IFSR #221

Flux and Differences in Action for Continuous Time Hamiltonian Systems

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4 December 1985

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Abstract For a time periodic Hamiltonian $H(p,q,t)$ of period T, the area crossing a collection of curves at time 0 spanning two homotopic orbits of common period nT, in a time T, is shown to be the difference between the actions, $\oint pdq-Hdt$, of the orbits. Similarly in an autonomous Hamiltonian system of two degrees of freedom the flux of energy surface volume per unit time through a surface spanning two homotopic orbits of the same energy is given by the difference between the actions, $\oint \mathbf{p}\cdot d\mathbf{q}$, of the orbits. Analogous results hold for pairs of orbits which converge together in both directions of time.

In dynamical systems described by area-preserving maps, one can interpret the difference between the actions of two periodic orbits of the same rotation number and period as the amount of area which crosses any curve which connects the orbits, per iteration of the map[1]. Similar interpretations hold for pairs of orbits which converge together in both directions of time ("homoclinic pairs"), such as an orbit on a cantorus and an orbit homoclinic to it. In this note we obtain analogous results for continuous time Hamiltonian systems of $1\,^1/_2$ and 2 degrees of freedom. This allows the direct application of the results of MacKay, Meiss and Percival[1] to the continuous time case which appears most frequently in applications (e.g. Ref. 2).

Statement of the Results

A. $1\,^1/_2$ Degrees of Freedom

Let H be the Hamiltonian for a time periodic, one degree of freedom system on a symplectic manifold M. Denote the period by T.

1. Consider two periodic orbits of the same homotopy class on M (i.e. continuously deformable into each other), of period nT. Take a surface, σ, in the extended (three dimensional) phase space $M\times\{t \bmod T\}$, which spans the two orbits (see Fig. 1); such surfaces exist because of the homotopy condition. Let γ be the collection of curves formed by the intersection of σ with any constant time section $t=t_0$ modulo T. Then the area crossing γ in time T is given by

$$F = \oint_1 pdq - Hdt \; - \oint_2 pdq - Hdt \qquad (1)$$

where (p,q) are local canonical coordinates in a simply connected neighborhood of the pair of orbits, and the loop integrals are taken around the orbits.

2. Consider a homoclinic pair of orbits, such that $(p^1,q^1)(t)-(p^2,q^2)(t) \to 0$ as $t \to \pm\infty$, and which are homotopic to zero in the following sense: there exists $\varepsilon > 0$ such that for all large enough positive and negative times $t_\pm$, the closed curve formed by connecting the pair of orbits by curves of length less than ε at times $t_\pm$ is homotopic to zero. Let σ and γ be defined as before. The area crossing γ per period T is

$$F = \lim_{t_\pm \to \pm\infty} \int_{t_-}^{t_+} (pdq - Hdt)_1 - (pdq - Hdt)_2 \qquad (2)$$

where the integrals are taken along the two orbits.

B. Two Degrees of Freedom

Let H be the Hamiltonian for an autonomous two degree of freedom system.

1. Consider two periodic orbits with the same energy and of the same homotopy class. Take any surface, σ, in the energy surface which spans from one orbit to the other (see Fig. 2) and which does not contain a critical point of H. The energy surface volume crossing σ per unit time, which we call the flux, is

$$F = \oint_1 \mathbf{p}\cdot d\mathbf{q} \; - \oint_2 \mathbf{p}\cdot d\mathbf{q} \qquad (3)$$

where $(\mathbf{p},\mathbf{q})$ are local canonical coordinates.

2. Take any homoclinic pair of orbits $(\mathbf{q}^1,\mathbf{p}^1)$ and $(\mathbf{q}^2,\mathbf{p}^2)$ with the same energy, and which are homotopic as in **A2.** Parametrize the orbits by a parameter τ which increases with time, such that $\mathbf{q}^1(\tau) - \mathbf{q}^2(\tau) \to \mathbf{0}$ and $\mathbf{p}^1(\tau) - \mathbf{p}^2(\tau) \to \mathbf{0}$ as $\tau \to \pm\infty$. Then the flux through any surface σ chosen as before is

$$F = \lim_{\tau_\pm \to \pm\infty} \int_{q^1(\tau_-)}^{q^1(\tau_+)} \mathbf{p}\cdot d\mathbf{q} - \int_{q^2(\tau_-)}^{q^2(\tau_+)} \mathbf{p}\cdot d\mathbf{q} \qquad (4)$$

where the integrals are taken along the two orbits.

These results can be summarized by the statement that the flux through a surface containing two homotopic orbits is the difference between the actions of the orbits. In the case of $1\,^1/_2$ degrees of freedom the action is defined as the integral of pdq-Hdt. For two degrees of freedom the action is defined as the integral of $\mathbf{p}\cdot d\mathbf{q}$.

These formulae allow the calculation of the flux, for example, passing between the stable and unstable periodic orbits which form an island chain, between a cantorus and an orbit homoclinic to it, or between the two orbits formed by the tranversal intersections of the stable manifold of one periodic orbit with the unstable manifold of another periodic orbit.

Proof of A

Let ω be the symplectic form ($\omega = dp \wedge dq$ in canonical coordinates) on the phase space M for the Hamiltonian system H(p,q,t) where H is time periodic with period T. The flow vector for the dynamics, ξ, satisfies

$$\omega(\eta,\xi) = dH(\eta) \qquad (5)$$

for all vectors η. Extend the flow to the space $M \times S^1$, where the third dimension corresponds to time modulo T. The extended flow vector is $\xi_e = (\xi, 1)$. Define a volume form on $M \times S^1$ by $dt \wedge \omega$. The "flux two form" is defined by the contraction of the volume form with the flow:

$$\varphi(\eta_1,\eta_2) = dt \wedge \omega\,(\xi_e,\eta_1,\eta_2) \qquad (6)$$

for any η_1, η_2 in $M \times S^1$. The integral of φ over a surface in $M \times S^1$ gives the rate at which three-volume crosses the surface. In particular choose a surface σ which spans two orbits C_1 and C_2 chosen as in the statement of **A1** or **A2**. The orientation of σ is chosen so that $\partial\sigma = C_1 - C_2$. Using equation (5) one can see that

$$\varphi = \omega - dH \wedge dt \tag{7}$$

Therefore since $d\omega=0$ we have $d\varphi=0$, i.e. the flow is incompressible.

Choose a time section M_0, defined by $t=t_0$ modulo T, and let $\gamma = \sigma \cap M_0$. In general γ has many pieces, denoted γ_i, corresponding to the successive intersections of the orbits with M_0. Let σ_i be the part of σ between γ_{i-1} and γ_i . Define the surfaces $\overline{\sigma}_i$ as those formed by evolving γ_{i-1} with the flow for one period T (see Fig. 3), and $\overline{\gamma}_i$ as the time T image of γ_{i-1}. We claim that $\gamma_i-\overline{\gamma}_i$ is homotopic to zero in M_0 because (1) $\overline{\gamma}_i$ can be continuously deformed to γ_{i-1} in M_0 by following the flow in M_0, and (2) γ_{i-1} can be continuously deformed to γ_i by following the projection of σ_i on M_0. Let δ_i be the surface in M_0 bounded by $\gamma_i-\overline{\gamma}_i$, which exists because of this homotopy. The surface $\sigma_i - \overline{\sigma}_i - \delta_i$ is a closed surface in $M \times S^1$ and since φ is a closed form, its integral over this surface is zero. Thus we have

$$\int_{\sigma_i} \varphi = \int_{\overline{\sigma}_i} \varphi + \int_{\delta_i} \varphi$$

On the surface $\overline{\sigma}_i$, φ is identically zero since ξ_e is tangent to the flow, so we obtain the result

$$\int_{\sigma_i} \varphi = \int_{\delta_i} \varphi \tag{8}$$

The right hand side of (8) can be interpreted as the area crossing γ_i per period. Since γ is the union of the γ_i, the total area crossing γ is the sum of (8) over i, which is the flux we desire to calculate. Because σ is simply connected, local canonical coordinates (p,q) can be defined so that $\omega = d(pdq)$. From (7) and Stokes' theorem, the left hand side of (8) can be written

$$\int_{\sigma_i} \varphi = \int_{\partial\sigma_i} pdq - Hdt \qquad (9)$$

Summing (9) over i we obtain the difference in action of the orbits since $\sum_i \partial\sigma_i$ is composed of the two orbits with opposite orientation. Thus we obtain (1) or (2) depending on the choice of orbit.

Proof of B

Let ω be the symplectic form ($\omega = dp_1 \wedge dq_1 + dp_2 \wedge dq_2$ in canonical coordinates) on the phase space M for Hamiltonian H. As before, the flow vector ξ satisfies $\omega(\eta,\xi) = dH(\eta)$ for all η. The symplectic form induces a volume 4-form, $\Omega = {}^1/_2 \omega \wedge \omega$. The restriction of the volume to the energy surface gives a 3-form, ε, except at critical points of the Hamiltonian (where dH=0), defined uniquely through

$$\Omega = dH \wedge \varepsilon \qquad (10)$$

The flux of energy surface volume is obtained from the flux form

$$\varphi(\eta_1,\eta_2) = \varepsilon(\xi,\eta_1,\eta_2) \qquad (11)$$

Given two homotopic orbits C_1 and C_2 and a two dimensional surface σ whose boundary is $C_1 - C_2$, all contained in an energy surface, such that σ contains no critical points of H, the flux through σ is

$$F = \int_\sigma \varphi$$

To compute this flux, take any vectors η_1 and η_2 tangent to σ and η_3 arbitrary. Then

$$\Omega\,(\xi,\eta_1,\eta_2,\eta_3) = \omega(\xi,\eta_1)\omega(\eta_2,\eta_3) + \omega(\xi,\eta_2)\omega(\eta_3,\eta_1) + \omega(\xi,\eta_3)\omega(\eta_1,\eta_2)$$

$$= -dH(\eta_1)\omega(\eta_2,\eta_3) - dH(\eta_2)\omega(\eta_3,\eta_1) - dH(\eta_3)\omega(\eta_1,\eta_2)$$

However, since η_1 and η_2 are tangent to the energy surface, both $dH(\eta_1)$ and $dH(\eta_2)$ are zero, so only the last term contributes. Similarly, equation (10) implies $dH \wedge \varepsilon(\zeta,\eta_1,\eta_2,\eta_3) = -dH(\eta_3)\varepsilon(\zeta,\eta_1,\eta_2)$ since $dH(\zeta)=0$. Thus (11) and the assumption $dH \neq 0$ imply

$$\varphi(\eta_1,\eta_2) = \omega(\eta_1,\eta_2)$$

for any η_1,η_2 tangent to energy surface. Since σ is simply connected we can choose local canonical coordinates $(\mathbf{p},\mathbf{q})$, so that $\omega = d(\mathbf{p}\cdot d\mathbf{q})$. Then the flux is

$$F = \int_\sigma \varphi = \int_\sigma \omega = \int_{\partial\sigma} \mathbf{p}\cdot d\mathbf{q} \qquad (12)$$

The boundary of σ is $C_1 - C_2$, thus we have shown, as explicitly written in (3) and (4), that the difference of action of the two orbits is the flux of energy surface volume per unit time through the surface σ spanning the orbits.

Acknowledgements

This research was sponsored by NATO Research Grant RG 85/0461 for international collaboration. We are grateful to A. Weinstein for useful hints.

References

1). R.S. MacKay, J.D. Meiss and I.C. Percival, "Transport in Hamiltonian Systems," Physica **13D**, 55 (1984).

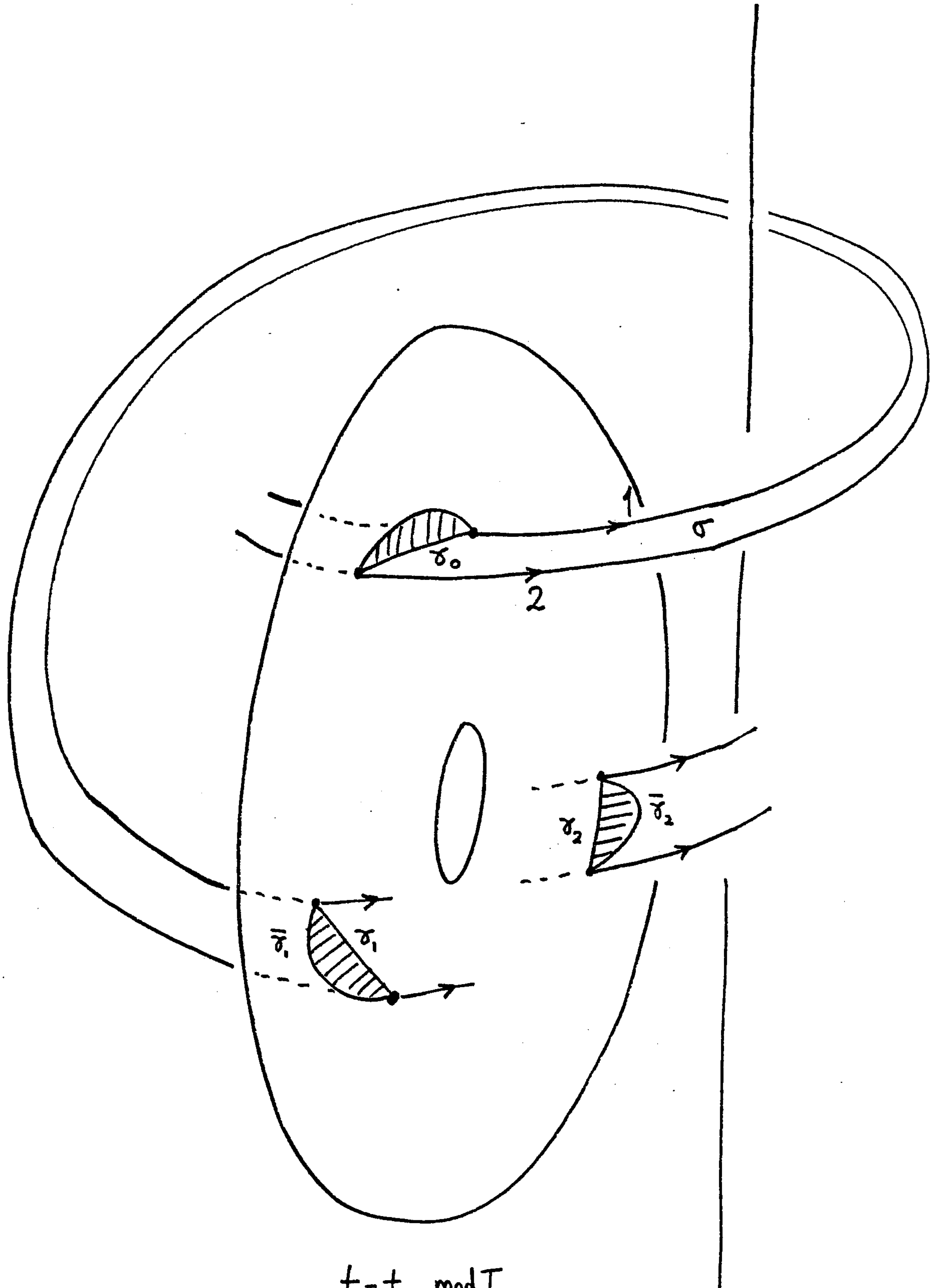
2). M.J. Davis, "Bottlenecks to Intramolecular Energy Transfer and the Calculation of Relaxation Rates," submitted to J. Chem. Phys. (1985).

Figure Captions

Figure 1: Two periodic orbits of the same period and homotopy class, in the extended phase space of a T-periodic one degree of freedom system, with a spanning surface σ intersecting a section $t = t_0$ mod T in a collection of curves γ_i.

Figure 2: Flux through a surface σ spanning two periodic orbits of the same homotopy class, all lying in the same (three-dimensional) energy surface.

Figure 3: Construction for the proof of A.



$t = t_0 \mod T$

Figure 1

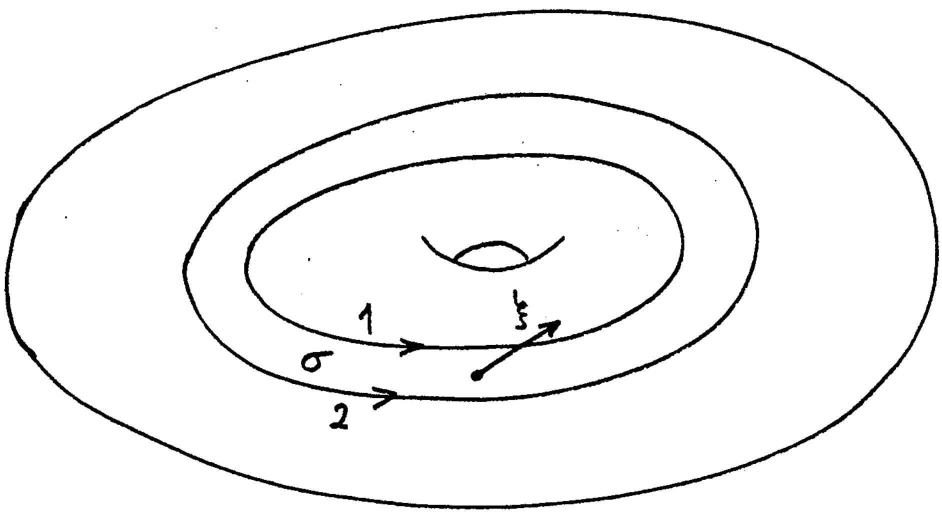


Figure 2

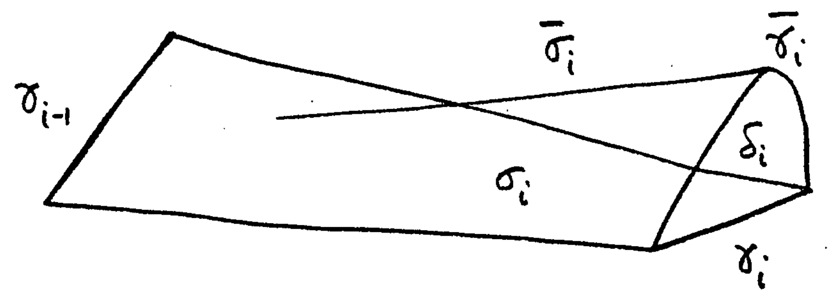


Figure 3