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THE SUFFICIENT CONDITION FOR AN EXTREMUM

IN THE CLASSICAL ACTION INTEGRAL AS AN EIGENVALUE PROBLEM†

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ABSTRACT

The sufficient condition for an extremum in the classical action integral is studied using Morse's theory. Applications to the classical harmonic and anharmonic oscillators are made. The analogy of the calculations to the quantum mechanical problems in one dimension is stressed.

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I. Introduction

Although the development of classical dynamics requires basically the necessary condition of extremum of the classical action integral,[1] the extention to quantum dynamics in its semiclassical approximate form requires a detailed knowledge of the consequences of the sufficient conditions[2] for obtaining such an extremum. Morse[3] has developed powerful methods for dealing with this problem. By considering the infinitesimal variations of the classical path that minimizes (or maximizes) the action integral to span a linear finite-dimensional Hilbert space, Morse transformed the sufficient condition problem into a boundary value problem. The resemblance to quantum mechanics becomes quite apparent when one discusses specific problems. We found the application of Morse's theory to the usual and familiar problems encountered in advanced undergraduate classical mechanics courses quite useful and intriguing calculations. On the other hand, the assumed familiarity of undergraduates taking such courses with intermediate quantum mechanics makes such calculations within their grasp. In this paper we shall discuss the sufficient condition for an extremum in the classical action integral using simple boundary value problem language. The usual discussion of the sufficient condition using geometrical consideration can be found in Ref. 4.

In Section II we give a brief introduction to Morse's theory and discuss the general case of systems with n-degree of freedom. In Section III we apply the method to the harmonic oscillator as well as to the symmetric and asymmetric anharmonic oscillator, and show the analogy to one-dimensional quantum mechanical problems. In Section IV we present the results of numerical calculations for the three systems considered. Finally, in Section V we present some discussions of our work and end the section with several conclusions.

II. Sufficient and Necessary Conditions for Extremum in the Classical Action Integral (Hamilton Function)

The starting point of analytical mechanics is Hamilton's principal expressed by

$$\delta\, I(t_1,t_2) = 0$$

where (1)

$$I(t_1,t_2) = \int_{t_1}^{t_2} dt\, \mathcal{L}(q(t),\dot{q}(t),t)$$

and $\mathcal{L}$ is the Lagrangian function pertaining to a general classical system with n degrees of freedom. We shall assume no constraints so that the generalized coordinates $\{q(t)\} = q_1,q_2 \ldots q_n$ are linearly independent. We consider conservative systems only.

The symbol δ stands for the variation of the classical path $\{q_{cl}(t)\}$ which leaves the endpoints unchanged. The resultant equation for $\{q_{cl}(t)\}$ are the Lagrange equations of motion. The above condition on I constitutes a necessary condition for extremum. In order to investigate the sufficient condition, one has to investigate the second variation of I

$$\delta^2\, I \gtreqless 0 \tag{2}$$

where the first inequality stands for a minimum, the second for a maximum, and the equality sign stands for an inflection point in $I(t_1,t_2)$.

Realizing the variation δ by considering the change $q_i \to q_i(t) + \eta_i(t)$ one can write Eq. (2) as follows

$$\delta^2 I = \sum_{ij} \int_{t_1}^{t_2} \left[\left(\frac{\partial^2}{\partial q_i \partial q_j}\right)_{\{q_{cl}\}} \eta_i \eta_j + 2\left(\frac{\partial^2}{\partial q_i \partial \dot{q}_j}\right)_{\{q_{cl}\}} \eta_i \dot{\eta}_j + \left(\frac{\partial^2}{\partial \dot{q}_i \partial \dot{q}_j}\right)_{\{q_{cl}\}} \dot{\eta}_i \dot{\eta}_j \right] dt \tag{3}$$

$$\equiv \frac{1}{2} \int_{t_1}^{t_2} \mathcal{L}^{(2)} \, dt \gtrless 0$$

with $\eta_i(t_1) = \eta_i(t_2) = 0$. In Eq. (3) the quantities in round brackets are evaluated at $q_i = q_{cl_i}$ which solves Lagrange's equation of motion.

The quantity $\mathcal{L}^{(2)}$ which is defined in Eq. (3) is called the secondary Lagrangian. By performing partial integration of the second and third term in Eq. (3) we cast Eq. (3) in the following form:

$$\delta^2 I = \sum_{ij} \int_{t_1}^{t_2} \eta_i(t) \, \Lambda_{ij} \, \eta_j(t) \, dt$$

where (4)

$$\Lambda_{ij} = -\frac{d}{dt}\left(P_{ij} \frac{d}{dt} + Q_{ij}\right) + \left(Q_{ij} \frac{d}{dt} + R_{ij}\right)$$

and

$$P_{ij} \equiv \left(\frac{\partial^2}{\partial \dot{q}_i \partial \dot{q}_j}\right)_{\{q_{cl}\}}$$

$$Q_{ij} = \left(\frac{\partial^2}{\partial q_i \partial \dot{q}_j}\right)_{\{q_{cl}\}}$$

$$R_{ij} = \left(\frac{\partial^2}{\partial q_i \partial q_j}\right)_{\{q_{cl}\}} .$$

The form of $\delta^2 I$ in Eq. (4) is quite convenient as one is expressing $\delta^2 I$ as a sum of matrix element involving the vectors $\{\eta_i\}$ and the operator Λ.

Defining a scalar product

$$(\eta_i, \eta_j) = \int_{t_1}^{t_2} dt\ \eta_i(t)\ \eta_j(t)\ , \tag{5}$$

we are then dealing with variations $\{\eta_i\}$ that span an n-dimentional linear vector (Hilbert) space.

We seek to diagonalize the operator Λ. This is done easily by expanding η in an orthonormal basis in the Hilbert space

$$\eta(t) = \sum_n a^n\ u^n(t)$$

with

$$\int_{t_1}^{t_2} u^n(t) u^{n'}(t) dt = \delta_{nn'} . \tag{6}$$

Then

$$\delta^2 I = \sum_{n,n'} A_{nn'}\ a^n a^{n'}$$

$$A_{nn'} = (u^n,\ \Lambda u^{n'}) \tag{7}$$

$$= \sum_{ij} \int_{t_1}^{t_2} u_i^n(t)\ \Lambda_{ij}\ u_j^{n'}\ dt\ .$$

A basis $\{u^n(t)\}$ which diagonalizes $\{A_{nn'}\}$ is given by the solution of Morse's boundary value problem[3)]

$$\Lambda_{ij}\ u_j^n = \lambda_n\ u_i^n \tag{8}$$

with $u_i(t_1) = u_i(t_2) = 0$, $(i = 1, \ldots n)$ then

$$\delta^2 I = \sum_n \lambda_n (a^n)^2 \ . \tag{9}$$

It is clear that $\{\lambda_n\}$ are all real since Λ is a self-conjugate ($\Lambda = \Lambda^+$) operator[3]. Equation (9) is an important result as it shows that the conditions in Eq. (2) can be recast into conditions on the eigenvalues $\{\lambda_n\}$. In the case that all $\{\lambda_n\} > 0$, one would have an absolute minimum in the action.

It is interesting to note that in cases where P_{ij} is independent of time and $Q_{ij} = 0$, Eq. (8) can be written as

$$\begin{gathered}[-P_{ij} \frac{d^2}{dt^2} + R_{ij}(t)]\ u_j^n(t) = \lambda_n u_i^n(t) \\ u(t_1) = u(t_2) = 0\end{gathered} \tag{10}$$

For systems with one degree of freedom Eq. (10) is analogous to the one-dimensional quantum mechanical problem of a particle of "mass" $m = \frac{\hbar^2}{2P}$ confined in the "space" $t_1 - t_2$ by two infinite barriers at "distances" t_1 and t_2 and subject to a potential $R(t)$. The time t plays the role of distance. The "quantized energy" of the particle is given by λ_n.

III. The Harmonic and Anharmonic Oscillator in One Dimension

In the case of the one-dimensional harmonic oscillator whose Lagrangian is given by

$$\mathcal{L} = \frac{1}{2} m\dot{q}^2 - \frac{1}{2} kq^2 \tag{11}$$

where m is the mass and k is the strength constants respectively, Eq. (10) takes the simple form

$$\left[\frac{-d^2}{dt^2} - \omega_o^2 \right] u^n(t) = \frac{\lambda_n}{m} \; u^n(t) \tag{12}$$

$$u^n(t_1) = u^n(t_2) = 0$$

$$\omega_o^2 = \frac{k}{m} \quad .$$

Thus the "potential" $R(t) = -\omega_o^2 m$ is attractive and constant. The solution of Eq. (12) is well-known and can be found in most quantum mechanics text books. Taking $t_1 = 0$, we have

$$\frac{\lambda_n}{m} = \left(\frac{n\ \pi}{t_2}\right)^2 - \omega_o^2 \ , \tag{13}$$

$$n = 1,\ 2,\ \ldots$$

The solutions $u^n(t)$ take the form:

$$u^n(t) = \sqrt{\frac{2}{t_2}} \ \sin(\frac{n\pi}{t_2})t \ . \tag{14}$$

It is clear from Eqs. (9) and (13) that the action integral for the simple harmonic oscillator is minimum for time intervals t_2 that satisfy the inequality:

$$t_2 < \frac{T}{2} \tag{15}$$

where T is the period $T = \dfrac{2\pi}{\omega_o}$.

For t_2 larger than $\frac{T}{2}$ there would be several eigenvalues λ_n whose contribution to $\delta^2 I$ is negative. The number, ν, of such negative eigenvalues is called the index of the classical path $q_{cl}(t)$.[2)] For a given value of t_2, ν is given by

$$\nu = \frac{\omega_o t_2}{\pi} \quad . \tag{16}$$

Considering now the case of the anharmonic oscillator whose Lagrangian we write as:

$$= \frac{1}{2} m\dot{q}^2 - \frac{1}{2} kq^2 + \frac{\alpha m}{s} q^s \tag{17}$$

where $s > 2$ and α could be positive or negative.

In this case Eq. (10) becomes

$$\left\{- \frac{d^2}{dt^2} - \left[\omega_o^2 - \alpha(s-1)\ q_{cl}^{s-2}(t)\right]\right\} u^n(t) = \lambda_n\ u^n(t) \tag{18}$$

with

$$u^n(t_1=0) = 0 = u^n(t_2) \quad .$$

One sees that now the "potential" $R(t) = -\omega_o^2 m + \alpha m(s-1)q^{s-2}\ (t)$ is an explicit function of time and has to be constructed from the knowledge of the solution, $q_{cl}(t)$, of the equation of motion:

$$\left(\frac{d^2}{dt^2} + \omega_o^2\right) q_{cl}(t) = \alpha\ q_{cl}^{s-1}(t) \tag{19}$$

with the appropriate initial conditions, e.g.,

$$q_{cl}(0) = A \quad , \quad \dot{q}_{cl}(0) = 0 \quad .$$

It is important to note that in the case of the anharmonic oscillator the eigenvalues $\dot{\lambda}_n$ depend on the initial conditions. This fact is to be contrasted with our results for the harmonic oscillator Eq. (13). Short of obtaining an exact analytical solution for $q_{cl}(t)$ and thus for $R(t)$ in the case of the anharmonic oscillator, we resort to perturbation treatment. We follow the renormalization techniques described by Marion[5] through which one can get rid of unwanted nonperiodic terms in the solution. We find for the renormalized frequency of the AHO to second order in α:

$$\omega_o^2 \to \omega^2 \cong \omega_o^2 - \alpha \frac{A^{s-2}}{2^{s-2}} \frac{(s-1)!}{(\frac{s}{2}-1)!(\frac{s}{2})!}$$

$$+ \alpha^2 \frac{2A^{2s-4}}{2^{2s-4}\omega^2} \left[\sum_{f=3}^{s-3} \frac{[(s-1)!]^2}{(\frac{s-1-f}{2})!(\frac{s-1+f}{2})!} \left(\frac{s-3}{s+f-3}\right) \right.$$

$$\times \frac{1}{(\frac{s-2-f+1}{2})!(\frac{s-2+f-1}{2})!} \frac{1}{f^2-1} \tag{20}$$

$$\left. + \frac{s-1}{[(s-1)^2-1]} \right], \qquad s = \text{even}$$

$$\omega_o^2 \to \omega^2 \cong \omega_o^2 - \alpha^2 \frac{(s-1)A^{2s-4}}{2^{2s-4}\omega^2} \left[\frac{(s-1)!}{(\frac{s-1}{2})!(\frac{s-1}{2})!} \frac{(s-2)!}{(\frac{s-3}{2})!(\frac{s-1}{2})!} - \frac{1}{(s-1)^2-1} \right.$$

$$- \sum_{f=2}^{s-3} \frac{(s-1)!}{(\frac{s-1-f}{2})!(\frac{s-1+f}{2})} \left(\frac{s-3}{s=3+f}\right)$$

$$\left. \times \frac{(s-2)!}{(\frac{s-f-3}{2})!(\frac{s-f-1}{2})!} \frac{2}{(f^2-1)} \right], \qquad s = \text{odd}$$

It is easy to show that with the above renormalized frequencies the resulting solution of the AHO is a sum of periodic terms. To first order in α we obtain:

$$q(t) = A\cos\omega t - \alpha \sum_{f=3}^{s-1} a_f \cos f\omega t \quad , \qquad s = \text{even}$$

$$q(t) = A\cos\omega t + \alpha \frac{A^{s-1}}{2^{s-1}\omega^2} \frac{(s-1)!}{(\frac{s-1}{2})!\,(\frac{s-1}{2})!} \tag{21}$$

$$- \alpha \sum_{f=2}^{s-1} a_f \cos f\omega t \quad , \qquad s = \text{odd}$$

where the coefficient a_f is given by

$$a_f = \frac{A^{s-1}}{2^{s-2}} \frac{1}{\omega^2(f^2-1)} \frac{(s-1)!}{(\frac{s-1-f}{2})(\frac{s-1+f}{2})!}$$

Given the above solution one may then construct the potential R(t) to the desired order. To second order in α we obtain:

$$R(t) = -k + m\alpha(s-1)A^{s-2}(\cos\omega t)^{s-2}$$

$$- m\alpha^2(s-1)(s-2)\, A^{s-3}(\cos\omega t)^{s-3} \sum_{f=3}^{s-1} a_f \cos f\omega t \; ; \qquad s = \text{even}$$

$$R(t) = -k + m\alpha(s-1)\, A^{s-2}(\cos\omega t)^{s-2} \tag{22}$$

$$+m\alpha^2(s-1)(s-2) \frac{A^{2s-4}}{2^{s-1}\omega^2} (\cos\omega t)^{s-3} \frac{(s-1)!}{[(\frac{s-1}{2})!]^2}$$

$$-m\alpha^2(s-1)(s-2)A^{s-3}(\cos\omega t)^{s-3} \sum_{f=2}^{s-1} a_f \cos f\omega t \quad ; \qquad s = \text{odd}$$

It should be clear that since the frequency ω which appears in $R(t)$ is the renormalized frequency the above expression implicitly contains terms higher than second order in α. The dependence of $R(t)$ on the initial conditions, i.e., $A \equiv q_o$ is quite apparent in Eq. (22).

In obtaining an approximate solution, $u^n(t)$, of Eq. (18), we use the usual non-degenerate perturbation theory. Expanding $u^n(t)$ in terms of the HO solutions of Eq. (14) and grouping terms of different orders in α, we obtain to second order in α for λ_n:

$$u^n(t) = u^n_{HO}(t) + \alpha(s-1) \sum_{m\neq n} \frac{(u^n_{HO}, q^{s-2}_{HO}\ u^m_{HO})}{\frac{\lambda^{HO}_n}{m} - \frac{\lambda^{HO}_m}{m}} u^m_{HO}(t) + 0(\alpha^2) \quad ;$$

$$\lambda_n = \lambda^{HO}_n + \alpha(s-1)(u^n_{HO}, q^{s-2}_{cl}(t)\ u^n_{HO}) + \tag{23}$$

$$+ \alpha^2(s-1)^2 \sum_{m\neq n} \frac{(u^n_{HO}, q^{s-2}_{HO}\ u^m_{HO})(u^m_{HO}, q^{s-2}_{HO}\ u^n_{HO})}{\lambda^{HO}_n - \lambda^{HO}_m}$$

$$+ \alpha^2(s-1)(s-2)\ (u^n_{HO}, q^{s-3}_{HO}\ u^n_{HO}) + 0(\alpha^3) \quad ,$$

where $q_{HO}(t)$ is the classical solution of the simple harmonic oscillator's equation of motion.

Equations (23) are the ones that we shall use to obtain numerical results for the asymmetrical ($s = 3$) and symmetrical ($s = 4$) anharmonic oscillators.

In the following we consider anharmonic oscillators whose deviations from the harmonic oscillator are given by $\frac{\alpha m}{3} q^3$ and $\frac{\beta m}{4} q^4$ respectively. Moreover, we assume for the strength α and β the following form:

$$\alpha = \frac{3\omega_o^2}{cq_o}$$

$$\beta = \frac{4\omega_o^2}{c' q_o^2} \tag{24}$$

with c and c' varied to strengthen or weaken the anharmonic terms.

In Fig. 1 we present the numerical results of our work based on the perturbative result Eq. (23). The number of terms included in the α^2 term of Eq. (23) is 4. As can be seen, with the values $c = \frac{15}{m}$ and $c' = \frac{20}{m}$ taken as representing small perturbation and taking $t_2 = 0.5\ T_H o \equiv \frac{\pi}{\omega_o}$, the quantity $\frac{\lambda_n}{m\omega_o^2}$, which represents the spectrum of the "Hamiltonian"-like operator $-\frac{d^2}{dt^2} + R(t)$ becomes negative at n=1 only in the case of the symmetrical anharmonic oscillator. It should be clear, however, that for larger value of anharmonic terms (in which case a more exact diagonalization procedure is required to get λ_n) the λ_n of the asymmetrical anharmonic oscillator would also become negative at some permissible integer n. Moreover, changing the value of the time interval, t_2, would also change the result. As we have seen from Eq. (13) the λ_n of the harmonic oscillator becomes negative at several n's in the case $t_2 > T/2$. Finally, since the initial conditions do become relevant in determining λ_n for the anharmonic oscillator, it is obvious that our results would be altered through changes in the initial velocity and/or initial position of the system.

IV. Discussions and Conclusions

We have shown in this paper how a simple and interesting way to discuss the sufficient condition of extremum in the classical action integral can be developed using Morse's theory. The analogy with one-dimensional quantum mechanical problems becomes quite apparent for the several cases worked out here. This then leads to methods of calculation which are quite familiar and easy to use. In the case of the one-dimensional harmonic and anharmonic oscillators we have seen that the initial conditions are relevant only to the latter case, and these initial values of q and $\dot{q}$ do have a role in determining the part of the spectrum, λ_n, which gives a negative contribution to $\delta^2 I$. This is an interesting point insofar as determining the index of the classical trajectory, ν, is concerned.

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FIGURE CAPTIONS

Fig. 1 The spectrum of the Hamiltonian-like operator $-\frac{d^2}{dt^2} + R(t)$ for the three cases indicated. The details of the calculation are given in the text.

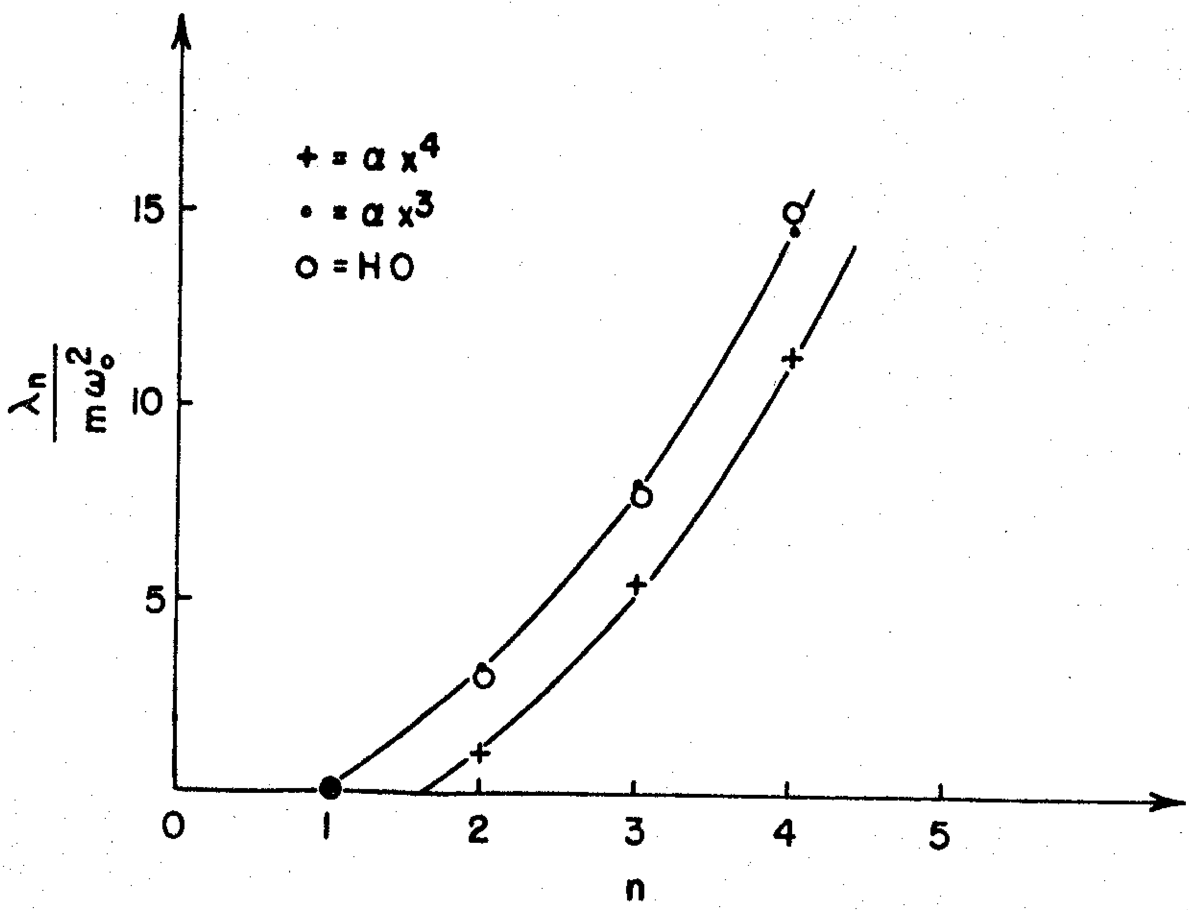

Figure 1