

# PRINCIPLE OF LEAST ACTION: DOES PHYSICAL MOTION GIVE THE *LEAST* ACTION? AN EXAMPLE: THE SIMPLE HARMONIC OSCILLATOR

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## I. AN OVERVIEW OF THE ANSWER

We study the simple harmonic oscillator, since we can solve the problem exactly. Let us consider a one-dimensional oscillator with angular frequency  $\omega > 0$ . The Lagrangian is

$$(1) \quad \mathcal{L} = \frac{1}{2}m\dot{q}^2 - \frac{1}{2}m\omega^2 q^2 .$$

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We study motion on the time interval  $[T_1, T_2]$  and fix the values of  $q(t)$  at the two endpoints: the time interval is  $T = T_2 - T_1$ , and we require  $q(T_1) = Q_1$  and  $q(T_2) = Q_2$ . Let us denote  $Q(t)$  to be the solution to Lagrange's equations for the oscillator with these end-point conditions.

**I.1. A Partial Answer.** Does the physical orbit  $Q(t)$  minimize the action  $S_{[T_1, T_2]}(q)$  for the simple harmonic oscillator? We first show

$$(2) \quad S_{[T_1, T_2]}(q) = S_{[T_1, T_2]}(Q) + S_{[T_1, T_2]}(\eta) .$$

Then we find a particular  $\eta(t)$  such that for  $T > \pi/\omega$ , one has  $S(\eta) < 0$ . This shows that the action  $S_{[T_1, T_2]}(q)$  for the simple harmonic oscillator is not minimized by  $S_{[T_1, T_2]}(Q)$  for large time intervals  $T$ . In fact we give an example where the principle of least action breaks down for  $T > \pi/\omega$ .

**I.2. A Complete Answer.** We show in these notes that for the oscillator, the answer to question “is the principle of least action correct?” is: The solution  $Q(t)$  minimizes the action  $S_{[T_1, T_2]}(q)$  for the simple harmonic oscillator, if and only if the magnitude  $T$  of the time interval satisfies

$$(3) \quad T \leq \frac{\pi}{\omega} .$$

For the oscillator we can find an exact formula for  $S(\eta)$  for arbitrary  $\eta$ , in terms of an eigenvalue problem. In §IV we relate this to determining the eigenvalues of a linear, self-adjoint transformation  $T = -\frac{d^2}{dt^2}$  on the interval  $[T_1, T_2]$ . This transformation  $T$  is not a matrix, but a linear, self-adjoint differential operator. It acts on the Hilbert space  $L^2([T_1, T_2], dt)$  of square-integrable functions on the interval. Nevertheless, this eigenvalue problem is similar to the eigenvalue problem for a hermitian matrix. In other words, the eigenfunctions  $e_j(t)$  of  $T$  that satisfy

$$(4) \quad T e_j(t) = \lambda_j e_j(t) , \text{ with } \eta_j(T_1) = \eta_j(T_2) = 0 ,$$

are a basis for the space  $L^2([T_1, T_2], dt)$ . Thus one can expand any  $\eta$  as a sum of normalized eigenfunctions  $\eta(t) = \sum_j c_j e_j(t)$ .

For this oscillator problem, one can calculate  $e_j(t)$  and the eigenvalues  $\lambda_j$  in closed form. Then one can show that the action satisfies

$$(5) \quad \begin{aligned} S_{[T_1, T_2]}(q) &= S_{[T_1, T_2]}(Q) + S_{[T_1, T_2]}(\eta) \\ &= S_{[T_1, T_2]}(Q) + \frac{m}{2} \sum_{j=1}^{\infty} c_j^2 \left( \left( \frac{j\pi}{T} \right)^2 - \omega^2 \right) , \end{aligned}$$

where  $c_j = \int_{T_1}^{T_2} e_j(t) \eta(t) dt$ . In other words,

$$(6) \quad S_{[T_1, T_2]}(\eta) = \frac{m}{2} \sum_{j=1}^{\infty} c_j^2 \left( \left( \frac{j\pi}{T} \right)^2 - \omega^2 \right) .$$

Thus we have a formula for the value of  $S_{[T_1, T_2]}(\eta)$  that depends only on our choice the coefficients  $c_j$ , which are up to us to choose. Each  $c_j^2$  is multiplied by a corresponding eigenvalue of  $-\frac{d^2}{dt^2} - \omega^2$  and by  $\frac{m}{2}$ . The smallest eigenvalue  $\lambda_1$  is negative in case  $T > \pi/\omega$ . If we choose  $c_1 = 1$  and all the other  $c_j = 0$  for  $j > 1$ , then (5) shows that  $S_{[T_1, T_2]}(\eta) = \frac{m}{2} \left( \frac{\pi^2}{T^2} - \omega^2 \right)$  is negative for the small  $T > \pi/\omega$  as claimed above. Any other  $\eta$  will have a larger contribution to  $S_{[T_1, T_2]}(q)$ , so this is the answer for the minimum! If  $T \leq \pi/\omega$ , then  $S_{[T_1, T_2]}(\eta) \geq 0$ . We now show that these claims are true!

## II. DETAILS OF THE SIMPLE HARMONIC OSCILLATOR

**II.1. Review.** Given a Lagrangian  $\mathcal{L}(q, \dot{q}, t)$ , for one degree of freedom, the Lagrange equation of motion is

$$(7) \quad \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}} - \frac{\partial \mathcal{L}}{\partial q} = 0.$$

One often studies solutions to the initial-value problem for this equation; one specifies a position  $q(T_1) = Q_1$  and velocity  $\dot{q}(T_1) = \dot{Q}_1$  at a particular initial time  $T_1$ , and asks for the solution  $q(t)$  to the equations for a later time  $t > T_1$  that agrees with the initial position and velocity. On the other hand, in the derivation of Lagrange's equations by the variational principle we studied the action  $S_{[T_1, T_2]}(q)$ , defined for a particular time interval  $t \in [T_1, T_2]$  with  $T_1 < T_2$ . This action is

$$(8) \quad S_{[T_1, T_2]}(q) = \int_{T_1}^{T_2} \mathcal{L}(q(t), \dot{q}(t)) dt.$$

The action is a function of an arbitrary trajectory  $q(t)$  from time  $T_1$  to time  $T_2$ , whether or not that trajectory satisfies Lagrange's equations. In this case we have specified both the starting point of the trajectory  $q(T_1) = Q_1$  and the ending point of the trajectory  $q(T_2) = Q_2$ , rather than the initial velocity. In studying variation of the action, we did not require that the trajectory have a particular initial velocity, but rather we fix the starting and ending points of the trajectory. One could also consider the situation for Lagrange's equations where one specifies the endpoints of a trajectory, rather than initial conditions.

**Hamilton's principle** relates these two situations. It is the statement that any solution  $q(t)$  to the Lagrange equations (7) which starts at  $q(T_1) = Q_1$  and ends at  $q(T_2) = Q_2$ , is a stationary point of the action (8). And conversely, any trajectory  $q(t)$  starting from  $Q_1 = q(T_1)$  and ending at  $Q_2 = q(T_2)$  that is a stationary point of the action (8) is a solution to Lagrange's equations (7).

In more detail, a stationary point of the action  $S_{[T_1, T_2]}(q)$  is defined to be a trajectory  $q(t)$  for which the first directional derivative  $D_\eta S_{[T_1, T_2]}(q)$  vanishes for all variations  $\eta(t)$  of  $q(t)$  for which  $\eta(T_1) = \eta(T_2) = 0$ . One calls this variation with vanishing endpoints; in such a situation, the varied trajectory  $\tilde{q}(t) = q(t) + \eta(t)$  always starts at  $Q_1$  and ends at  $Q_2$ . We

defined the variational derivative in direction  $\eta$  at the trajectory  $q$  as

$$(9) \quad D_\eta S_{[T_1, T_2]}(q) = \lim_{\epsilon \rightarrow 0} \frac{S_{[T_1, T_2]}(q + \epsilon \eta) - S_{[T_1, T_2]}(q)}{\epsilon}$$

In some physics books, Hamilton's principle is called the *principle of least action*. This is meant to assert that a solution  $q(t)$  to Lagrange's equations minimizes the action  $S_{[T_1, T_2]}(q)$ . In these notes we investigate this statement for the simple harmonic oscillator.

**II.2. Oscillator Basics.** Consider a one-dimensional, simple harmonic oscillator with mass  $m$ , angular frequency  $\omega$ , and Lagrangian

$$(10) \quad \mathcal{L} = T - V = \frac{1}{2} m \dot{q}^2 - \frac{1}{2} m \omega^2 q^2 .$$

The action for a trajectory  $q(t)$  on the time interval  $t \in [T_1, T_2]$  is  $S_{[T_1, T_2]}(q) = \int_{T_1}^{T_2} \mathcal{L} dt$ , namely

$$(11) \quad S_{[T_1, T_2]}(q) = \frac{1}{2} m \int_{T_1}^{T_2} \dot{q}(t)^2 dt - \frac{1}{2} m \omega^2 \int_{T_1}^{T_2} q(t)^2 dt .$$

The Euler-Lagrange equation of motion is

$$(12) \quad \ddot{q}(t) = -\omega^2 q(t) .$$

We assume that the angular frequency  $\omega > 0$ .

**II.3. The Solution with Given Initial Conditions.** Here we denote a solution to the equation of motion by  $Q(t)$ . We use the upper-case  $Q(t)$ , in order to distinguish clearly a solution to Lagrange's equations from a general trajectory  $q(t)$  that may or may not solve the equation (12).

The initial conditions for position and velocity at one time, say  $T_1$ , uniquely determine the solution to (12). Let us assume that  $Q(T_1) = Q_1$  and  $\dot{Q}(T_1) = \dot{Q}_1$  at time  $t = T_1$ . The corresponding solution is

$$(13) \quad Q(t) = Q_1 \cos(\omega(t - T_1)) + \frac{\dot{Q}_1}{\omega} \sin(\omega(t - T_1)) .$$

In the zero-frequency limit, the solution does not oscillate; rather it becomes the free-particle motion,

$$(14) \quad Q(t) = Q_1 + (t - T_1)\dot{Q}_1 , \quad \text{in the limit } \omega = 0 .$$

One easily checks that (13) satisfies the equation of motion and the initial conditions. In fact there is only one such solution: for assume that there is a second one  $\tilde{Q}(t)$ . then  $R(t) = Q(t) - \tilde{Q}(t)$  also satisfies the equation of motion and has  $R(T_1) = \dot{R}(T_1) = 0$ . This means that

$$(15) \quad \frac{d^n R(t)}{dt^n} = -\omega^2 \frac{d^{n-2} R(t)}{dt^{n-2}} ,$$

for all  $n$ . So

$$(16) \quad \left. \frac{d^n R(t)}{dt^n} \right|_{t=T_1} = 0, \quad \text{for all } n.$$

One can show that the solution to the oscillator is analytic in time, so vanishing of all the time derivatives at a particular times ensures that  $R(t) \equiv 0$  for all  $t$ . Thus  $\tilde{Q}(t) = Q(t)$ .

subsection The Action of the Solution: We calculate the action  $S_{[T_1, T_2]}(Q)$  of the solution (13). Insert the formula for  $Q(t)$  into the expression for the action of the solution given initial data (13). Then,

$$\begin{aligned} \int_{T_1}^{T_2} \mathcal{L} dt &= \frac{1}{2} m \omega^2 \left( Q_1^2 - \frac{\dot{Q}_1^2}{\omega^2} \right) \int_{T_1}^{T_2} (\sin^2(\omega(t - T_1)) - \cos^2(\omega(t - T_1))) dt \\ &\quad - m \omega Q_1 \dot{Q}_1 \int_{T_1}^{T_2} \sin 2\omega(t - T_1) dt \\ &= \frac{1}{4} m \omega \left( \frac{\dot{Q}_1^2}{\omega^2} - Q_1^2 \right) \sin 2\omega(T_2 - T_1) + \frac{1}{2} m \dot{Q}_1 Q_1 (\cos 2\omega(T_2 - T_1) - 1). \end{aligned}$$

Thus (with  $T = T_2 - T_1$ ),

$$(17) \quad S_{[T_1, T_2]}(Q) = \frac{1}{4} m \omega \left( \frac{\dot{Q}_1^2}{\omega^2} - Q_1^2 \right) \sin 2\omega T + \frac{1}{2} m \dot{Q}_1 Q_1 (\cos 2\omega T - 1).$$

As a function of the size of the time interval  $T$ , the action oscillates in sign with period  $\frac{\pi}{\omega}$ . For small  $T$  the first term dominates; so the sign of the action depends on the sign of  $(\dot{Q}_1^2 - \omega^2 Q_1^2)$ .

**II.4. The Solution with Fixed Endpoints.** Let us convert the solution with given initial conditions to a solution with given endpoints. We choose initial and final points  $Q_1, Q_2$  and wish to require that  $Q(T_1) = Q_1$  and  $Q(T_2) = Q_2$ . Let us see what is possible for the actual solution (13).

So to begin, set  $Q(T_2) = Q_2$  in (13) and solve this relation for the initial velocity  $\dot{Q}_1$ ; then replace this function of  $Q_1$  and  $Q_2$  in (13). If

$$(18) \quad Q_2 = Q_1 \cos \omega T + \frac{\dot{Q}_1}{\omega} \sin \omega T,$$

then one can solve for  $\dot{Q}_1$ , only if  $\omega T \neq n\pi$  for integer  $n$ . Since  $T > 0$  and  $\omega > 0$ , we require that

$$(19) \quad \frac{\omega T}{\pi} \neq 1, 2, \dots$$

If (19) is the case, then

$$(20) \quad \frac{\dot{Q}_1}{\omega} = \frac{Q_2 - Q_1 \cos \omega T}{\sin \omega T},$$

and

$$(21) \quad Q(t) = Q_1 \cos(\omega(t - T_1)) + \frac{Q_2 - Q_1 \cos(\omega T)}{\sin(\omega T)} \sin(\omega(t - T_1)).$$

The forbidden values  $\omega T = \pi, 2\pi, \dots$  either are values for which the motion is *periodic* with period  $T$ , for then

$$(22) \quad Q(T_2) = Q(T_1), \text{ and } \dot{Q}(T_2) = \dot{Q}(T_1), \quad \text{the case when } n \text{ is even,}$$

or else values for which the motion is said to satisfy *anti-periodic boundary conditions*, namely

$$(23) \quad Q(T_2) = -Q(T_1), \text{ and } \dot{Q}(T_2) = -\dot{Q}(T_1), \quad \text{the case when } n \text{ is odd.}$$

In either case there is no way to determine the initial velocity  $\dot{Q}_1$  just from knowing  $Q_1$ .

Let us return to an elementary example to compute the action of the trajectory in terms of the endpoints. Let us suppose that we start the system at time  $T_1 = 0$  and position  $Q_1 = Q(T_1) = 0$ . Then the formula (20) reduces to

$$\frac{\dot{Q}_1}{\omega} = \frac{Q_2}{\sin \omega T_2},$$

and the expression (17) becomes

$$(24) \quad S_{[0, T_2]}(Q) = \frac{1}{4} m \omega \frac{Q_2^2}{\sin^2 \omega T_2} \sin 2\omega T_2 = \frac{m \omega}{2 \tan \omega T_2} Q_2^2.$$

**II.5. Perturbation of the Action for a Physical Orbit.** We observe that the perturbed action away from a physical orbit  $Q$  for action  $S_{[T_1, T_2]}(q)$  for the oscillator has a very special property. It is additive, because the action is quadratic in  $q$ . If  $Q(t)$  is a solution to the equation of motion, and if  $\eta(t)$  vanishes at the endpoints, then

$$(25) \quad \boxed{S_{[T_1, T_2]}(Q + \eta) = S_{[T_1, T_2]}(Q) + S_{[T_1, T_2]}(\eta)}.$$

**Warning:** this simple relation holds for the oscillator, but not for most actions!

To demonstrate the relation (25), note that  $S_{[T_1, T_2]}(Q + \epsilon \eta)$  has a power series in  $\epsilon$  that terminates at degree 2. And the second order term is just  $S_{[T_1, T_2]}(\eta)$ . Thus

$$\begin{aligned} S_{[T_1, T_2]}(Q + \epsilon \eta) &= S_{[T_1, T_2]}(Q) + \epsilon \left. \frac{d}{d\epsilon} S_{[T_1, T_2]}(Q + \epsilon \eta) \right|_{\epsilon=0} + S_{[T_1, T_2]}(\eta) \\ &= S_{[T_1, T_2]}(Q) - \langle \mathbb{L}(Q), \eta \rangle_{[T_1, T_2]} + S_{[T_1, T_2]}(\eta) \\ (26) \quad &= S_{[T_1, T_2]}(Q) + S_{[T_1, T_2]}(\eta). \end{aligned}$$

Here we use the fact that  $\langle \mathbb{L}(Q), \eta \rangle_{[T_1, T_2]} = 0$  characterizes the solution  $Q$  to Lagrange's equation. Thus (25) is valid for the expansion about the physical trajectory.

### III. DOES PHYSICAL MOTION MINIMIZE THE ACTION?

Let us suppose we consider Hamilton's principle for a simple harmonic oscillator with angular frequency  $\omega$ . We look for a critical point of the action  $S_{[T_1, T_2]}(q)$ , with fixed endpoints. In order to ensure that the endpoints (rather than initial conditions) determine the trajectory, we only consider time intervals that satisfy the condition (19). *It is interesting that we will discover that this same condition relates to whether physical motion minimizes the action.*

**III.1. An  $\eta$  for which  $S_{[T_1, T_2]}(\eta)$  is negative:** Once we know that  $S(q)$  has the property (25), we have a very simple test whether the physical trajectory  $Q$  yields the least action  $S_{[T_1, T_2]}(Q)$  for  $S(q)$ . We only need to determine whether or not it is the case that

$$(27) \quad 0 \leq S_{[T_1, T_2]}(\eta), \quad \text{whenever} \quad \eta(T_1) = \eta(T_2) = 0. \quad \textbf{Test for Least Action}$$

The explicit form for  $S_{[T_1, T_2]}(\eta)$  is

$$(28) \quad S_{[T_1, T_2]}(\eta) = \frac{m}{2} \left( \int_{T_1}^{T_2} \dot{\eta}(t)^2 dt - \omega^2 \int_{T_1}^{T_2} \eta(t)^2 dt \right), \quad \text{with } \eta(T_1) = \eta(T_2) = 0.$$

The first term in (28) is positive; the second term in (28) is negative. So the question is *which term wins?* In order to answer this question, we start by repeating the argument leading to (25). Write  $\dot{\eta}^2 = \frac{d}{dt}(\eta\dot{\eta}) - \eta\ddot{\eta}$ , and substitute this into the first term. The boundary term vanishes, and (28) becomes

$$(29) \quad S_{[T_1, T_2]}(\eta) = \frac{m}{2} \int_{T_1}^{T_2} \eta(t) \left( -\frac{d^2}{dt^2} - \omega^2 \right) \eta(t) dt, \quad \text{with } \eta(T_1) = \eta(T_2) = 0.$$

Let us choose for  $\eta(t)$  the expression

$$(30) \quad \eta(t) = \sin\left(\frac{\pi(t - T_1)}{T}\right), \quad \text{so} \quad -\frac{d^2}{dt^2} \eta(t) = \frac{\pi^2}{T^2} \eta(t).$$

Clearly  $\eta(T_1) = \eta(T_2) = 0$ . Putting this  $\eta(t)$  into (29) shows that,

$$(31) \quad S_{[T_1, T_2]}(\eta) = \frac{m}{2} \left( \frac{\pi^2}{T^2} - \omega^2 \right) \int_{T_1}^{T_2} \eta(t)^2 dt.$$

Thus whenever  $T > \frac{\pi}{\omega}$ , we know that the variation of the action (31) is negative. Thus for  $T > \frac{\pi}{\omega}$ , the physical solution  $Q(t)$  does not minimize the action.

### IV. THE GENERAL SOLUTION: AN EIGENVALUE PROBLEM

With finite dimensional matrices, we know there is a relation between a variational approach and the eigenvalue problem for a Hermitian matrix  $T$ . Let us denote vectors by  $q$  with components  $q_i$  or by  $\eta$  with components  $\eta_i$ . Also let  $\langle q, \eta \rangle$  denote the standard inner product  $\langle q, \eta \rangle = \sum_i \bar{q}_i \eta_i$ . The real-valued function  $F(q)$ , defined for vectors  $q$  by

$$(32) \quad F(q) = \frac{\langle q, Tq \rangle}{\langle q, q \rangle},$$

is stationary at  $q = Q$  if  $Q$  is an eigenvector of  $T$  with eigenvalue  $\lambda = \frac{\langle Q, TQ \rangle}{\langle Q, Q \rangle}$ .

The directional derivative of  $F(q)$  in the direction  $\eta$  is

$$(33) \quad \begin{aligned} (D_\eta F)(q) &= \lim_{\epsilon \rightarrow 0} \frac{F(q + \epsilon \eta) - F(q)}{\epsilon} \\ &= \frac{\langle \eta, Tq \rangle + \langle q, T\eta \rangle}{\langle q, q \rangle} - \frac{\langle q, Tq \rangle (\langle \eta, q \rangle + \langle q, \eta \rangle)}{\langle q, q \rangle^2}. \end{aligned}$$

Replace  $q$  by the unit vector  $f = \frac{q}{\langle q, q \rangle^{1/2}}$ , so using the reality of  $\langle f, Tf \rangle$ ,

$$(34) \quad \begin{aligned} (D_\eta F)(f) &= \langle \eta, (Tf - \langle f, Tf \rangle f) \rangle + \overline{\langle (Tf - \langle f, Tf \rangle f), \eta \rangle} \\ &= \langle \eta, (Tf - \langle f, Tf \rangle f) \rangle + \overline{\langle \eta, (Tf - \langle f, Tf \rangle f) \rangle}. \end{aligned}$$

For  $q$  to be a stationary point  $Q$ , this derivative must vanish for all  $\eta$ . Therefore at a stationary point,

$$(35) \quad Tf = \langle f, Tf \rangle f.$$

In other words, at a stationary point  $f$  is a unit eigenvector of  $T$  with eigenvalue  $\lambda = \langle f, Tf \rangle$ .

Since any  $N \times N$  Hermitian matrix has an orthonormal basis  $e^{(1)}, \dots, e^{(N)}$  of eigenvectors, with eigenvalues  $\lambda_1, \dots, \lambda_N$ , one can expand any vector  $q$  into a sum of such vectors,  $q = \sum_{j=1}^N q_j e^{(j)}$ , where  $q_j = \langle e^{(j)}, q \rangle$ . Then for an arbitrary unit vector  $f$ ,

$$(36) \quad F(f) = \sum_{j=1}^N |c_j|^2 \lambda_j, \quad \text{where} \quad \sum_{j=1}^N |c_j|^2 = 1.$$

Hence  $F(f)$  is minimized by the minimum eigenvalue of  $T$ . and it is maximized by the maximum eigenvalue of  $T$ .

If we now order the eigenvectors so that the eigenvalues are increasing,

$$(37) \quad \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_N,$$

then at the stationary point  $e^{(1)}$ , the function  $F(e^{(1)}) = \lambda_1$  has  $N - 1$  increasing directions. At the stationary point  $e^{(k)}$ , the function  $F(e^{(k)}) = \lambda_k$  has  $N - k$  increasing directions and  $k - 1$  decreasing directions. And at the maximum  $F(e^{(N)}) = \lambda_N$  the function has  $N - 1$  decreasing directions.

The analysis of  $T = -\frac{d^2}{dt^2}$  is the infinite dimensional generalization of the case for a Hermitian matrix. The fact that  $T$  is hermitian depends on the boundary condition  $f(0) = f(T) = 0$ . In this case  $T$  does have an orthonormal basis of eigenvectors, namely the functions

$$(38) \quad e^{(j)} = \left(\frac{2}{T}\right)^{\frac{1}{2}} \sin\left(\frac{j\pi}{T}(t - T_1)\right),$$

with eigenvalues

$$(39) \quad \lambda_j = \left(\frac{j\pi}{T}\right)^2, \quad \text{for } j = 1, 2, \dots$$



The eigenvalue  $\lambda_1$  is the minimum value of  $F(f)$  for  $\langle f, f \rangle = \int_{T_1}^{T_2} |f(t)|^2 dt = 1$ , and there is no maximum eigenvalue nor a maximum value of  $F(f)$ .

## V. ANALYSIS WITH FOURIER SERIES (OPTIONAL)

The rest of these notes are more advanced. I recommend reading this section in case you know the mathematics of quantum theory: in that case you will find it very interesting.

The formula (29) for the variation of the action has the form of an “expectation” of a linear transformation  $-\frac{d^2}{dt^2} - \omega^2$  in the state  $\eta$ , namely

$$(40) \quad S_{[T_1, T_2]}(\eta) = \left\langle \eta, \left( -\frac{d^2}{dt^2} - \omega^2 \right) \eta \right\rangle .$$

Let us explain this in the context of orbits that are square integrable functions of time, namely elements of  $L^2[T_1, T_2]$ . Suppose that we consider the function  $\eta(t)$ , vanishing at the endpoints, as an element in the Hilbert space  $L^2[T_1, T_2]$  of square integrable functions on the interval  $[T_1, T_2]$ . The set of all square-integrable functions for which  $\eta(T_1) = \eta(T_2) = 0$ , is a linear subspace of  $L^2$ . For two different functions  $\eta_1(t)$  and  $\eta_2(t)$ , both vanishing at the endpoints,  $\eta_1(T_1) = \eta_1(T_2) = \eta_2(T_1) = \eta_2(T_2) = 0$ , we can for real numbers  $\lambda_1, \lambda_2$  form a new function  $\eta(t) = \lambda_1 \eta_1(t) + \lambda_2 \eta_2(t)$ . This also satisfies the boundary condition  $\eta(T_1) = \eta(T_2) = 0$ . Thus the space of real functions vanishing at the endpoints is a “space of real vectors.” This is a subspace of the space of the bigger space of vectors made of functions  $\eta(t)$  on the interval  $[T_1, T_2]$  where we do not require that the functions vanish at the endpoints.

We can introduce the scalar product between the real vectors  $\eta_1$  and  $\eta_2$  as

$$(41) \quad \langle \eta_1, \eta_2 \rangle = \int_{T_1}^{T_2} \eta_1(t) \eta_2(t) dt .$$

Also we can define the transformation

$$K = -\frac{d^2}{dt^2}$$

that takes a twice differentiable vector  $\eta$  into the vector  $T\eta$  defined by

$$(K\eta)(t) = -\ddot{\eta}(t) .$$

**V.1. Symmetry of  $K$ :** The transformation  $K$  is symmetric when defined on twice-differentiable functions  $\eta$  that vanish at the endpoints. It is always the case that  $\eta_1 \ddot{\eta}_2 =$

$\frac{d}{dt}(\eta_1 \dot{\eta}_2) - \dot{\eta}_1 \dot{\eta}_2$ . Therefore

$$\begin{aligned}
 \langle \eta_1, K \eta_2 \rangle &= - \int_{T_1}^{T_2} \eta_1(t) \ddot{\eta}_2(t) dt \\
 &= \int_{T_1}^{T_2} \dot{\eta}_1(t) \dot{\eta}_2(t) dt - \eta_1(t) \dot{\eta}_2(t) \Big|_{T_1}^{T_2} \\
 (42) \qquad &= \int_{T_1}^{T_2} \dot{\eta}_1(t) \dot{\eta}_2(t) dt = \langle \dot{\eta}_1, \dot{\eta}_2 \rangle .
 \end{aligned}$$

Now repeat the same argument, but use  $\dot{\eta}_1 \dot{\eta}_2 = \frac{d}{dt}(\dot{\eta}_1 \eta_2) - \ddot{\eta}_1 \eta_2$ . Thus

$$(43) \qquad \langle \eta_1, K \eta_2 \rangle = - \int_{T_1}^{T_2} \ddot{\eta}_1(t) \eta_2(t) dt = \langle K \eta_1, \eta_2 \rangle .$$

Note that in deriving (43), the boundary terms arising from integration by parts in (43) vanish as we assume  $\eta(T_1) = \eta(T_2) = 0$ .

We interpret  $K$  as a linear transformation on the space of twice differentiable vectors (not necessarily satisfying the vanishing boundary conditions). In other words  $K$  acts like a real, symmetric matrix on a space of vectors, taking one vector into another. The transformation  $K$  is linear in the sense that  $K(\eta_1 + \eta_2) = K\eta_1 + K\eta_2$ . Similarly we interpret  $\langle \eta_1, K \eta_2 \rangle$  as a matrix element of the transformation  $K$ . The diagonal matrix element (or expectation)  $\langle \eta, K \eta \rangle$  of  $K$  occurs for  $\eta_1 = \eta_2 = \eta$ , and

$$(44) \qquad \langle \eta, K \eta \rangle = \int_{T_1}^{T_2} \dot{\eta}(t)^2 dt .$$

Comparing (44) with (28)–(29), we see that the action  $S_{[T_1, T_2]}(\eta)$  is proportional to the expectation of  $K - \omega^2$ , namely

$$(45) \qquad S_{[T_1, T_2]}(\eta) = \frac{1}{2} m \langle \eta, (K - \omega^2) \eta \rangle .$$

**V.2. Relation of  $S_{[T_1, T_2]}(\eta)$  to Eigenvalues and Eigenvectors:** Suppose that the vector  $\eta$  is an eigenvector for  $K$  with eigenvalue  $\lambda$  (a real number). This means that

$$(46) \qquad K \eta = \lambda \eta .$$

Consequently

$$(47) \qquad \langle \eta, K \eta \rangle = \lambda \langle \eta, \eta \rangle .$$

In the case that  $\eta$  is an eigenvector of  $K$ , with eigenvalue  $\lambda$ ,

$$(48) \qquad S_{[T_1, T_2]}(\eta) = \frac{m}{2} (\lambda - \omega^2) \langle \eta, \eta \rangle .$$

Hence if  $\lambda < \omega^2$ , the corresponding eigenvector  $\eta$  yields  $S_{[T_1, T_2]}(\eta) < 0$ . In that case,  $S_{[T_1, T_2]}(Q + \eta) = S_{[T_1, T_2]}(Q) + S_{[T_1, T_2]}(\eta) < S_{[T_1, T_2]}(Q)$ . In this case, the trajectory  $Q(t)$  does *not* minimize the action.

**V.3. All the Eigenfunctions of  $K$ :** Understanding *all* the eigenvalues of  $K$  with vanishing boundary conditions, means solving the differential equation

$$(49) \quad -\ddot{\eta}(t) = \lambda\eta(t) \quad \text{with} \quad \eta(T_1) = \eta(T_2) = 0 .$$

This is called the *Dirichlet problem* or the problem of *Dirichlet boundary conditions* for  $-\frac{d^2}{dt^2}$  with vanishing boundary conditions at the endpoints  $t = T_1, T_2$ . Let  $T = T_2 - T_1$  denote the time difference. The normalized eigenfunctions for this Dirichlet problem are

$$(50) \quad \eta_j(t) = \left(\frac{2}{T}\right)^{1/2} \sin\left(\frac{\pi j(t - T_1)}{T}\right) , \quad \text{where } j = 1, 2, 3, \dots ,$$

and the corresponding eigenvalues are

$$(51) \quad \lambda_j = \left(j\frac{\pi}{T}\right)^2 .$$

For a given  $j$ , there is only one function (up to a multiple) satisfying the equation and the boundary condition. For different values of  $j$ , the  $\lambda_j$  are different, so the eigenfunctions are mutually orthogonal. The minimum eigenvalue comes from  $j = 1$  and this is  $\eta_1$ .

**V.4. Expansion in Eigenfunctions:** Suppose we consider a linear combination  $\eta$  of the eigenfunctions  $\eta_j$ . Namely inspect a sum of the form

$$(52) \quad \eta = \sum_{j=1}^{\infty} c_j \eta_j .$$

As the eigenfunctions  $\eta_j$  are orthogonal and normalized, the coefficients  $c_j$  can be found from  $\eta$  by the relation  $c_j = \langle \eta, \eta_j \rangle$ . If the set of eigenvectors  $\{\eta_j\}$  are actually a basis, then any  $\eta$  can be expanded in this fashion. (We do not address that here.)

In any case, the orthonormality also shows

$$(53) \quad S_{[T_1, T_2]}(\eta) = \frac{m}{2} \sum_{j=1}^{\infty} c_j^2 (\lambda_j - \omega^2) = \frac{m}{2} \sum_{j=1}^{\infty} c_j^2 \left( \left(j\frac{\pi}{T}\right)^2 - \omega^2 \right) .$$

Those terms in the sum for which  $\lambda_j > \omega^2$  are positive. The smallest eigenvalue is  $\lambda_1$ , and  $\lambda_j$  increases with  $j^2$ , so at most a finite number of terms can be negative. They are the terms for which  $\lambda_j < \omega^2$ .

**V.5. Remark: Relation to a Variational Problem:** The normalized action functional (real valued function)

$$(54) \quad F(\eta) = \frac{\langle \eta, K\eta \rangle}{\langle \eta, \eta \rangle}$$

plays a major role in the study of  $K$ . The eigenvectors  $\eta$  of  $K$  are critical points of  $F(\eta)$ . The eigenvalues are  $F(\eta)$  when  $\eta$  is an eigenvector. As in the notes on matrices, this functional is used to study the eigenvalue for the Dirichlet problem and to prove that the eigenfunctions are a basis.

**V.6. Remark: Relation of “Least Action” to “Quantum Theory of a Particle in a Box”:** For those of you who have studied quantum theory, you might recognize the transformation  $K$ . In quantum theory the variable is not the time  $t$ . Rather the variable is the position  $x$  of a particle on an interval  $Q_1 \leq x \leq Q_2$ . Then the study of  $K = -\frac{d^2}{dx^2}$  as a transformation on the real subspace of  $L^2[Q_1, Q_2]$  with the Dirichlet boundary condition  $\eta(Q_1) = \eta(Q_2) = 0$  is called “the study of the Schrödinger Hamiltonian for a *particle in a box*.” (Here we use units for which the constants  $m$  and  $\hbar$  equal 1.)

The minimal eigenvalue of the kinetic energy  $K$  is

$$(55) \quad \lambda_1 = \pi^2(Q_2 - Q_1)^{-2} .$$

This is called the *zero-point energy* of a particle in a box of length  $\ell = Q_2 - Q_1$ . The corresponding eigenfunction is

$$(56) \quad \psi(x) = \sin \lambda_1^{1/2}(x - Q_1) = \sin \left( \frac{\pi(x - Q_1)}{Q_2 - Q_1} \right) .$$

This function corresponds to the function (30), proportional to  $\eta_1(x)$ , considered earlier, but with the variable  $x$  replacing the variables  $t$ . The fact that the zero-point energy  $\lambda_1 \propto \ell^{-2} > 0$  is important in the interpretation of quantum theory.