invariant for Euler's equations, the total angular momentum.

2.2 Noether's Theorem

For a canonical system, if a particular generalized coordinate q_j does not appear in the Hamiltonian, then the Hamiltonian is invariant under changes in that coordinate; in other words, there is a coordinate symmetry. Translational and rotational symmetries are common examples. Hamilton's equations [1] then immediately imply that the corresponding generalized momentum is conserved: $dp_j/dt = 0$.

This connection between symmetries and conservation laws has a more general and far more powerful form. Given a function $\mathcal{F}(\mathbf{u})$, define $\delta_{\mathcal{F}} u_i \equiv \varepsilon J_{ij} \frac{\partial \mathcal{F}}{\partial u_j}$, where ε is an infinitesimal parameter; $\delta_{\mathcal{F}} \mathbf{u}$ is called the infinitesimal variation in \mathbf{u} generated by \mathcal{F} . (In the canonical case, $\delta_{\mathcal{F}} \mathbf{u}$ is an infinitesimal canonical transformation.) It then follows that the infinitesimal variation in \mathcal{H} generated by \mathcal{F} is given by eqn [9].

$$\delta_{\mathcal{F}} \mathcal{H} = \frac{\partial \mathcal{H}}{\partial u_i} \delta_{\mathcal{F}} u_i = \varepsilon \frac{\partial \mathcal{H}}{\partial u_i} J_{ij} \frac{\partial \mathcal{F}}{\partial u_j} \quad [9]$$

On the other hand, the time evolution of \mathcal{F} is given by eqn [10].

$$\frac{d\mathcal{F}}{dt} = \frac{\partial \mathcal{F}}{\partial u_i} \frac{du_i}{dt} = \frac{\partial \mathcal{F}}{\partial u_i} J_{ij} \frac{\partial \mathcal{H}}{\partial u_j} \quad [10]$$

Using the skew-symmetry of J , eqns [9] and [10] then imply that $\delta_{\mathcal{F}} \mathcal{H} = 0$ if and only if $\frac{d\mathcal{F}}{dt} = 0$. This connects symmetries and conservation laws: the Hamiltonian is invariant under the variation generated by \mathcal{F} (i.e., that variation represents a symmetry of the Hamiltonian) if and only if \mathcal{F} is a conserved quantity. This result, known as Noether's theorem, is one of the central results of Hamiltonian dynamics (Arnold, 1989) and underpins many of its applications to dynamical meteorology.

Casimir invariants are special because $\delta_{\mathcal{C}} \mathbf{u} = \mathbf{0}$. This suggests that they correspond to invisible symmetries. For example, in rigid-body dynamics the total angular momentum is a conserved quantity in any description of the motion. In the original canonical description it corresponds to the rotational symmetry of the dynamics, but in Euler's equations, where angles have been eliminated, it enters as a Casimir because the underlying physical symmetry is no longer explicit.

3. Barotropic Dynamics

In what sense are the models of dynamical meteorology Hamiltonian? Consider what is probably the simplest such model, the barotropic vorticity equation (eqn [11]), which describes two-dimensional, nondivergent flow.

$$\frac{\partial \omega}{\partial t} = -\mathbf{v} \cdot \nabla \omega = -\partial(\psi, \omega) \quad [11]$$

Here $\omega(x, y, t) = \hat{\mathbf{z}} \cdot (\nabla \times \mathbf{v}) = \nabla^2 \psi$ is the vorticity, $\hat{\mathbf{z}}$ is the unit vector in the vertical direction, $\mathbf{v}(x, y, t) = \hat{\mathbf{z}} \times \nabla \psi$ is the horizontal velocity, $\psi(x, y, t)$ is the streamfunction, and $\partial(f, g) \equiv f_x g_y - f_y g_x$ is the two-dimensional Jacobian. The candidate Hamiltonian is the conserved energy of this system, which is just the kinetic energy. The obvious dynamical variable is the vorticity. In order to cast eqn [11] in the form of eqn [4], we need to regard every point (x, y) in space as indexing a degree of freedom analogous to the index i ; the sum over i then becomes an integral over space, functions become functionals, and partial derivatives become functional or variational derivatives. Thus we write eqn [12].

$$\delta \mathcal{H} = \delta \iint \frac{1}{2} |\nabla \psi|^2 dx dy = \iint \nabla \psi \cdot \delta \nabla \psi dx dy = \iint \{\nabla \cdot (\psi \delta \nabla \psi) - \psi \delta \omega\} dx dy \quad [12]$$

Assuming for now that the boundary terms vanish, we identify the variational derivative as $\delta \mathcal{H} / \delta \omega = -\psi$. The need to integrate by parts reflects the fact that the effect of a vorticity perturbation on the kinetic energy density is nonlocal; thus, partial derivatives at fixed points in space make no sense and variational derivatives are essential. Equation [11] can now be cast in Hamiltonian form as eqn [13].

$$\frac{\partial \omega}{\partial t} = J \frac{\delta \mathcal{H}}{\delta \omega} \quad \text{where} \quad J \equiv -\partial(\omega, \cdot) \quad [13]$$

Note that J is now a differential operator rather than a matrix. It is evidently skew-symmetric since $\iint f J g dx dy = - \iint g J f dx dy$ (under suitable boundary conditions) for arbitrary functions f, g .

3.1 Conservation Laws

The form of J in eqn [13] is clearly singular: any function of ω inserted in the argument gives zero. These then represent Casimir invariants of the system: functionals of the form [14], where $C(\cdot)$ is an arbitrary differentiable function, evidently satisfy $J(\delta C/\delta\omega) = 0$.

$$C = \iint C(\omega) \, dx dy \quad \text{with} \quad \frac{\delta C}{\delta\omega} = C'(\omega) \quad [14]$$

The fact that such functionals are conserved in time corresponds to the material conservation of vorticity expressed by eqn [11].

To identify the momentum invariants, we need to apply Noether's theorem to the various spatial symmetries. Suppose that the domain is unbounded, with decay conditions at infinity, so that there is symmetry in all directions. The variation in ω corresponding to a translation by δx in the coordinate x is given by $\delta\omega = -(\partial\omega/\partial x) \delta x$. Setting $\varepsilon = \delta x$, we then need to solve for the momentum invariant \mathcal{M} according to eqn [15].

$$-\varepsilon \frac{\partial\omega}{\partial x} = \delta_{\mathcal{M}}\omega = \varepsilon J \frac{\delta\mathcal{M}}{\delta\omega} = -\varepsilon \partial(\omega, \frac{\delta\mathcal{M}}{\delta\omega}) \quad [15]$$

To within the addition of a Casimir, the solution of eqn [15] is given by $\delta\mathcal{M}/\delta\omega = y$. Hence we may choose \mathcal{M} as in eqn [16], where $\mathbf{v} = (u, v)$.

$$\mathcal{M} = \iint y\omega \, dx dy = \iint y \left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \right) \, dx dy = \iint u \, dx dy \quad [16]$$

The first, elementary form of \mathcal{M} given by eqn [16] is known as Kelvin's impulse (Benjamin, 1984). It represents the y 'center-of-mass' of the vorticity distribution, and is in many ways the preferable form because it is local in ω . The final form, however, shows that the invariant \mathcal{M} corresponding to symmetry in x is ultimately just the x -momentum, as expected. The same argument applied to translation in the coordinate y yields eqn [17].

$$\mathcal{M} = -\iint x\omega \, dx dy = \iint v \, dx dy \quad [17]$$

Finally, rotational symmetry leads to eqn [18], where $\mathbf{r} \equiv (x, y)$ and $r = |\mathbf{r}|$, which is the angular momentum about the origin.

$$\mathcal{M} = - \iint \frac{1}{2} r^2 \omega \, dx dy = \iint \hat{\mathbf{z}} \cdot (\mathbf{r} \times \mathbf{v}) \, dx dy \quad [18]$$

The discussion has so far neglected any contribution from boundary terms. They are easily included. In the presence of rigid lateral boundaries, for a complete mathematical specification of the problem, eqn [11] must be supplemented with the conditions [19] on each connected portion of the boundary.

$$\mathbf{v} \cdot \hat{\mathbf{n}} = 0, \quad \frac{d}{dt} \oint \mathbf{v} \cdot d\mathbf{s} = 0 \quad [19]$$

Here $\hat{\mathbf{n}}$ is the outward-pointing normal, and s is the vector arc length along the boundary. The second of eqns [19] represents conservation of circulation, which follows from the underlying momentum equations but must be included as a separate condition in the vorticity formulation of the dynamics. Although the circulation integrals along each connected portion of the boundary are constants in time, they are independent dynamical variables and are needed to determine \mathbf{v} from ω . The Hamiltonian formulation of eqn [13] may easily be extended to include the circulation integrals in addition to ω as dynamical variables. The Casimir invariants then include functions of these circulation integrals. With regard to the momentum invariants, of course, the rigid boundaries must respect the same symmetries; a zonal channel flow with walls at constant y breaks the translational symmetry in y and the rotational symmetry, leaving only the zonal impulse of eqn [16] as an invariant. The final equality of eqn [16] is then no longer strictly true, but the impulse and momentum differ only by terms involving the circulations along the channel walls, which are Casimirs. Since symmetry-based invariants are only defined to within the addition of a Casimir in any case, the impulse and momentum are essentially equivalent.

A simplified model of barotropic dynamics is the point-vortex model, where the vorticity is concentrated in Dirac delta functions. The point-vortex model has been used to study two-dimensional turbulence and certain kinds of atmospheric flow structures. It also turns out to be Hamiltonian, and is in fact a canonical system: the Casimirs are built into the model as parameters through the choice of the point-vortex strengths.

4. Other Balanced Models

The barotropic vorticity equation has a mathematical structure that is analogous to that of many models of balanced, or potential-vorticity-driven, flow and the results derived above extend in an obvious way to such systems. Inclusion of the beta effect means simply a change from ω to the potential vorticity $q = \omega + \beta y$. Since $\delta y = 0$ (recalling that the coordinate y is like an index), $\delta q = \delta \omega$ and eqns [11], [12], [13] and [14] go through unchanged with q in place of ω . However the beta effect breaks translational symmetry in y and rotational symmetry, leaving only the translational symmetry in x represented by the zonal impulse invariant of eqn [16]. Strictly speaking the latter should be written with q in place of ω , but the integrals differ by a constant and so represent the same invariant. Inclusion of topography is no more difficult; one simply includes an additional topographic term $h(x, y)$ in the definition of q . This will generally break all spatial symmetries, leaving only the energy \mathcal{H} and Casimirs \mathcal{C} as invariants. This illustrates a general and important point, namely, that symmetry-based invariants are fragile: a slight change in the conditions of the problem destroys their conservation properties. In contrast, the energy and the Casimirs are robust invariants (robust within the conservative context, of course) that survive such perturbations.

Stratification is most easily introduced in the context of the quasi-geostrophic (QG) model. Layered QG models are completely trivial extensions of the barotropic system: their evolution is

determined by the potential vorticity $q_i(x, y, t)$ in each layer i , governed by eqn [11] with q_i in place of ω , together with conservation of circulation along any rigid lateral boundaries that may be present. These are then the dynamical variables. The energy now includes available potential as well as kinetic energy, but, apart from some geometric factors representing the layer depths, one still recovers $\delta\mathcal{H}/\delta q_i = -\psi_i$ in each layer as well as eqn [13] with q_i in place of ω . The various invariants follow in the obvious way with the spatial integrals summed over the different layers. The same considerations, incidentally, apply to layered non-QG ‘intermediate’ models that still have the form of eqn [11] – namely, nondivergent horizontal advection of the potential vorticity q_i within each layer, with the flow in each layer driven by the potential vorticity in all layers (as described by the particular definition of q_i).

With continuous stratification and with upper and lower boundaries (at $z = 1$ and $z = 0$, say), there is an additional effect. It is well known that the temperature distribution along the upper and lower boundaries is equivalent to potential vorticity, and independent evolution equations for these temperature distributions are required to fully specify the continuously stratified QG system, in addition to the equation for the interior potential vorticity (the latter being eqn [11], with q in place of ω , applied at every value of z ; thus, the advection of q remains purely horizontal). The Eady model is an extreme case where the interior potential vorticity is uniform and the flow is driven entirely by the temperature distributions on the upper and lower boundaries; the dynamical structures driven from each boundary are known as Eady edge waves. Since these temperature distributions also evolve according to eqn [11], with the QG temperature ψ_z in place of ω , it is not surprising that the same kind of Hamiltonian structure also applies to this model (McIntyre and Shepherd, 1987). The energy is given by eqn [20].

$$\mathcal{H} = \iiint \frac{\rho_s}{2} \left\{ |\nabla \psi|^2 + \frac{1}{s} \psi_z^2 \right\} dx dy dz \quad [20]$$

In eqn [20], the reference-state density $\rho_s(z)$ and stratification function $S(z) = N^2/f^2$ are both prescribed, with $N(z)$ the buoyancy frequency and f the Coriolis parameter, and where ∇ is still just the horizontal gradient operator. With the potential vorticity given by eqn [21], where f and β are constants, eqn [22] follows.

$$q(x, y, z, t) = \psi_{xx} + \psi_{yy} + \frac{1}{\rho_s} \left(\frac{\rho_s}{S} \psi_z \right)_z + f + \beta y \quad [21]$$

$$\delta\mathcal{H} = \left[\iint \frac{\rho_s}{S} \psi \delta \psi_z \, dx dy \right]_{z=0}^{z=1} + \iiint \{ \nabla \cdot (\rho_s \psi \delta \nabla \psi) - \rho_s \psi \delta q \} \, dx dy dz \quad [22]$$

This is like eqn [12], but with an additional term involving the temperature variations $\delta\psi_z$ at the upper and lower boundaries. Including these as independent dynamical variables, in addition to q (and possibly also circulation terms), the governing equations can be cast in the symplectic form of eqn [13]. The Casimirs now involve integrals of arbitrary functions of the temperature on the upper and lower boundaries, in addition to integrals of arbitrary functions of potential vorticity in the interior (eqn [23]).

$$\mathcal{C} = \iiint C(q) \, dx dy dz + \iint C_0(\psi_z) \, dx dy|_{z=0} + \iint C_1(\psi_z) \, dx dy|_{z=1} \quad [23]$$

The momentum invariants similarly extend in obvious ways: for example, the zonal impulse invariant is given by eqn [24].

$$\mathcal{M} = \iiint \int \rho_s y q \, dx dy dz + \iint \frac{\rho_s}{S} y \psi_z \, dx dy|_{z=0} - \iint \frac{\rho_s}{S} y \psi_z \, dx dy|_{z=1} \quad [24]$$

The semi-geostrophic (SG) model is widely used in mesoscale dynamics because of its ability to represent realistic frontal structures. It turns out that the SG model can also be cast in the form of eqn [11], and hence in the symplectic form of eqn [13], provided the equations are written in isentropic-geostrophic coordinates. However, in these coordinates rigid boundaries appear to move in time (Kushner and Shepherd, 1995a,b). The SG equations, in contrast to the QG equations, make no geometrical distinction between horizontal and vertical boundaries – this is

why they are also useful for the study of coastal dynamics in physical oceanography – and the same kind of independent dynamical degrees of freedom encountered in the QG system on upper and lower boundaries also appear on lateral boundaries. In the special case of channel walls, these degrees of freedom correspond to coastal Kelvin waves and are analogous in some respects to the Eady edge waves represented by both the QG and SG systems. They must be taken into account in the variational calculations, and enter into many of the resulting expressions.

5. Unbalanced Models

Balanced models are controlled by the advection of potential vorticity (perhaps augmented by the advection of isentropic surfaces on rigid boundaries), so for such models it is natural to seek a Hamiltonian description analogous to eqn [13]. However, models that include a representation of gravity waves or other high-frequency oscillations, called unbalanced models, do not fit within this framework. They necessarily have additional degrees of freedom. For such models, a description in terms of the velocity field is a more natural way to reflect the Hamiltonian structure. For example, the rotating shallow-water equations [25] with $\mathbf{v}(x, y, t) = (u, v)$ the horizontal velocity, $h(x, y, t)$ the fluid depth, g the gravitational acceleration, and with constant f , conserve energy (eqn [26]).

$$\frac{\partial \mathbf{v}}{\partial t} + (f\hat{\mathbf{z}} + \nabla \times \mathbf{v}) \times \mathbf{v} + \nabla \left(\frac{1}{2} |\mathbf{v}|^2 \right) = -g\nabla h, \quad \frac{\partial h}{\partial t} + \nabla \cdot (h\mathbf{v}) = \mathbf{0} \quad [25]$$

$$\mathcal{H} = \iint \frac{1}{2} \{h|\mathbf{v}|^2 + gh^2\} \, dx dy \quad [26]$$

The dynamical variables are \mathbf{v} and h , for which eqns [27] hold.

$$\frac{\delta \mathcal{H}}{\delta \mathbf{v}} = h\mathbf{v}, \quad \frac{\delta \mathcal{H}}{\delta h} = \frac{1}{2} |\mathbf{v}|^2 + gh \quad [27]$$

Note that no integration by parts is necessary in this case; this is characteristic of velocity-based representations of the dynamics. It can easily be verified that eqns [25] may be cast in the

symplectic form $\partial\mathbf{u}/\partial t = J(\delta\mathcal{H}/\delta\mathbf{u})$ with $\mathbf{u} = (u, v, h)$ and J given by eqn [28], where $q =$

$(f + \hat{\mathbf{z}} \cdot \nabla \times \mathbf{v})/h$ is the potential vorticity of the shallow-water system.

$$J = \begin{pmatrix} 0 & q & -\partial_x \\ -q & 0 & -\partial_y \\ -\partial_x & -\partial_y & 0 \end{pmatrix} \quad [28]$$

The matrix (28) is evidently skew-symmetric; the signs on the derivative terms are indeed correct, since first-order differential operators are themselves skew-symmetric, as with the J in eqn [13]. The zonal (absolute) momentum invariant is given as expected by eqn [29], for which it is easy to verify that $J(\delta\mathcal{M}/\delta\mathbf{u}) = -\partial\mathbf{u}/\partial x$ in line with Noether's theorem, and the other momentum invariants follow similarly.

$$\mathcal{M} = \iint h(u - fy) \, dx \, dy \quad [29]$$

The Casimirs are given by eqn [30] for arbitrary functions $C(\cdot)$.

$$\mathcal{C} = \iint h C(q) \, dx \, dy \quad [30]$$

Thus, potential vorticity still plays a crucial role in the Hamiltonian description of the dynamics.

Special cases of Casimirs are total mass ($C = 1$) and total circulation ($C = q$).

Stratification is easily incorporated. The hydrostatic primitive equations can be cast in Hamiltonian form isomorphic to that of eqn [28] when expressed in isentropic coordinates. Even the fully compressible stratified Euler equations, which form the most general system imaginable for (dry) dynamical meteorology, can be cast in an analogous form, although there are now additional dynamical variables associated with compressibility. The Casimirs are in this case given by eqn [31], where $\rho(x, y, z, t)$ is the density, $\theta(x, y, z, t)$ is the potential temperature, and $q = [(f\hat{\mathbf{z}} + \nabla \times \mathbf{v}) \cdot \nabla \theta]/\rho$ is the Ertel potential vorticity, with \mathbf{v} and ∇ now acting in all three spatial dimensions.

$$\mathcal{C} = \iiint \rho C(q, \theta) \, dx \, dy \, dz \quad [31]$$

The invariance of the Casimirs is of course evident directly from the dynamical equations (eqn [32]) and reflects the material invariance of q and θ .

$$\frac{\partial q}{\partial t} + \mathbf{v} \cdot \nabla q = 0, \quad \frac{\partial \theta}{\partial t} + \mathbf{v} \cdot \nabla \theta = 0, \quad \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \quad [32]$$

The fully compressible stratified Euler equations are, in fact, a straightforward expression of Newton's second law, without constraints such as hydrostatic balance, provided they are expressed in Lagrangian coordinates (Morrison, 1998). In Lagrangian coordinates, the dynamical variables are the positions and momenta of fluid elements, which are natural canonical variables. The thermodynamic fields can be expressed in terms of these variables: ρ can be written in terms of the Jacobian of particle positions (which describes the compression of the fluid), while θ can just be chosen as one of the Lagrangian coordinates. In this way, the fully compressible stratified Euler equations represent a canonical Hamiltonian system. But there are six dynamical variables in the Lagrangian description, compared with only five in the Eulerian description; in transforming to Eulerian coordinates, a reduction of the phase space takes place. This is where the potential vorticity comes in. In Lagrangian coordinates, the potential vorticity is still materially conserved; but what symmetry does it correspond to? The answer is a particle-relabeling symmetry: if one rearranges fluid elements while preserving the same Eulerian fields, then the dynamics is unchanged. There is just enough freedom to do this, because there is one more Lagrangian than Eulerian variable. Upon reduction to the Eulerian description, this additional degree of freedom disappears, and the particle-relabeling symmetry becomes invisible. That is why potential vorticity conservation then appears in the form of a Casimir invariant.

6. Disturbance Invariants

Probably the most powerful application of Hamiltonian dynamics to dynamical meteorology arises in the context of studying the properties of disturbances to basic states. In fluid dynamics,

the question of how to define the energy of a wave has often been a point of confusion if not contention. For example, in the case of a basic flow, if the wave energy is defined as the energy in the frame of reference moving with the basic flow, then it is positive definite but not conserved. On the other hand, if it is defined as the difference energy relative to the basic-flow energy, then it is conserved but not positive definite. One would like both properties in order to define normal modes, spectra, etc. Another problem, at first sight unrelated, arises with momentum. The momentum of a wave would appear to be zero (the average of a sinusoid is zero), yet waves can certainly transfer momentum; this is what drives the quasi-biennial oscillation in the tropical stratosphere, for example. How is one to describe this wave momentum?

In canonical Hamiltonian mechanics, the disturbance energy about an equilibrium is always quadratic; from this one assesses stability and defines normal modes. There is no ambiguity. So why are things not equally clear for fluid dynamics? The answer lies in the noncanonical Hamiltonian structure of virtually every fluid dynamical system in the Eulerian representation. If $\mathbf{u} = \mathbf{U}$ is a steady solution of a Hamiltonian system, then eqn [33] holds.

$$J \frac{\delta \mathcal{H}}{\delta \mathbf{u}} |_{\mathbf{u} = \mathbf{U}} = 0 \quad [33]$$

For a canonical system, the invertibility of J then implies that $\delta \mathcal{H} / \delta \mathbf{u} = 0$ at $\mathbf{u} = \mathbf{U}$. This means that \mathbf{U} is a conditional extremum of \mathcal{H} , and $\mathcal{H}[\mathbf{u}] - \mathcal{H}[\mathbf{U}]$ is quadratic in the disturbance. However, for a noncanonical system none of this follows and the disturbance energy is generally linear in the disturbance.

6.1 Pseudoenergy

Hamiltonian structure provides the solution to this quandary. Equation [33] is locally the same as the equation defining the Casimirs, which means that $\delta\mathcal{H}/\delta\mathbf{u}$ is locally parallel to $\delta\mathcal{C}/\delta\mathbf{u}$ for some \mathcal{C} (a different \mathcal{C} for each choice of \mathbf{U}). In other words, there exists a Casimir \mathcal{C} such that eqn [34] holds.

$$\frac{\delta\mathcal{H}}{\delta\mathbf{u}}|_{\mathbf{u}=\mathbf{U}} = -\frac{\delta\mathcal{C}}{\delta\mathbf{u}}|_{\mathbf{u}=\mathbf{U}} \quad [34]$$

Now, both \mathcal{H} and \mathcal{C} are invariants, and the combined invariant $\mathcal{H} + \mathcal{C}$ satisfies the extremal condition $\delta(\mathcal{H} + \mathcal{C}) = 0$ at $\mathbf{u} = \mathbf{U}$. We have thus constructed what we wanted, namely a disturbance quantity that is conserved and is locally quadratic in the disturbance (eqn [35]).

$$\mathcal{A} = (\mathcal{H} + \mathcal{C})[\mathbf{u}] - (\mathcal{H} + \mathcal{C})[\mathbf{U}] \quad [35]$$

This quantity is known as the pseudoenergy. Provided one has a complete set of Casimirs, eqn [34] can always be solved for a Hamiltonian system and the pseudoenergy can always be constructed according to eqn [35]. This is one of the great attractions of Hamiltonian dynamics: it provides systematic recipes in abstract terms, which can be worked out for any particular application.

A particularly illuminating application is the subject of available potential energy, highly useful in energy budget analyses (Shepherd, 1993). We demonstrate the method in the case of the three-dimensional stratified Boussinesq equations. The energy is given by eqn [36].

$$\mathcal{H} = \iiint \left\{ \frac{\rho_s}{2} |\mathbf{v}|^2 + \rho g z \right\} dx dy dz \quad [36]$$

Here ρ_s is the constant reference-state density, and the dynamical variables are \mathbf{v} and ρ , for which eqns [37] hold.

$$\frac{\delta\mathcal{H}}{\delta\mathbf{v}} = \rho_s \mathbf{v}, \quad \frac{\delta\mathcal{H}}{\delta\rho} = g z \quad [37]$$

The term $\rho g z$ in eqn [36] is the gravitational potential energy, and is linear in the dynamical variables. Now consider disturbances to a stably stratified, resting basic state $\mathbf{v} = 0, \rho = \rho_0(z)$.

Although the Casimirs of this system include functions of the potential vorticity, because the basic state is at rest, $\delta\mathcal{H}/\delta\mathbf{v} = \mathbf{0}$ at $\mathbf{v} = 0$ and this dependence is unnecessary, so we may consider Casimirs of the form of eqn [38].

$$\mathcal{C} = \iiint C(\rho) dx dy dz \quad \text{with} \quad \frac{\delta \mathcal{C}}{\delta \rho} = C'(\rho) \quad [38]$$

Equation [34] then leads to the condition $C'(\rho_0) = -gz$. This is the defining relation for the function $C(\cdot)$. Thus, one has to express gz in terms of the same argument ρ_0 . This can be done by inverting the functional dependence $\rho_0(z)$ to obtain $Z(\rho_0)$, where $Z(\rho_0(z)) = z$. This is always possible provided $\rho_0(z)$ is monotonic, which is the case for a stably stratified basic state. This yields eqn [39].

$$C(\rho) = - \int_{\rho_0}^{\rho} g Z(\tilde{\rho}) d\tilde{\rho} \quad [39]$$

From this the pseudoenergy of eqn [35] takes the form [40].

$$\mathcal{A} = \iiint \left\{ \frac{\rho_s}{2} |\mathbf{v}|^2 + (\rho - \rho_0) gz - \int_{\rho_0}^{\rho} g Z(\tilde{\rho}) d\tilde{\rho} \right\} dx dy dz \quad [40]$$

The first term in the spatial integrand is the kinetic energy and is positive definite; the last two terms can be rewritten as in eqn [41].

$$- \int_0^{\rho - \rho_0} g [Z(\rho_0 + \tilde{\rho}) - Z(\rho_0)] d\tilde{\rho} \quad [41]$$

This is self-evidently positive definite for $d\rho_0/dz < 0$ and has the small-amplitude quadratic approximation [42].

$$- \frac{g(\rho - \rho_0)^2}{2(d\rho_0/dz)} \quad [42]$$

Equation [41] is the exact, finite-amplitude expression for the available potential energy (see **General Circulation of the Atmosphere: Energy Cycle**) of disturbances to a stably stratified, resting basic state $\rho_0(z)$, while eqn [42] is its more familiar small-amplitude counterpart, widely

used in the theory of internal gravity waves. Similar constructions can be performed to define the available potential energy of any stratified fluid system. Although the small-amplitude expression of eqn [42] appears to be singular in regions where $d\rho_0/dz = 0$, the finite-amplitude expression of eqn [41] remains perfectly well-defined in such regions.

A benefit of the Hamiltonian perspective on available potential energy is that it is immediately clear from the derivation that the basic state around which the pseudoenergy is defined need not be at rest. In the case of symmetric circulations, Codoban and Shepherd (2003) generalized the concept of available potential energy to include the momentum constraints associated with a non-resting basic state, such that centrifugal potential energy is included along with gravitational potential energy. This formulation addressed a challenge posed by Lorenz (1955) in his original derivation of available potential energy, and showed how within such a perspective, the energetics of a mechanically-forced, thermally-damped circulation (as is the case in the middle atmosphere) always reflects its causality. For the very different problem of subgrid-scale parameterization in numerical models of the atmosphere, where the resolved scales provide the basic state for the unresolved scales, Shaw and Shepherd (2009) applied the concepts of pseudoenergy and pseudomomentum (see next section) to derive a theoretical framework ensuring the joint conservation of energy and momentum.

6.2 Pseudomomentum

The same kind of reasoning can be applied for disturbances to zonally symmetric (x -invariant) basic states, assuming that the underlying system possesses the same symmetry. For such states, with $\partial \mathbf{U}/\partial x = 0$, Noether's theorem implies that the zonal impulse or momentum invariant satisfies eqn [43].

$$J \frac{\delta \mathcal{M}}{\delta \mathbf{u}} |_{\mathbf{u} = \mathbf{U}} = 0 \quad [43]$$

But just as with eqn [33], there is a Casimir \mathcal{C} such that $\delta(\mathcal{M} + \mathcal{C}) = 0$ at $\mathbf{u} = \mathbf{U}$; with this \mathcal{C} , one may immediately construct the invariant [44], which is quadratic to leading order in the disturbance.

$$\mathcal{A} = (\mathcal{M} + \mathcal{C})[\mathbf{u}] - (\mathcal{M} + \mathcal{C})[\mathbf{U}] \quad [44]$$

This quantity is known as the pseudomomentum.

We calculate the pseudomomentum for the case of barotropic flow on the beta-plane. Suppose we are given a monotonic basic state $q_0(y)$. From eqns [14] and [16], with q in place of ω , we have eqn [45].

$$\frac{\delta\mathcal{M}}{\delta q} = y, \quad \frac{\delta\mathcal{C}}{\delta q} = C'(q) \quad [45]$$

The extremal condition $\delta(\mathcal{M} + \mathcal{C}) = 0$ at $q = q_0$ then leads to $C'(q_0) = -y$. This is now isomorphic to the construction of the available potential energy, replacing gz with y and ρ with q . If we define the function $Y(\cdot)$ by $Y(q_0(y)) = y$, then evidently eqn [46] holds.

$$\mathcal{A} = \iint \left\{ - \int_0^{q-q_0} [Y(q_0 + \tilde{q}) - Y(q_0)] d\tilde{q} \right\} dx dy \quad [46]$$

The small-amplitude approximation to the spatial integrand is given by eqn [47].

$$- \frac{(q-q_0)^2}{2(dq_0/dy)} \quad [47]$$

Equations [46] and [47] are evidently negative definite for $dq_0/dy > 0$, which is the case when q_0 is dominated by βy . These rather peculiar expressions have no obvious relation to zonal momentum at first sight, but they nevertheless explain why it is that Rossby waves always exert an eastward (positive) force when they leave a source region, and a westward (negative) force when they dissipate and deposit their momentum in a sink region: they carry negative pseudomomentum (see Shepherd, 2020).

The general nature of the derivation ensures that exactly the same expressions hold for any balanced model having the basic form of eqn [13]. If the basic state q_0 is chosen to be the zonal mean \bar{q} , then the zonal mean of eqn [47] becomes eqn [48], where $q' \equiv q - \bar{q}$.

$$-\frac{\overline{q'^2}}{2\bar{q}_y} \quad [48]$$

In the case of stratified QG dynamics, the negative of eqn [48] is known as the Eliassen–Palm wave activity, which has been widely used in dynamical meteorology to assess the effect of Rossby waves on the zonal mean flow. It is such an effective diagnostic precisely because it represents negative pseudomomentum. Moreover, and importantly, its use is not restricted to waves. The exact, finite-amplitude expression of eqn [46] ensures that the concept of pseudomomentum applies to fully nonlinear, even turbulent disturbances (McIntyre and Shepherd, 1987).

The robust negative definiteness of the pseudomomentum of balanced disturbances explains a great deal about the general circulation of the atmosphere. Propagation of synoptic-scale Rossby waves away from their source region in the baroclinic storm tracks implies an eastward force in the storm track regions, accounting for the maintenance of the westerlies. The westward momentum deposition associated with breaking planetary-scale Rossby waves in the stratosphere drives the poleward Brewer–Dobson circulation, which is responsible for the observed distribution of ozone and other chemical species in the stratosphere.

7. Stability Theorems

The pseudoenergy and pseudomomentum are, by their construction, conserved quantities that are quadratic to leading order in the disturbance quantities. In fact, their quadratic approximations are exactly conserved by the linearized dynamics. (The quadratic approximation

to the pseudoenergy is the Hamiltonian of the linearized dynamics.) When either of these quantities is sign-definite for a given basic state, it follows that that basic state is stable to normal-mode instabilities. Indeed, in order to reconcile exponentially growing disturbances with conservation of pseudoenergy and pseudomomentum, the latter quantities must vanish for such disturbances. This fact provides a useful constraint on the structure of normal-mode instabilities, as well as a powerful unifying framework between different models.

This simple framework accounts for virtually every known stability theorem in dynamical meteorology. For resting, stratified basic states in unbalanced models, with pseudoenergy like eqn [40] for the Boussinesq model, the condition of positive definite pseudoenergy is the statement of static stability. For basic flows in axisymmetric or symmetric stratified unbalanced models, the same condition is the statement of symmetric stability, which reduces to Rayleigh's centrifugal stability theorem in the special case of axisymmetric homogeneous flow. These stability theorems are all quite analogous to static stability. A different situation arises for balanced models. There, the pseudoenergy can take either sign depending on the basic flow. The positive-definite and negative-definite cases correspond respectively to Arnold's first and second stability theorems (McIntyre and Shepherd, 1987). (They are analogous to the stability of a rigid body rotating about an axis of symmetry corresponding respectively to a maximum or minimum moment of inertia.) In the special case of a parallel basic flow, Arnold's first theorem states that the flow is stable if $u_0/(dq_0/dy) < 0$, which is the Fjørtoft–Pedlosky theorem.

With regard to pseudomomentum for balanced models, eqn [46] is sign-definite whenever dq_0/dy is sign-definite. For barotropic flow with $q = \omega$, this corresponds to Rayleigh's inflection-point theorem; on the beta-plane with $q = \omega + \beta y$, to the Rayleigh–Kuo theorem; and for stratified QG flow with q given either by its multilevel forms q_i or by eqn [21] in the

continuously stratified case, to the Charney–Stern theorem. For stratified QG dynamics in the presence of a lower boundary, the second terms of eqns [23] and [24] become relevant and there is an additional contribution to the pseudomomentum involving the temperature distribution on the lower boundary; it is isomorphic to the interior eqns [46], [47] and [48], replacing q with ψ_z . Since the climatological temperature gradient along the Earth’s surface is towards the Equator, the pseudomomentum associated with surface disturbances is generally positive. In this case the Charney–Stern stability criterion is not satisfied for observed flows; on the other hand, normal-mode instabilities are generally required to involve both temperature disturbances on the lower boundary and potential-vorticity disturbances in the interior, in order to create a disturbance with zero total pseudomomentum. The Charney model of baroclinic instability is the best-known example of this. In the presence of an upper boundary, there is a further contribution to the pseudomomentum, with opposite sign to the lower contribution in accord with eqn [24]. Thus in the Eady model of baroclinic instability, where the potential vorticity is uniform and the interior contribution to the pseudomomentum disappears, the instability can arise from the interaction of disturbances on the upper and lower boundaries that together add up to zero total pseudomomentum.

These statements all concern normal-mode stability. But what can be said about stability goes much further than this. The existence of finite-amplitude disturbance invariants suggests the possibility of nonlinear, or Liapunov stability: namely, that small disturbances stay small for all time, where small is defined in terms of some disturbance norm (Holm et al., 1985).

Mathematically, we say that a basic state \mathbf{U} is Liapunov stable to disturbances \mathbf{u}' in a given norm $\|\mathbf{u}'\|$ if for all $\varepsilon > 0$ there exists a $\delta(\varepsilon) > 0$ such that eqn [49] holds.

$$\|\mathbf{u}'(0)\| < \delta \implies \|\mathbf{u}'(t)\| < \varepsilon \quad \forall t \quad [49]$$

Let us see how this applies to static stability for the Boussinesq model considered earlier.

Suppose that the basic state has $d\rho_0/dz < 0$ and that furthermore the basic-state density gradients are bounded according to [50] for some constants c_1, c_2 .

$$0 < c_1 \leq -g \frac{dz}{d\rho_0} = -\frac{g}{d\rho_0/dz} \leq c_2 < \infty \quad [50]$$

Then eqn [41] for the available potential energy is bounded from above and below according to eqn [51].

$$\frac{1}{2}c_1(\rho - \rho_0)^2 \leq [41] \leq \frac{1}{2}c_2(\rho - \rho_0)^2 \quad [51]$$

Define the disturbance norm by eqn [52], with $c_1 \leq \lambda \leq c_2$.

$$\|(\mathbf{v}, \rho - \rho_0)\|^2 = \iiint \frac{1}{2} \{ \rho_s |\mathbf{v}|^2 + \lambda(\rho - \rho_0)^2 \} \, dx dy dz \quad [52]$$

Then using eqn [51] we obtain the chain [53] of inequalities, valid for any time t , involving the pseudoenergy \mathcal{A} of eqn [40].

$$\|(\mathbf{v}, \rho - \rho_0)(t)\|^2 \leq \frac{\lambda}{c_1} \mathcal{A}(t) = \frac{\lambda}{c_1} \mathcal{A}(t) \leq \frac{c_2}{c_1} \|(\mathbf{v}, \rho - \rho_0)(0)\|^2 \quad [53]$$

With the choice $\delta = \sqrt{c_1/c_2} \varepsilon$, eqn [53] establishes Liapunov stability in the norm defined by eqn [52]. Conservation of pseudoenergy is clearly central to the proof.

The finite-amplitude stability of stably stratified flow is not too surprising; it corresponds to physical intuition, and indeed motivates the very concept of available potential energy, which has a long pedigree. What is perhaps more surprising is that exactly the same kinds of constructions can be made for all of the stability theorems mentioned above, and for virtually any model within the same family. They can also be used to obtain rigorous upper bounds on the saturation of normal-mode instabilities, by considering the initial unstable flow (plus infinitesimal disturbance) to be a finite-amplitude disturbance to a stable basic state (Shepherd, 1988a,b).

8. Conclusion

Hamiltonian dynamics is considered to provide the backbone of many branches of physics, as it represents a ‘metatheory’ that can encompass a variety of detailed theoretical models of the phenomena under study and thereby provide a connection between them. In dynamical meteorology, there has long been a call for the use of model hierarchies as a way of understanding the complexity of the real atmosphere (Hoskins, 1983). Dynamical meteorology is part of classical physics, and Hamiltonian dynamics provides the backbone for the model hierarchy in this context too. The abstract unifying concepts of pseudoenergy and pseudomomentum map directly onto longstanding and widely-used theoretical concepts in dynamical meteorology such as (respectively) available potential energy and momentum transfer by waves, and explain why they take slightly different forms in different models. Whenever there is a theoretical challenge in dynamical meteorology, Hamiltonian dynamics is invariably lying below the surface and can often be usefully exploited to provide a solution that can be generalized to other models. It deserves to be part of the canon of dynamical meteorology.

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