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## LETTER TO THE EDITOR

## A variational principle for invariant tori of fixed frequency

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**Abstract.** A fixed frequency Lagrangian variational principle is formulated for the invariant tori of conservative dynamical systems. It avoids the singularities due to small frequency divisors, and for pure rotation provides a strict bound which can be used as a basis for an effective variational method.

Variational principles for orbits have guided the development of classical dynamics since Maupertuis and Hamilton (Lanczos 1949, Landau and Lifshitz 1969). Hamilton's principle also helped Born and Jordan (1925) formulate the general theory of quantum mechanics (see also Van der Waerden 1967, p 289). However, the variational principles of dynamics have had less influence on the theory and practice of approximation in classical dynamics than the Rayleigh–Ritz principle has had in quantum mechanics. In particular the perturbation theories of classical dynamics are usually obtained without applying variational principles, and the important theorems of Kolmogorov, Arnol'd (1961, 1963) and Moser (1962) (hereafter referred to as KAM) are proved without them.

For regular bounded motion (see Whiteman 1977) we can name three reasons for this:

(i) For a system of n freedoms the regular orbit lies in an invariant torus of n dimensions in the 2n-dimensional phase space. We need variational principles for the tori, not for the orbits.

(ii) The famed small frequency divisors produce singularities arbitrarily close to every torus in phase space, thus reducing the radius of convergence of the usual perturbation expansions to zero.

(iii) Unlike the Rayleigh-Ritz principle, the usual classical variational principles do not provide bounds (Helleman 1978).

Reason (i) is no longer a problem as variational principles have been formulated for invariant tori (Percival 1974; see also Trkal 1922 and Van Vleck 1923) and used to obtain the usual form of the classical perturbation theory (Percival and Pomphrey 1976).

In these variational principles and in the corresponding perturbation theories the action variables are held fixed and the frequencies allowed to vary. Moser (1974) has remarked that an alternative perturbation theory, in which the frequencies are held fixed, has finite radii of convergence. This result follows from the KAM theorems. Poincaré already knew of the fixed frequency perturbation theory.

In this Letter we introduce fixed frequency variational principles for invariant tori, overcoming the difficulties of reason (ii), and then show that for coupled rotors one of these principles provides a strict bound, by contrast to reason (iii).

There are two new principles, based on the Lagrangian function  $L(q, \dot{q})$  and on the Hamiltonian function H(p, q), where q represents n configuration coordinates and p represents n conjugate generalised momentum coordinates.

For the Lagrangian variational principle the torus  $\Sigma$  is represented parametrically by a configuration function

$$\boldsymbol{q}_{\boldsymbol{\Sigma}}(\boldsymbol{\theta}) = (\boldsymbol{q}_{\boldsymbol{\Sigma}1}(\boldsymbol{\theta}), \boldsymbol{q}_{\boldsymbol{\Sigma}2}(\boldsymbol{\theta}), \dots, \boldsymbol{q}_{\boldsymbol{\Sigma}n}(\boldsymbol{\theta})) \tag{1}$$

of the vector angle variable

$$\boldsymbol{\theta} = (\theta_1, \theta_2, \dots, \theta_n) \tag{2}$$

which is periodic of period  $2\pi$  in each  $\theta_i$ .

Let

$$\boldsymbol{\omega} = (\omega_1, \omega_2, \dots, \omega_n) \tag{3}$$

be the vector angular frequency for the motion in the invariant torus, and let

$$\nabla_{\boldsymbol{\theta}} = (\partial/\partial \theta_1, \partial/\partial \theta_2, \dots, \partial/\partial \theta_n)$$
(4)

be the gradient operator with respect to  $\theta$ .

Using  $a \cdot b$  to denote the usual scalar product, the dynamical differential operator  $D_{\omega}$  on the torus is defined by

$$\mathbf{D}_{\boldsymbol{\omega}} f(\boldsymbol{\theta}) = \boldsymbol{\omega} \cdot \boldsymbol{\nabla}_{\boldsymbol{\theta}} f(\boldsymbol{\theta}). \tag{5}$$

According to the 1974 Lagrangian fixed action variational principle for invariant tori, the functional

$$\Psi = \langle L(\boldsymbol{q}(\boldsymbol{\theta}), \mathbf{D}_{\boldsymbol{\omega}}\boldsymbol{q}(\boldsymbol{\theta})) - \boldsymbol{\omega} \cdot \boldsymbol{I} \rangle$$
(6)

is stationary at  $q_{\Sigma}(\theta)$  with respect to the variation of both the function  $q(\theta)$  and the angular frequency  $\omega$ , with the *I* held constant. The mean of a function  $f(\theta)$  over a torus is defined by

$$\langle f(\boldsymbol{\theta}) \rangle = (2\pi)^{-n} \oint d^n \boldsymbol{\theta} \cdot f(\boldsymbol{\theta}).$$
 (7)

The variation in  $q(\theta)$  provides Lagrange's equation for the torus, which is

$$\mathbf{D}_{\boldsymbol{\omega}}[\boldsymbol{\nabla}_{\boldsymbol{\phi}} L(\boldsymbol{q}, \mathbf{D}_{\boldsymbol{\omega}} \boldsymbol{q})] = \boldsymbol{\nabla}_{\boldsymbol{q}} L(\boldsymbol{q}, \mathbf{D}_{\boldsymbol{\omega}} \boldsymbol{q}) \tag{8}$$

where  $\nabla_{\dot{q}}$  represents a gradient with respect to the second vector argument of *L*. It may be verified that if  $q_{\Sigma}(\theta)$  is a solution of (8), then  $q_{\Sigma}(\omega t + \theta^0)$  represents an orbit satisfying Lagrange's equations of motion with initial condition  $\theta(0) = \theta^0$ . The variation in  $\omega$ provides a definition of the vector action variable *I* in terms of  $q(\theta)$ . It is

$$I_{j} = \langle \nabla_{\dot{\boldsymbol{q}}} L \cdot (\partial/\partial \theta_{j}) \boldsymbol{q} \rangle.$$
<sup>(9)</sup>

In this variational principle the vector action variable I is held constant and the tori are distinguished from one another by differing values of I. There are strong arguments in favour of using the action I in this way, which follow from the fact that  $(I, \theta)$  are canonical variables. However, it leads to difficulties because of the singularities due to small frequency divisors which occur where the frequency vector  $\boldsymbol{\omega}$  satisfies a relation of the form

$$\boldsymbol{k} \cdot \boldsymbol{\omega} = 0 \qquad (\boldsymbol{k} \neq 0) \tag{10}$$

where k is any non-zero vector with integer components. Any  $\omega$  which does not satisfy equation (10) for any such k is named a proper frequency vector. Since any real number may be arbitrarily closely approximated by a rational number, there are improper  $\omega$ satisfying (10), and therefore small divisors, arbitrarily close to any proper  $\omega$ . If  $\omega$  is allowed to vary, then arbitrarily small variations of the torus encounter singularities due to small frequency divisors, causing difficulties for both the theory and application of the variational principle.

These difficulties are overcome by using a variational principle at fixed proper frequency  $\omega$ . Let the functional be

$$\Phi = \langle L(\boldsymbol{q}(\boldsymbol{\theta}), \mathbf{D}_{\boldsymbol{\omega}}\boldsymbol{q}(\boldsymbol{\theta})) \rangle. \tag{11}$$

Fixing  $\boldsymbol{\omega}$  and allowing the  $\boldsymbol{q}(\boldsymbol{\theta})$  to vary we obtain

 $0 = \Delta \Phi \tag{12}$ 

$$= \langle \Delta \boldsymbol{q} \cdot \boldsymbol{\nabla}_{\boldsymbol{q}} L(\boldsymbol{q} \cdot \boldsymbol{D} \boldsymbol{q}) + (\boldsymbol{D}_{\boldsymbol{\omega}} \Delta \boldsymbol{q}) \cdot \boldsymbol{\nabla}_{\boldsymbol{q}} L(\boldsymbol{q} \cdot \boldsymbol{D}_{\boldsymbol{\omega}} \boldsymbol{q}) \rangle$$
(13)

$$= \langle \Delta \boldsymbol{q} \cdot \boldsymbol{\nabla}_{\boldsymbol{q}} L(\boldsymbol{q} \cdot \mathbf{D} \boldsymbol{q}) - \Delta \boldsymbol{q} \cdot \mathbf{D}_{\boldsymbol{\omega}} (\boldsymbol{\nabla}_{\boldsymbol{\dot{q}}} L(\boldsymbol{q} \cdot \mathbf{D}_{\boldsymbol{\omega}} \boldsymbol{q})) \rangle$$
(14)

where integration by parts and periodicity of all functions in  $\theta_i$  have been used to obtain equation (14). Lagrange's equations (8) for the torus follow on equating first-order variations to zero.

For the special but important case of coupled rotors and equivalent systems the Lagrangian functional (11) can provide a strict bound. In that case the coordinates  $q_i$  are chosen so that the configuration is periodic of period  $2\pi$  in each of the  $q_j$ . The configuration space is a torus of dimension n, and the function  $q(\theta)$  represents a mapping of an *n*-torus onto itself. If the mapping can be obtained by continuous deformation then  $q_j$  increases by  $2\pi$  when  $\theta_j$  increases by  $2\pi$ , and since  $\theta_i$  is linear in time the motion is a rotation in all the  $q_j$ . The direction of rotation for  $\theta_i$  is determined by the sign of  $\omega_j$ . The bound applies to rotations only.

The Lagrangian can be put into the form

$$L(\boldsymbol{q}, \, \boldsymbol{\dot{q}}) = T(\boldsymbol{\dot{q}}) - V(\boldsymbol{q}) \tag{15}$$

$$= (1/2m)\dot{q}^2 - V(q)$$
(16)

where V(q) is continuous and therefore bounded. In that case the functional

$$\Phi_T(\boldsymbol{q}) = \langle T(\mathbf{D}_{\omega}\boldsymbol{q}(\boldsymbol{\theta})) \rangle \tag{17}$$

is positive semi-definite and

$$\Phi_{V}(\boldsymbol{q}) = \langle V(\boldsymbol{q}(\boldsymbol{\theta})) \rangle \tag{18}$$

is bounded above by Sup V(q). Therefore the Lagrangian functional

$$\Phi(\boldsymbol{q}) = \Phi_T(\boldsymbol{q}) - \Phi_V(\boldsymbol{q}) \tag{19}$$

is bounded below, and provided that it is twice differentiable with respect to its functional argument at a point  $q_{\Sigma}(\theta)$  in the function space where it attains its minimum, then  $q_{\Sigma}(\theta)$  satisfies the toric Lagrange equations (8). There is an invariant torus at the minimum of  $\Phi$  for all proper values of  $\omega$  satisfying the above condition.

By analogy with the Rayleigh-Ritz principle, the better of two approximate tori is that which has the lesser value of the functional  $\Phi$ . However, the dependence is nonlinear, so other solutions with the same  $\omega$  can exist.

This minimum principle does not apply when one of the coordinates  $q_i$  does not rotate, but vibrates, and even the variational principle (12) cannot be used for purely harmonic motion.

There is a Hamiltonian fixed frequency variational principle for tori, whereby the functional

$$\bar{\Phi}(\boldsymbol{q},\boldsymbol{p}) = \langle \boldsymbol{p}(\boldsymbol{\theta}) \cdot \mathbf{D}_{\boldsymbol{\omega}} \boldsymbol{q}(\boldsymbol{\theta}) - H(\boldsymbol{q}(\boldsymbol{\theta}),\boldsymbol{p}(\boldsymbol{\theta})) \rangle$$
(20)

is stationary for variations in the functions  $q(\theta)$ ,  $p(\theta)$ .  $\overline{\Phi}$  is not an extremum, even for the case of pure rotation.

In conclusion, the Lagrangian fixed frequency variational principle (12) for invariant tori avoids the singularities due to small frequency divisors, and given a functional differentiability condition which appears to be satisfied in practice, it provides a strict bound for pure rotation, and can be used as a basis for an effective variational method. Given the condition, there are invariant tori for all proper frequency vectors  $\boldsymbol{\omega}$ . Of course this does not imply that there are tori for all vector actions  $\boldsymbol{I}$ , as  $\boldsymbol{I}$  is a discontinuous function of  $\boldsymbol{\omega}$ .

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