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Variational principles for the invariant toroids of classical dynamics

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Abstract. Kolmogorov, Arnol'd and Moser proved that invariant toroids of N dimensions occupy a finite volume of the $2N$-dimensional phase space of nearly integrable bounded systems of N degrees of freedom. Variational principles are stated for such invariant toroids.

1. Introduction

It is well known that variational principles lie at the heart of mechanics (Lanczos 1966). It is less well known that invariant toroids are essential to the modern general theory of dynamical systems of N degrees of freedom. In this paper variational principles are obtained for invariant toroids.

If a conservative system of N degrees of freedom is integrable, the motion of a phase point in the $2N$-dimensional phase space is confined to an 'invariant toroid' of N dimensions; such invariant toroids occupy almost the whole phase space of bounded integrable motions. If the system is sufficiently close to being integrable, Kolmogorov (1954, 1957), Arnol'd (1963a, b), and Moser (1962) (to be referred to as KAM), have shown that invariant toroids occupy a finite $2N$-dimensional volume (positive measure) of the phase space, provided certain conditions of analyticity or differentiability are satisfied. Even if the system is far from being integrable, numerical experiments (for example, Hénon and Heiles 1964, Contopoulos 1963, 1971) suggest that much of phase space may be occupied by invariant toroids.

Both analytic and numerical work on invariant toroids was stimulated by problems of celestial mechanics, including the stability of the solar system and the velocity distribution of stars in the galaxy. In addition to these fields, the theory has applications to the particle dynamics of plasmas (Whiteman and McNamara 1968), to the stability of particles in accelerators (Symon and Sessler 1956), to magnetic surfaces (Arnol'd 1963b), to the theory of certain molecular processes (Thiele and Wilson 1961), to the foundations of classical statistical mechanics (Arnol'd and Avez 1968, Wightman 1971, Ford 1972), and to the semi-classical quantization of bound systems (Einstein 1917, Keller 1958, Percival 1973). The earlier workers were not aware of the KAM theorem.

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For details of the analytic theory of invariant toroids the reader is referred to the quoted papers of Kolmogorov, Arnol'd and Moser and to the books of Arnol'd and Avez (1968), Abraham (1967) and Siegel and Moser (1971).

In this paper we obtain variational principles for invariant toroids and discuss only briefly their application. Abraham (1967, § 19) points out that it is quite difficult to be rigorous in the calculus of variations, and rigour is not attempted here.

2. Invariant toroids of integrable systems

Consider a conservative dynamical system with N-dimensional canonical vector coordinate and momentum

$$q = (q_1, q_2, \ldots, q_N), \qquad p = (p_1, p_2, \ldots, p_N), \tag{2.1}$$

whose motion satisfies Hamilton's equations

$$\dot{q}_k = \frac{\partial H(q, p)}{\partial p_k}, \qquad \dot{p}_k = \frac{-\partial H(q, p)}{\partial q_k} \qquad (k = 1, 2, \ldots, N). \tag{2.2}$$

Let $\mathscr{R}$ be a bounded $2N$-dimensional region in the phase space of phase points

$$X = (q, p) \tag{2.3}$$

within which $H(q, p)$ is everywhere analytic in (q, p). Consider only those classical phase trajectories

$$X(t) = (q(t), p(t)) \tag{2.4}$$

which satisfy Hamilton's equations (2.2) and which are confined to $\mathscr{R}$ for all times t. Suppose $\mathscr{R}$ consists entirely of such trajectories.

By the conservation of energy each trajectory is further confined to a $(2N-1)$-dimensional region or 'energy shell' defined by the equation

$$H(q, p) = E \tag{2.5}$$

for some fixed value of E.

A system is 'integrable' if there is a time-independent canonical transformation to a new N-dimensional coordinate q' and momentum p' for which the hamiltonian has the q'-independent form

$$H = H(p'). \tag{2.6}$$

A particular case is that of 'completely separable' systems for which it can be further simplified to the form

$$H(p') = \sum_{k=1}^{N} H_k(p'_k). \tag{2.7}$$

In each case a classical trajectory is confined to an N-dimensional region defined by the initial values of the momenta p'_k. According to the usual theory of action-angle variables for the bounded motion of integrable systems (Landau and Lifshitz 1969, § 50, Goldstein 1953, § 9.5, Born 1960, chap 2) a further transformation can be made to canonical coordinate and momentum

$$\theta = (\theta_1, \theta_2, \ldots, \theta_N), \qquad I = (I_1, I_2, \ldots, I_N), \tag{2.8}$$

where θ is in an N-dimensional angle variable; that is, θ_k lies in the range

$$-\pi < \theta_k \leqslant \pi \tag{2.9}$$

and a phase point $X(\theta, I)$ is periodic of period 2π in each of the θ_k variables†. The hamiltonian is independent of the θ_k,

$$H = H(I), \tag{2.10}$$

so that the action vector I is constant. For a given $I = I^0$ a classical trajectory which passes through the phase point $\theta = \theta^0$ at time $t = 0$ is given by

$$X(I^0, \theta), \tag{2.11a}$$

$$\theta_k = \omega_k t + \theta_k^0, \qquad (k = 1, 2, \ldots, N) \tag{2.11b}$$

where ω_k is an angular frequency which generally depends on all the $I_{k'}$, but for completely separable systems depends on I_k alone.

For each fixed value I^0 of the N-dimensional action I, the dependence of the phase point $X(\theta, I^0)$ on the N-dimensional angle variable θ parametrically defines an N-dimensional region in the phase space, where θ is the N-dimensional parameter. Because the dependence of X on θ is periodic in each of the θ_k, the region is a toroid.

For a system of two degrees of freedom, the toroid is a two-dimensional surface lying in a three-dimensional energy shell of a four-dimensional phase space. For any N, a phase point which lies in the toroid at any time and which moves according to the classical equations of motion, remains in it for all time. The toroid is therefore invariant under the classical motion of its phase points.

Since the canonical transformation to (θ, I) is possible for all points X of trajectories $X(t)$ in $\mathscr{R}$, every such trajectory is confined to an invariant toroid, and cannot wander freely within the energy shell. The $2N$-dimensional region $\mathscr{R}$ of phase space consists almost entirely of invariant toroids, the exceptions being regions of lower dimension.

3. Invariant toroids of general systems

Suppose our system of N degrees of freedom is not necessarily integrable. An N-dimensional toroid Σ in the $2N$-dimensional phase space can still be represented parametrically by a phase point which is a sufficiently well behaved function of an N-dimensional angle variable θ:

$$X = X_\Sigma(\theta) = [q_\Sigma(\theta), p_\Sigma(\theta)], \tag{3.1}$$

where q, p are the original coordinate and momentum of the phase point X. The toroid is invariant if it contains all of the classical trajectory which passes through any one of its phase points. We shall refer to it as an invariant toroid only if, in addition, the motion along each classical trajectory of the surface satisfies equation (2.11b) for some set of N angular frequencies ω_k.

This parametric representation is suggested by the work of Siegel and Moser (1971, § 36).

According to the theorem of Kolmogorov, Arnol'd and Moser, invariant toroids occupy a region of finite volume (positive measure) of the phase space of a system which is sufficiently close to integrability. We shall name this a 'regular' region. Numerical

† Where notation differs from the quoted texts: $J_k = 2\pi I_k$, $w_k = \theta_k/2\pi$.

experiment suggests that regular regions are still significant even when the system is far from being integrable. The residual (irregular) region also appears to be of finite volume, in many cases consisting of unstable trajectories which do not seem to be in invariant surfaces. The geometrical structure of both regular and irregular regions is very complicated.

The condition for a toroid represented by (3.1) to be invariant can be expressed independently of the time by using equation (2.11*b*) to obtain the operator relation

$$\frac{\mathrm{d}}{\mathrm{d}t} = \sum_k \frac{\mathrm{d}\theta_k}{\mathrm{d}t}\frac{\partial}{\partial\theta_k} = \sum_k \omega_k \frac{\partial}{\partial\theta_k}. \tag{3.2}$$

Hamilton's equations then take the form of first-order differential equations in θ_k:

$$\sum_k \omega_k \frac{\partial}{\partial\theta_k} q = \frac{\partial H}{\partial p} \tag{3.3a}$$

$$\sum_k \omega_k \frac{\partial}{\partial\theta_k} p = -\frac{\partial H}{\partial q} \tag{3.3b}$$

where the vector operators $\partial/\partial q$, $\partial/\partial p$ are defined as

$$\begin{aligned}\frac{\partial}{\partial q} &= \left(\frac{\partial}{\partial q_1}, \frac{\partial}{\partial q_2}, \ldots, \frac{\partial}{\partial q_N}\right)\\ \frac{\partial}{\partial p} &= \left(\frac{\partial}{\partial p_1}, \frac{\partial}{\partial p_2}, \ldots, \frac{\partial}{\partial p_N}\right).\end{aligned} \tag{3.4}$$

If the angle Hamilton equations (3.3) and equation (2.11*b*) are satisfied for any N angular frequencies $(\omega_1, \omega_2, \ldots, \omega_N)$, then the toroid is invariant.

The condition (3.3) relates phase points of the toroid along the trajectories only. There is no condition across these trajectories, except that $q(\theta)$, $p(\theta)$ should be a well behaved, in particular a continuous, function of the N-dimensional angle variable θ.

Invariant toroids are related to solutions of the time-independent Hamilton–Jacobi (HJ) equation

$$H(q, \partial S_E/\partial q) - E = 0 \tag{3.5}$$

for an action function (characteristic function) $S_E(q)$. Given a solution of equation (3.5), the momentum

$$p = \partial S_E/\partial q \tag{3.6}$$

may be considered as a function of q, thus defining an N-dimensional region in the $2N$-dimensional phase space of points $X = (q, p)$. From the Hamilton–Jacobi theory this region is made up of parts of classical trajectories, but it is not necessarily an invariant toroid, as it may not be closed.

Unfortunately the definition of an invariant toroid from the HJ equation requires a detailed study of multi-valued action functions, as may be seen by considering the simple one-dimensional oscillator. The complicated analytic properties of these multi-valued functions are discussed in general terms by Einstein (1917).

Because of these complications the parametric representation of invariant toroids is chosen as the basis of the following theory, despite the apparent advantages of defining them through a single function $S_E(q)$ of the vector coordinate q.

Conversely, however, line integrals of the form

$$S(q^1) = \int_{q^0}^{q^1} p \, . \, dq \tag{3.7}$$

on an invariant toroid provide a special multivalued solution of the HJ equation (3.5), which is the classical analogue of the bound state solution of the Schrödinger equation of quantum mechanics. The dot represents a scalar product.

4. Variational principle in hamiltonian form

Denote an integral over the entire space of the angle variables by

$$\oint d(\theta)F(\theta) = \int_{-\pi}^{\pi} d\theta_1 \ldots \int_{-\pi}^{\pi} d\theta_N F(\theta_1, \ldots, \theta_N) \tag{4.1}$$

and a normalized integral by

$$\oint' d(\theta)F(\theta) = (2\pi)^{-N} \oint d(\theta)F(\theta). \tag{4.2}$$

The mean value of the kth action integral for an N-dimensional toroid Σ (not necessarily invariant) is defined as

$$I_k(\Sigma) = \oint' d(\theta)p_\Sigma(\theta) \, . \, \partial q_\Sigma(\theta)/\partial\theta_k, \tag{4.3}$$

where the dot represents a scalar product.

Introduce the mean energy on the toroid, which is

$$E = \oint' d(\theta)H(q(\theta), p(\theta)), \tag{4.4}$$

where $H(q, p)$ is the hamiltonian function and suffices Σ have been dropped. By analogy with the stationary principle for bound state solutions of the Schrödinger wave equation (Landau and Lifshitz 1958, § 18) we require that this energy be stationary with respect to small smooth periodic variations in $q(\theta), p(\theta)$ subject to the action integrals (4.3) remaining constant. This suggests a stationary principle for the classical functional

$$\Phi = \oint' d(\theta)\left(H(q(\theta), p(\theta)) - \sum_{k=1}^{N} \omega_k p \, . \, \partial q/\partial\theta_k\right), \tag{4.5}$$

where the ω_k are Lagrange multipliers. According to this principle and ignoring terms of second order in the variations:

$$0 = \Delta\Phi \tag{4.6a}$$

$$= \oint' d(\theta)\left(\frac{\partial H}{\partial q} \, . \, \Delta q(\theta) - \sum_k \omega_k p \, . \, \frac{\partial}{\partial\theta_k}\Delta q(\theta)\right)$$

$$+ \oint' d(\theta)\left(\frac{\partial H}{\partial p} \, . \, \Delta p(\theta) - \sum_k \omega_k \frac{\partial q}{\partial\theta_k} \, . \, \Delta p(\theta)\right)$$

$$= \oint' d(\theta)\left(\frac{\partial H}{\partial q} + \sum_k \omega_k \frac{\partial p}{\partial\theta_k}\right) . \, \Delta q(\theta) + \oint' d(\theta)\left(\frac{\partial H}{\partial p} - \sum_k \omega_k \frac{\partial q}{\partial\theta_k}\right) . \, \Delta p(\theta). \tag{4.6b}$$

Integration by parts is used in the third equality; the periodicity of q and p in each of the θ_k ensures that the boundary terms are zero.

Since $\Delta q(\theta)$ and $\Delta p(\theta)$ are arbitrary, their coefficients must be zero, giving

$$\sum_k \omega_k \frac{\partial q}{\partial \theta_k} = \frac{\partial H}{\partial p} \tag{4.7a}$$

$$\sum_k \omega_k \frac{\partial p}{\partial \theta_k} = -\frac{\partial H}{\partial q}. \tag{4.7b}$$

These are the angle Hamilton equations (3.3) for an invariant toroid. When the ω_k are interpreted as angular frequencies, the linear combination of partial derivatives with respect to the θ_k becomes a total derivative with respect to the time as in equation (3.2).

The usual relations (2.11b) between the angle variables and the time for a particular orbit follow and equations (4.7) become Hamilton's equations.

The explicit form of the trajectory in phase space is given as a function of time by $[q_\Sigma(\theta(t)), p_\Sigma(\theta(t))]$ with $\theta(t)$ given by (2.11b) with fixed phase shifts θ_k^0.

Thus a toroid with parametric representation (3.1) and satisfying the variational principle (4.6) is an invariant toroid. Conversely, because an invariant toroid Σ with parametric representation (3.1) satisfies the surface Hamilton equations (4.7), the integral (4.5) may be shown to be stationary for variations about Σ.

We now have a variational principle for invariant toroids in hamiltonian form.

When the hamiltonian function has the form

$$H = \sum_l \frac{1}{2m_l} p_l^2 + V(q), \tag{4.8}$$

equation (4.7a) requires the momentum coordinate p_l to be

$$p_l = \sum_k \omega_k \frac{\partial}{\partial \theta_k}(m_l q_l), \tag{4.9}$$

so that from (4.7b) the angle equations may be written in newtonian form in terms of the coordinates q_l alone:

$$\left(\sum_k \omega_k \frac{\partial}{\partial \theta_k}\right)^2 m_l q_l = F_l = -\frac{\partial V}{\partial q_l}. \tag{4.10}$$

For this hamiltonian the action integrals (4.3) can also be written in terms of the coordinates:

$$I_k = \sum_j G_{kj} \omega_j, \tag{4.11}$$

where G_{kj} is a generalized moment of inertia tensor, given by

$$G_{kj} = \oint' \mathrm{d}(\theta) \frac{\partial q}{\partial \theta_k} \cdot \frac{\partial}{\partial \theta_j}(mq) \tag{4.12}$$

and mq is an N-vector with elements $m_l q_l$.

5. Variational principle in lagrangian form

Let $L(q, \dot{q})$ be the lagrangian. Suppose from the start that ω_k is the angular frequency corresponding to the angle variable θ_k, and that the total time derivative is given by equation (3.2). Then the lagrangian is the following function of $q(\theta)$, $\partial q/\partial\theta_k$ and ω_k:

$$L\left(q, \sum_k \omega_k \frac{\partial q}{\partial \theta_k}\right). \tag{5.1}$$

Let I_k be fixed and initially undefined constants, of the dimensions of action, and consider the functional

$$\Psi = \oint' \mathrm{d}(\theta) L\left(q, \sum_k \omega_k \frac{\partial q}{\partial \theta_k}\right) - \sum_k \omega_k I_k. \tag{5.2}$$

For the variational principle, suppose that Ψ is stationary with respect to small smooth periodic variations in $q(\theta)$ and also with respect to small variations in the angular frequencies ω_k. According to this principle and neglecting terms of second order in the variations:

$$0 = \Delta\Psi = \oint' \mathrm{d}(\theta)\left(\frac{\partial L}{\partial q} . \Delta q(\theta) + \frac{\partial L}{\partial \dot{q}} . \sum_k \omega_k \frac{\partial \Delta q}{\partial \theta_k} + \frac{\partial L}{\partial \dot{q}} . \sum_k \frac{\partial q}{\partial \theta_k} \Delta\omega_k\right) - \sum_k \omega_k I_k \tag{5.3a}$$

$$= \oint' \mathrm{d}(\theta)\left[\frac{\partial L}{\partial q} - \sum_k \omega_k \frac{\partial}{\partial \theta_k}\left(\frac{\partial L}{\partial \dot{q}}\right)\right] . \Delta q(\theta) + \sum_k \left(\oint' \mathrm{d}(\theta) \frac{\partial L}{\partial \dot{q}} . \frac{\partial q}{\partial \theta_k} - I_k\right) \Delta\omega_k . \tag{5.3b}$$

Equate the coefficients of the variations to zero and obtain

$$\sum_k \omega_k \frac{\partial}{\partial \theta_k}\left(\frac{\partial L}{\partial \dot{q}}\right) = \frac{\partial L}{\partial q} \tag{5.4a}$$

$$\oint \mathrm{d}(\theta) \frac{\partial L}{\partial \dot{q}} . \frac{\partial q}{\partial \theta_k} = I_k. \tag{5.4b}$$

These are the angle form of Lagrange's equations and the equations for the action integrals; in this case the latter are obtained from the variational principle.

The functions

$$q(\theta), \qquad p(\theta) = \frac{\partial L}{\partial \dot{q}}(\theta) \tag{5.5}$$

define an invariant toroid when they satisfy the variational principle or the equations (5.4).

Since the number of unknowns $q(\theta)$, ω_k for the lagrangian form is less than for the hamiltonian form, the lagrangian form is used in the following.

6. Fourier expansion

An approximation to an invariant toroid is obtained by restricting it to a specific functional form and then applying a variational principle which preserves that form. A particularly simple form is the finite Fourier sum. For simplicity consider the case of motion of a particle of mass m in two dimensions with position $\boldsymbol{r} = (x, y)$, velocity $\boldsymbol{v} = (v_x, v_y)$ and lagrangian

$$L = \tfrac{1}{2}m\boldsymbol{v}^2 - V(\boldsymbol{r}). \tag{6.1}$$

The position and velocity can be expanded in Fourier series, which may be truncated for an approximation:

$$\boldsymbol{r}(\theta_1, \theta_2) = \sum_{s_1 s_2} \boldsymbol{r}_{s_1 s_2} \exp[\mathrm{i}(s_1\theta_1 + s_2\theta_2)] \tag{6.2}$$

$$\boldsymbol{v}(\theta_1, \theta_2) = \sum_{s_1 s_2} \mathrm{i}(s_1\omega_1 + s_2\omega_2)\boldsymbol{r}_{s_1 s_2} \exp[\mathrm{i}(s_1\theta_1 + s_2\theta_2)]. \tag{6.3}$$

The lagrangian functional is

$$\Psi = \tfrac{1}{2}m \sum_{s_1 s_2} (s_1\omega_1 + s_2\omega_2)^2 (x_{s_1 s_2} x_{-s_1-s_2} + y_{s_1 s_2} y_{-s_1-s_2})$$
$$- \oint' \mathrm{d}(\theta) V\left(\sum_{s_1 s_2} \boldsymbol{r}_{s_1 s_2} \exp[\mathrm{i}(s_1\theta_1 + s_2\theta_2)]\right) - \omega_1 I_1 - \omega_2 I_2. \tag{6.4}$$

The coefficients of the derivatives with respect to $x_{-s_1-s_2}$ and $y_{-s_1-s_2}$ are all zero, so that

$$m(s_1\omega_1 + s_2\omega_2)^2 \boldsymbol{r}_{s_1 s_2} = -\boldsymbol{F}_{s_1 s_2}, \tag{6.5}$$

where $\boldsymbol{F}_{s_1 s_2}$ is the Fourier component of the force:

$$\boldsymbol{F}(\boldsymbol{r}) = -\nabla V(\boldsymbol{r}) \tag{6.6}$$

$$\boldsymbol{F}_{s_1 s_2} = \oint' \mathrm{d}(\theta) \exp[-\mathrm{i}(s_1\theta_1 + s_2\theta_2)] \boldsymbol{F}(x(\theta), y(\theta)). \tag{6.7}$$

The Fourier equations (6.5) are truncated at the same point as the original expression (6.2). They are the same equations as are obtained by the corresponding truncation of the discrete Fourier transformation of the newtonian form (4.10). The variational principle shows that they are the best that can be obtained for an estimate of Ψ from a truncated Fourier expansion.

The variations in ω_1 and ω_2 provide the matrix equation for the action integrals

$$I = G\omega, \tag{6.8}$$

with

$$\left.\begin{aligned} G_{ii} &= m \sum_{s_1 s_2} s_i^2 |\boldsymbol{r}_{s_1 s_2}|^2 \\ G_{12} = G_{21} &= m \sum_{s_1 s_2} s_1 s_2 |\boldsymbol{r}_{s_1 s_2}|^2. \end{aligned}\right\} \tag{6.9}$$

Similar truncated Fourier expansions of the angle hamiltonian and Lagrange equations can be obtained from the corresponding variational principles. Various iterative procedures for the solution of these equations result in a variety of approximate methods for finding invariant surfaces. One can rederive in this way the classical method of Lindstedt (see Poincaré 1893) and the method used by Arnol'd (1963a) in his proof of the existence of invariant surfaces.

By substitution of particular restricted approximate analytic forms for the $q_\Sigma(\theta)$ (and $p_\Sigma(\theta)$) a wide variety of other approximations to invariant surfaces can be obtained.

7. Conclusion

The variational principles proposed for invariant surfaces have the properties of other dynamical variational principles. Their statement is very simple, they are independent of the canonical variables, they can be made the basis of a whole variety of approximations and they suggest interesting relations between classical and quantum mechanics but they are difficult to treat rigorously.

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† An English translation of this article forms appendix D of Abraham (1967).