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# New formulation of a forgotten old variational principle

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An old variational principle (Maupertuis principle), forgotten as inconvenient quirk of history, has been reformulated into the modified variational principle (MVP) along with its reciprocal principle (RMP) and both these principles have been derived classically as well as quantum mechanically. Wide scope of applicability of these new principles in classical mechanics has been demonstrated by solving the problems of Linear Oscillator, Anharmonic Oscillator and Anisotropic 2D-Quartic Oscillator (chaotic system).

Key words: Variational principle, anharmonic oscillator, chaotic system.

# INTRODUCTION

Classically a mechanical system of particles can be described by a Lagrangian  $L(q_i, \dot{q}_i, t)$  or by Hamiltonian  $H(q_i, p_i, t)$  where  $q_i$  are the generalized coordinates and  $p_i$  are the generalized momenta. The transformation from  $(q_i, \dot{q}_i, L)$  to  $(q_i, p_i, H)$  is the Legendre transformation (Rajput, 2005a)

$$H(q_{i}, p_{i}, t) = \sum_{i} p_{i} \dot{q}_{i} - L(q_{i}, \dot{q}_{i}, t)$$
(1)

Maupertuis proposed in 1744 a global integral quantity (Yourgan and Mandelstam, 1968) 'Action' which is least along the true path and greater for the unphysical virtual paths. Maupertuis definition of action and his corresponding variational principle were little vague, which were modified by Euler and Lagrange by taking the action as:

$$W = \int_{q_i}^{q_j} \sum_j p_j dq_j \tag{2}$$

Where the arbitrary path  $q_j(t')$  runs from an initial point  $q_i = q_j(0)$  to a final point  $q_f = q_j(t)$ . These end points are kept fixed but the duration t is path dependent.

Euler and Lagrange showed that for the true trajectory W is stationary provided that the virtual trajectories  $q_j(t')$  are all restricted to have the same fixed energy E= H=T+V. Thus the Maupertuis principle of least action may be written as:

$$\left(\delta W\right)_E = 0 \tag{3}$$

Where  $\partial W$  denotes a first order variation and the subscript E denotes that the energy is held fixed during the variation. This constraint of fixed energy brings several drawbacks in this Maupertuis variational principle given by Equation (3). It makes energy conservation an assumption and not a consequence, makes it cumbersome to convert this principle in to a differential equation for the trajectory, path becomes awkward to be handled analytically, and the virtual trajectories allowed by this principle in one dimension differ from the true trajectory by instantaneous velocity reversals. Due to these weaknesses the Maupertuis action (2) and his variational principle (3) were forgotten altogether.

In the present paper, Maupertuis variational principle (3) has been reformulated into a very useful modified variational principle (MVP) along with its reciprocal principle (RMP). Deriving both these principles classically as well as quantum mechanically, their very wide applicability has been demonstrated in the problems of Linear Oscillator, Anharmonic Oscillator and Anisotropic

2D-Quartic Oscillator (chaotic system).

# MODIFIED MAUPERTUIS VARIATIONAL PRINCIPLE (MVP) AND ITS RECIPROCAL PRINCIPLE (RMP)

Maupertuis variational principle (3) can be reformulated in to following very useful modified variational principle (MVP) by relaxing the constraint of fixed energy for virtual path, allowing a larger class of trial trajectories and keeping the mean energy  $\overline{E}$  fixed (not necessarily conserving the energy):

$$(\partial W)_{\overline{F}} = 0 \tag{4}$$

Where the mean energy may be defined as:

$$\overline{E} = \frac{1}{t} \int_{0}^{t} H(q_{j}, p_{j}, t') dt'$$
(5)

This modified variational principle (MVP), given by Equation (4) is free from weaknesses of the old principle (3) and it has the additional merit of allowing the reciprocal transformation interchanging  $Wand\overline{E}$  transforming it in to the following Reciprocal Maupertius Principle (RMP) with the same solution;

$$(\delta \overline{E})_W = 0 \tag{6}$$

The reciprocal pair of variational principles, MVP and RMP, given by Equation (4) and (2.3) respectively, may also be written in the following unconstrained form that is, Unconstrained Maupertuis Principle (UMP);

$$(\partial W) = t \partial \overline{E} \tag{7}$$

Where the time t, the duration of pure trajectory, is constant Lagrangian multiplier.

Let us derive these variational principles, MVP, RMP and UMP, classically as well as quantum mechanically in the following subsections.

### **Classical derivation**

Let us consider a function J[q(t')] such that:

$$J[q(t)] = \int_{0}^{t} F(q_1, q_2, \dots, \dot{q}_1, \dot{q}_2, \dots, \dot{t}') dt'$$
(8)

Where  $q_{1,}q_{2}$ ,.....are the generalized coordinates and  $\dot{q}_{1}, \dot{q}_{2}$ .....are the generalized velocities of the system

of any number of particles. Taking the variation of virtual trajectory

$$q_j(t') \rightarrow q_j(t') + \delta q_j(t')$$

Where the end point variation of  $q_j$ 's are zero but there is an arbitrary final end point variation in t, that is,

$$t \rightarrow t + \delta t$$

Then, on applying the first variation theorem of calculus of variations, we have:

$$\delta I = \int_{o}^{t} \sum_{i} \delta q_{i} \left[ \frac{\partial F}{\partial q_{i}} - \frac{d}{dt'} \left( \frac{\partial F}{\partial \dot{q}_{i}} \right) \right] dt' + \left[ F(t) - \sum \dot{q}_{i}(t) \left( \frac{\partial F}{\partial \dot{q}_{i}} \right) \right] \delta t$$
(9)

Let us apply this result on the action given by Equation (2) which may also be written as:

$$J = W = \int_{0}^{t} \sum_{i} p_{i}(t') \dot{q}_{i}(t'_{i}) dt'$$
(10)

Where we have:

$$F = \sum p_i(t) \dot{q}_i(t)$$

And hence Equation (9) gives:

$$\delta J = \delta W = \sum_{j=0}^{t} \delta q_{j} (-\dot{p}_{j}) dt' + \left[\sum_{i} p_{i}(t) \dot{q}_{i}(t) - \sum_{i} \dot{q}_{i}(t) p_{i}(t)\right] \delta t$$
$$= -\sum_{j=0}^{t} \delta q_{j} \dot{p}_{j} \delta t'$$
(11)

From Equation (5) for average energy we have:

$$\delta \overline{E} = -\frac{\delta t}{t^2} \int_0^t H(q_j, p_j, t') dt' + \frac{1}{t} \delta \int_0^t H(q_j, p_j, t') dt'$$
$$= -\frac{\delta t}{t} \overline{E} + \frac{1}{t} \delta \int_0^t (\sum_j p_j \dot{q}_j - L)$$
(12)

Where we have used Equation (1). This equation may also be written as:

$$t \, \delta \overline{E} = -\overline{E} \, \delta t + \delta \int_{0}^{t} (\sum_{j} p_{j} \dot{q}_{j} - L) dt'$$

Using relation (9), this equation may be written as:

$$t\delta\overline{E} = -\overline{E}\delta t + \int_{0}^{t} \sum_{j} \left[-\frac{\partial L}{\partial q_{j}} - \dot{p}_{j} + \frac{d}{dt}(\frac{\partial L}{\partial \dot{q}_{j}})\right]\delta q_{j}dt'$$
$$+ \left[\sum_{j} p_{j}\dot{q}_{j} - L - \sum_{j} p_{j}\dot{q}_{j} + (\dot{q}_{j}\frac{\partial L}{\partial \dot{q}_{j}})\right]\delta t$$
$$= -\overline{E}\delta t - \int_{0}^{t} \sum_{j} \dot{p}_{j}\delta q_{j}dt' - L\delta t + \sum_{j} \dot{q}_{j}p_{j}\delta t$$
(13)

Where in the first bracket we have used the well known Lagrangian equation,

$$\frac{\partial L}{\partial q_j} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_j} \right) = 0 ,$$

And in the second bracket we have used the well known relation

$$p_{j} = \frac{\partial L}{\partial \dot{q}_{j}}$$

For the holonomic conservative system. Now subtracting Equation (11) from (13), we have:

$$t\delta \overline{E} - \delta W = -\overline{E}\,\delta t + (\sum_{j} p_{j}\dot{q}_{j} - L)\delta t$$
$$= (H - \overline{E})\delta t \tag{14}$$

Where we have used relation (1).

If H(t) = E is constant of motion, then Equation (14) reduces to

$$t\,\partial\overline{E} - \partial W = 0\tag{15}$$

On setting  $\delta \overline{E} = 0$  that is, for fixed average energy, this equation leads to MVP given by Equation (4) whereas for fixed W that is, for  $\delta W = 0$ , it leads to RMP given by Equation (6). Equation may also be written as:

$$\delta W = t \, \delta \overline{E}$$

which is UMP given by Equation (7).

## Quantum mechanical derivation

Schrodinger (1926a) tried to derive the variational principle of wave mechanics from something like RMP but in another of his paper on wave mechanics (Schrödinger 1926b), he described his heuristic argument used in earlier paper as incomprehensible and presented

a second platform for Schrödinger equation based on the analogy between geometric and wave optics on one hand and particle and wave on the other hand. It is interesting to note that Klein et al. (1995) derived this. RMP directly from matrix mechanics. Following the arguments presented by Gray et al. (1996), it will be demonstrated here that RMP is the classical limit of quantum variational principle given by Rajput (2005),

$$\delta\left[\frac{\langle n|H|n\rangle}{\langle n|n\rangle}\right] = 0 \tag{16}$$

which turns in to RMP for large quantum number n. For simplicity, let us consider a one dimensional periodic motion, where the state  $|n\rangle$  corresponds to a classical periodic trajectory with precisely the same energy  $E_n$ . Using the WKB approximation for the trial wave functions  $\psi_n(q) = |n\rangle$ ,

we have

$$\langle n|n\rangle = \int \psi_n^* \psi_n dq = C \int_{q_{\min}}^{q_{\max}} \frac{dq}{v} = C \int_0^\tau dt = C\tau$$
(17)

where  $\nu$  is the velocity, C is a constant and  $\tau$  is the period of motion. Under the same approximation, we have:

$$\langle n | \hat{H} | n \rangle = C \int_{0}^{\tau} H(q, p, t) dt$$
(18)

For one dimensional periodic motion, the constraint on the energy for an allowed state  $|n\rangle$  for large *n* is

$$W(cycle) = \oint pdq = nh \tag{19}$$

which is famous Bohr-Sommerfeld-Wilson quantization rule (Rajput, 2005b). It shows that for fixed n the action W is to be kept fixed. Hence for fixed large value of n, the quantum variational principle (16) reduces to

$$\delta[\frac{1}{\tau}\int_{0}^{\tau}H(q, p, t)dt] = 0, \qquad (20)$$

for fixed W, that is,  $(\delta \overline{E})_W = 0$  showing that the quantum variational principle (16) transforms in to RMP for one dimensional periodic motion. It may also be demonstrated (Percival, 1974), that such transformation is valid for quasi-periodic case also.

#### APPLICATIONS OF MVP AND RMP

Reformulated MVP and RMP are the new and very useful principles of classical mechanics. Gray et al. (1996) have established the link of MVP and RMP with Hamilton variational principle (HP) and reciprocal Hamilton principle (RHP) and applied RMP to simple problems of physical interest. Here we shall demonstrate the wider applicability of RMP by applying it to the following problems.

#### Linear oscillator

Let us start with the following Hamiltonian for linear oscillator

$$H = \frac{1}{2}(m\dot{q}^2 + kq^2)$$
(21)

which corresponds to a simple pendulum, in square approximation of cosine term, for

$$q = l\theta$$
and
(22)

$$k = \frac{mg}{l}$$

Let us choose the trial trajectory as:

$$q(t) = A\sin \alpha t \tag{23}$$

where q = 0 at t = 0 and  $t = \frac{2\pi}{\omega} = \tau$  (at the end of the cycle). Using Equation (2), we have the action as:

$$W = \int_{0}^{\tau} p dq = m \int_{0}^{\tau} \dot{q} dq = m \int_{0}^{\tau} \dot{q}^{2} dt = m \omega^{2} A^{2} \int_{0}^{\tau} \cos^{2} \omega t dt$$
$$= \frac{1}{2} m \omega^{2} A^{2} \tau = \pi \omega m A^{2}$$
(24)

Using Equation (5), the average energy for this case may be written as:

$$\overline{E} = \frac{1}{2\tau} \int_{0}^{\tau} (m\dot{q}^{2} + kq^{2}) dt = \frac{A^{2}}{4} (m\omega^{2} + k)$$
$$= \frac{W}{4\pi m} (m\omega + \frac{k}{\omega})$$
(25)

Where we have used relation (24).

Now applying RMP and treating  $\boldsymbol{\varpi}$  as a variational parameter in relation

$$\left(\frac{\partial \overline{E}}{\partial \omega}\right)_{W} = 0$$

we get

$$m - \frac{k}{\omega^2} = 0$$
  
or  
$$\omega = \sqrt{\frac{k}{m}} = \omega_0$$

which leads to the following well known relation for the period of linear oscillator

$$\tau = 2\pi \sqrt{\frac{m}{k}} \tag{26}$$

which reduces to the standard relation for the time period of simple pendulum on using relation (22).

#### Anharmonic oscillator

Let us consider the following Hamiltonian for a one dimensional anharmonic oscillator (Rajput, 2005c)

$$H = \frac{1}{2}m\dot{q}^{2} + \frac{1}{2}kq^{2} + \mu q^{3} + \lambda q^{4}$$
<sup>(27)</sup>

For 
$$q = l\theta, k = \frac{mg}{l} = m\omega_0^2, \mu = 0, and\lambda = -\frac{k}{24l^2}$$
, it

reduces to the Hamiltonian of a plane pendulum in quadratic approximation of cosine.

We choose the same trial trajectory as given by Equation (23) and then we have:

$$W = \int_{0}^{\tau} p dq = \pi \omega m A^{2}$$
and
(28)

$$\overline{E} = \frac{1}{\tau} \int_{0}^{\tau} H dt$$

$$= \frac{W}{4\pi m} (m\omega + \frac{k}{\omega}) + \frac{\mu A^{3}}{\tau} \int (\sin\omega t)^{3} dt + \frac{\lambda A^{4}}{\tau} \int (\sin\omega t)^{4} dt$$

$$= \frac{W}{4\pi m} (m\omega + \frac{k}{\omega} + \frac{3\lambda W}{2\pi m\omega^{2}})$$
(29)

Then RMP (6) gives:

$$\omega^2 = \omega_0^2 + \frac{3\lambda A^2}{m}$$
(30)

Where  $\omega^2 = \frac{k}{m}$ . For  $\lambda = 0$ , we get the frequency of simple

pendulum that is,  $\boldsymbol{\varTheta} = \boldsymbol{\varOmega}_0$ . For plane pendulum with

$$q = l\theta, \lambda = -\frac{m\omega_0^2}{24l^2}, and\theta_{\max} = \frac{A}{l} = B,$$

we get

$$\omega = \omega_0 \left(1 - \frac{B^2}{8}\right)^{-\frac{1}{2}}$$
(31)

with the period given by:

$$\tau = \frac{2\pi}{\omega} = \tau_0 \left(1 - \frac{B^2}{8}\right)^{-\frac{1}{2}}$$
where
(32)

where

$$\tau_0=\frac{2\pi}{\omega_0}.$$

This relation gives

$$\tau = \tau_0 \left( 1 + \frac{B^2}{16} + \frac{3B^4}{512} + \dots \right)$$
(33)

which is correct to the order of  $B^2$ . For better accuracy we can take a more elaborate trial trajectory with more parameters.

#### A Chaotic system

Chaotic systems that is, non-integral systems have their own difficulties in finding their solutions. To demonstrate the applicability of the method of RMP to such systems, let us consider the case of 2D-guadratic oscillator with the Hamiltonian given by Dahlguist and Russberg (1990)

$$H = \frac{m}{2}(\dot{q}_1^2 + \dot{q}_2^2) + cq_1^2 q_2^2$$
(34)

where c is a constant. Let us choose the following quasi periodic anisotropic harmonic trajectory so that the semi-classical quantization via Einstein-Brillouin-Keller (EBK) rule (Percival, 1974) becomes simple;

$$q_1 = A_1 \cos \omega_1 t,$$
  

$$q_2 = A_2 \cos \omega_2 t$$
(35)

where, in general,  $\omega_1 and \omega_2$  are not equal.

Over a long period au the action becomes

$$W = \int_{0}^{\tau} m(q_{1}^{2} + q_{2}^{2}) dt = m(A_{1}^{2}\omega_{1}^{2} + A_{2}^{2}\omega_{2}^{2})\frac{\tau}{2}$$
$$= \frac{\tau}{2\pi}(\omega_{1}W_{1} + \omega_{2}W_{2})$$
(36)

Where:

$$W_1 = m \pi \omega_1 A_1^2$$
  
and  
$$W_2 = m \pi \omega_2 A_2^2$$

are the one cycle actions for  $q_1 and q_2$  motions respectively. The average energy for this case is

$$\overline{E} = \frac{1}{\tau} \int_{0}^{\tau} H dt = \frac{m}{4} (\omega_{1}^{2} A_{1}^{2} + \omega_{2}^{2} A_{2}^{2}) + \frac{c}{\tau} \int A_{1}^{2} A_{2}^{2} (\cos \omega_{1} t)^{2} (\cos \omega_{2} t)^{2} dt$$

$$= \frac{m}{4} (\omega_{1}^{2} A_{1}^{2} + \omega_{2}^{2} A_{2}^{2}) + \frac{c}{4} A_{1}^{2} A_{2}^{2}$$

$$= \frac{1}{4\pi} (\omega_{1} W_{1} + \omega_{2} W_{2} + \frac{c W_{1}^{2} W_{2}^{2}}{\pi m^{2} \omega_{1} \omega_{2}}$$
(37)

For simple trajectory like that given by Equation (35), the mean sub actions are

$$\overline{W_1} = W_1, \overline{W_2} = W_2$$

and for this trajectory, extremizing  $\overline{E}$  at fix W is equivalent to extremizing it at fixed  $\overline{W_1}, and \overline{W_2}$  treating  $\omega_1, and \omega_2$  as variational parameters. Thus applying RMP on  $\overline{E}$  given by Equation (37), we have:

$$\left(\frac{\partial \overline{E}}{\partial \omega_{1}}\right)_{W_{1},W_{2}}=0, and \left(\frac{\partial \overline{E}}{\partial \omega_{2}}\right)_{W_{1},W_{2}}=0$$

which gives

$$W_{1} - \frac{cW_{1}W_{2}}{\pi m^{2}\omega_{1}^{2}\omega_{2}} = 0,$$

$$W_{2} - \frac{cW_{1}W_{2}}{\pi m^{2}\omega_{1}\omega_{2}^{2}} = 0$$
(38)

These equations give

$$\omega_{1}^{2} \omega_{2} = \frac{cW_{2}}{\pi m^{2}}$$
and
$$\omega_{2}^{2} \omega_{1} = \frac{cW_{1}}{\pi m^{2}}$$
or
$$\frac{\omega_{2}}{\omega_{1}} = \frac{W_{1}}{W_{2}}$$
(39)

Substituting these relations in to Equation (38), we get the following relations for parameters  $\mathcal{O}_1$  and  $\mathcal{O}_2$  of the periodic harmonic

trajectory given by Equation (35);

$$\omega_1^3 = \frac{cW_2^2}{\pi m^2 W_1}$$

(40)

and

$$\omega_2^3 = \frac{cW_1^2}{\pi m^2 W_2}$$

Substituting these values in to Equation (37), we get

$$\overline{E} = \frac{3}{4\pi} \left(\frac{c}{\pi n^2}\right)^{\frac{1}{3}} \left(W_1 W_2\right)^{\frac{2}{3}}$$
(41)

which is the same result (with different numerical coefficients) as derived by Martens et al. (1989) by using the adiabatic approximation.

In order to get the semi classically quantized average energy from Equation (41) obtained on applying RMP on a chaotic system, let us substitute

$$W_1 = (n_1 + \frac{1}{2})h$$
and
(42)

 $W_2 = (n_2 + \frac{1}{2})h$ 

into Equation (41). Thus we get

$$\overline{E} = E_{n_1, n_2} = \frac{3}{4\pi} \left(\frac{ch^4}{\pi n^2}\right)^{\frac{1}{3}} \left(n_1 + \frac{1}{2}\right)^{\frac{2}{3}} \left(n_2 + \frac{1}{2}\right)^{\frac{2}{3}}$$
(43)

which is the same result as obtained by Gray et al. (1996). This result when compared with exact results obtained by the method of numerical calculation (Gray et al., 1996) shows the exciting accuracy for the lowest fifty levels. Thus the method of RMP can be applied to get almost accurate results even for the non-integrable (chaotic) systems. Other variable principles, known in classical mechanics, do not have this capability. This principle (RMP) for special cases for periodic and quassi-periodic motions is equivalent to Percival' principle of invariant tori (Percival, 1977).

## DISCUSSION

The variational principles MP, RMP and UMP given by Equations (4), (6) and (7) respectively, have been derived classically in the form of Equations (15) and (7) using  $\delta$  -variation and also quantum mechanically for one dimensional periodic motion as the as the classical limit of quantum mechanical principle (16). It may also be demonstrated (Percival, 1977), that such transformation is valid for quasi-periodic motion also. These new principles are the concise statements of laws of classical

mechanics. For instance, the energy conservation is the consequence of MP given by Equation (4). The RMP given by Equation (6) is also very useful principle of classical mechanics. Gray et al. (1996) have established the link of MP and RMP with Hamilton variational principle HP and its reciprocal RHP and also demonstrated that for guasi-periodic motion the RMP is equivalent to Percival's principle for invariant tori (Percival, 1977). Equation (26) shows that the variational principle RMP, when applied to the linear harmonic oscillator with the Hamiltonian given by Equation (21), gives the well known period which gives the standard relations (32). The RMP when applied to anharmonic oscillator with the Hamiltonian given by Equation (27), leads to the expression for angular frequency in the form of Equation (30). This relation leads to Equation (33) for the time period of plane pendulum in quadratic approximation of cosine. This result when compared with that computed directly through an elliptical integral is correct to the order of  $B^2$ . This accuracy order  $O(B^2)$ is expected with the trajectory Equation (23). For the better accuracy one can take a more elaborate trial trajectory with more parameters but then this method will become complicated mathematically.

Relation (41), obtained for the average energy on applying the variational RMP on a chaotic system like anisotropic 2D guartic oscillator with the Hamiltonian given by Equation (34), is similar, with slightly different numerical coefficient, to that obtained by Martens et al. (1989), by using the adiabatic approximation. The classically quantized energy, given by Equation (43) for this chaotic system, is exactly similar to that obtained by Gray et al. (1996). This result when compared with exact results obtained by the method of numerical calculations (Marten et al., 1989), shows the exciting accuracy for the lowest fifty levels. Thus the method of RMP can be applied to get the approximate results even for nonintegrable systems (that is, chaotic systems). Applying this method of variational RMP on the central force problem with inverse square potential, it may be demonstrated (Singh, 2008), that for the force constant of the potential  $C \ge Eb^2$ , where b is the impact parameter and E is the incident energy, there is no scattering under this attractive potential and the path becomes an equiangular spiral. Thus the method of variational RMP is a powerful classical method for solving the problems of linear, non-linear and chaotic oscillators. Recently, homotopy perturbation method and some nonperturbative methods have been developed (Ozis and Yildirim, 2007a, b, c, d; Yildirim and Momani, 2010) for linear as well as non-linear oscillators.

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