Chapter 5

Calculus of Variations

5.1 Snell's Law

Warm-up problem: You are standing at point (x_1, y_1) on the beach and you want to get to a point (x_2, y_2) in the water, a few meters offshore. The interface between the beach and the water lies at $x = 0$. What path results in the shortest travel time? It is not a straight line! This is because your speed v_1 on the sand is greater than your speed v_2 in the water. The optimal path actually consists of two line segments, as shown in Fig. 5.1. Let the path pass through the point $(0, y)$ on the interface. Then the time T is a function of y:

$$T(y) = \frac{1}{v_1}\sqrt{x_1^2 + (y - y_1)^2} + \frac{1}{v_2}\sqrt{x_2^2 + (y_2 - y)^2} \ . \tag{5.1}$$

To find the minimum time, we set

$$\begin{aligned} \frac{dT}{dy} = 0 &= \frac{1}{v_1}\frac{y - y_1}{\sqrt{x_1^2 + (y - y_1)^2}} + \frac{1}{v_2}\frac{y_2 - y}{\sqrt{x_2^2 + (y_2 - y)^2}} \\ &= \frac{\sin\theta_1}{v_1} - \frac{\sin\theta_2}{v_2} \ . \end{aligned} \tag{5.2}$$

Thus, the optimal path satisfies

$$\frac{\sin\theta_1}{\sin\theta_2} = \frac{v_1}{v_2} \ , \tag{5.3}$$

which is known as *Snell's Law.*

Snell's Law is familiar from optics, where the speed of light in a polarizable medium is written $v = c/n$, where n is the index of refraction. In terms of n,

$$n_1 \sin\theta_1 = n_2 \sin\theta_2 \ . \tag{5.4}$$

If there are several interfaces, Snell's law holds at each one, so that

$$n_i \sin\theta_i = n_{i+1} \sin\theta_{i+1} \ , \tag{5.5}$$

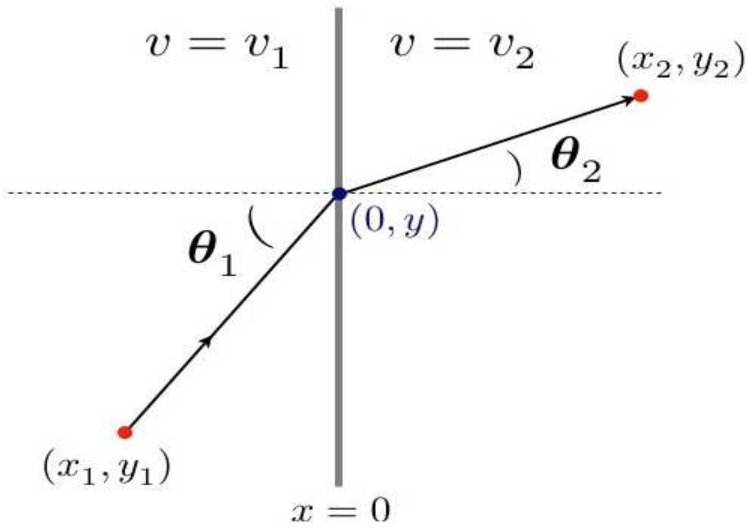

Figure 5.1: The shortest path between (x_1, y_1) and (x_2, y_2) is not a straight line, but rather two successive line segments of different slope.

at the interface between media i and $i+1$.

Now let us imagine that there are many such interfaces between regions of very small thicknesses. We can then regard n and θ as continuous functions of the coordinate x. The differential form of Snell's law is

$$\begin{aligned} n(x)\, \sin\big(\theta(x)\big) &= n(x+dx)\, \sin\big(\theta(x+dx)\big) \\ &= (n + n'\, dx)\, \big(\sin\theta + \cos\theta\, \theta'\, dx\big) \\ &= n\, \sin\theta + \big(n'\, \sin\theta + n\, \cos\theta\, \theta'\big)\, dx\ . \end{aligned} \tag{5.6}$$

Thus,

$$\text{ctn}\,\theta\, \frac{d\theta}{dx} = -\frac{1}{n}\, \frac{dn}{dx}\ . \tag{5.7}$$

If we write the path as $y = y(x)$, then $\tan\theta = y'$, and

$$\theta' = \frac{d}{dx}\, \tan^{-1} y' = \frac{y''}{1 + y'^2}\ , \tag{5.8}$$

which yields

$$-\frac{1}{y'} \cdot \frac{y''}{1+y'^2} = \frac{n'}{n}\ . \tag{5.9}$$

This is a differential equation that $y(x)$ must satisfy if the *functional*

$$T\big[y(x)\big] = \int \frac{ds}{v} = \frac{1}{c} \int\limits_{x_1}^{x_2} dx\, n(x)\, \sqrt{1 + y'^2} \tag{5.10}$$

is to be minimized.

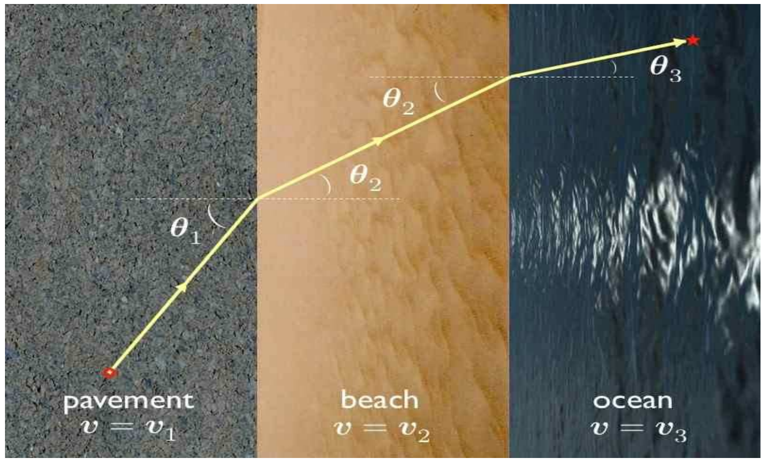

Figure 5.2: The path of shortest length is composed of three line segments. The relation between the angles at each interface is governed by Snell's Law.

5.2 Functions and Functionals

A *function* is a mathematical object which takes a real (or complex) variable, or several such variables, and returns a real (or complex) number. A *functional* is a mathematical object which takes an entire function and returns a number. In the case at hand, we have

$$T\big[y(x)\big] = \int\limits_{x_1}^{x_2} dx\, L(y, y', x) \ , \tag{5.11}$$

where the function $L(y, y', x)$ is given by

$$L(y, y', x) = c^{-1}\, n(x)\, \sqrt{1 + y'^2} \ . \tag{5.12}$$

Here $n(x)$ is a given function characterizing the medium, and $y(x)$ is the path whose time is to be evaluated.

In ordinary calculus, we extremize a function $f(x)$ by demanding that f not change to lowest order when we change $x \to x + dx$:

$$f(x + dx) = f(x) + f'(x)\, dx + \tfrac{1}{2}\, f''(x)\, (dx)^2 + \ldots \ . \tag{5.13}$$

We say that $x = x^*$ is an extremum when $f'(x^*) = 0$.

For a functional, the first *functional variation* is obtained by sending $y(x) \to y(x) + \delta y(x)$,

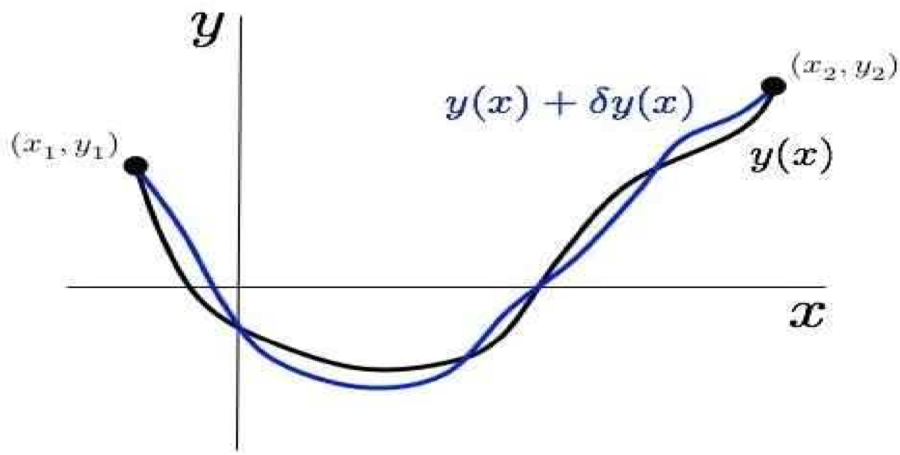

Figure 5.3: A path $y(x)$ and its variation $y(x) + \delta y(x)$.

and extracting the variation in the functional to order δy. Thus, we compute

$$\begin{aligned} T\big[y(x) + \delta y(x)\big] &= \int\limits_{x_1}^{x_2} dx\, L(y + \delta y, y' + \delta y', x) \\ &= \int\limits_{x_1}^{x_2} dx \left\{ L + \frac{\partial L}{\partial y}\,\delta y + \frac{\partial L}{\partial y'}\,\delta y' + \mathcal{O}\big((\delta y)^2\big) \right\} \\ &= T\big[y(x)\big] + \int\limits_{x_1}^{x_2} dx \left\{ \frac{\partial L}{\partial y}\,\delta y + \frac{\partial L}{\partial y'}\,\frac{d}{dx}\,\delta y \right\} \\ &= T\big[y(x)\big] + \int\limits_{x_1}^{x_2} dx \left[\frac{\partial L}{\partial y} - \frac{d}{dx}\left(\frac{\partial L}{\partial y'}\right)\right] \delta y + \frac{\partial L}{\partial y'}\,\delta y \,\bigg|_{x_1}^{x_2} . \end{aligned} \tag{5.14}$$

Now one very important thing about the variation $\delta y(x)$ is that it must vanish at the endpoints: $\delta y(x_1) = \delta y(x_2) = 0$. This is because the space of functions under consideration satisfy fixed boundary conditions $y(x_1) = y_1$ and $y(x_2) = y_2$. Thus, the last term in the above equation vanishes, and we have

$$\delta T = \int\limits_{x_1}^{x_2} dx \left[\frac{\partial L}{\partial y} - \frac{d}{dx}\left(\frac{\partial L}{\partial y'}\right)\right] \delta y \ . \tag{5.15}$$

We say that the first functional derivative of T with respect to $y(x)$ is

$$\frac{\delta T}{\delta y(x)} = \left[\frac{\partial L}{\partial y} - \frac{d}{dx}\left(\frac{\partial L}{\partial y'}\right)\right]_x , \tag{5.16}$$

where the subscript indicates that the expression inside the square brackets is to be evaluated at x. The functional $T\big[y(x)\big]$ is *extremized* when its first functional derivative vanishes, which results in a differential equation for $y(x)$,

$$\frac{\partial L}{\partial y} - \frac{d}{dx}\left(\frac{\partial L}{\partial y'}\right) = 0 \ , \tag{5.17}$$

known as the *Euler-Lagrange* equation. Since L is independent of y, we have

$$\begin{aligned} 0 = \frac{d}{dx}\left(\frac{\partial L}{\partial y'}\right) &= \frac{1}{c}\frac{d}{dx}\left[\frac{n\,y'}{\sqrt{1+y'^2}}\right] \\ &= \frac{n'}{c}\,\frac{y'}{\sqrt{1+y'^2}} + \frac{n}{c}\,\frac{y''}{\big(1+y'^2\big)^{3/2}} \ . \end{aligned} \tag{5.18}$$

We thus recover the second order equation in 5.9. However, note that the above equation directly gives

$$n(x)\,\sin\theta(x) = \text{const.} \ , \tag{5.19}$$

which follows from the relation $y' = \tan\theta$. For $y(x)$ we obtain

$$\frac{n^2\,y'^2}{1+y'^2} \equiv \alpha^2 = \text{const.} \quad \Rightarrow \quad \frac{dy}{dx} = \frac{\alpha}{\sqrt{n^2(x)-\alpha^2}} \ . \tag{5.20}$$

In general, we may expand a functional $F[y+\delta y]$ in a *functional Taylor series*,

$$\begin{aligned} F[y+\delta y] = F[y] &+ \int\! dx_1\, K_1(x_1)\,\delta y(x_1) + \tfrac{1}{2!}\int\! dx_1 \int\! dx_2\, K_2(x_1,x_2)\,\delta y(x_1)\,\delta y(x_2) \\ &+ \tfrac{1}{3!}\int\! dx_1 \int\! dx_2 \int\! dx_3\, K_3(x_1,x_2,x_3)\,\delta y(x_1)\,\delta y(x_2)\,\delta y(x_3) + \ldots \end{aligned} \tag{5.21}$$

and we write

$$K_n(x_1,\ldots,x_n) \equiv \frac{\delta^n F}{\delta y(x_1)\cdots\delta y(x_n)} \tag{5.22}$$

for the n^{th} functional derivative.

5.3 Examples from the Calculus of Variations

Here we present three useful examples of variational calculus as applied to problems in mathematics and physics.

5.3.1 Example 1 : minimal surface of revolution

Consider a surface formed by rotating the function $y(x)$ about the x-axis. The area is then

$$A\big[y(x)\big] = \int\limits_{x_1}^{x_2}\! dx\, 2\pi y\,\sqrt{1+\left(\frac{dy}{dx}\right)^2} \ , \tag{5.23}$$

and is a functional of the curve $y(x)$. Thus we can define $L(y, y') = 2\pi y\sqrt{1 + y'^2}$ and make the identification $y(x) \leftrightarrow q(t)$. We can then apply what we have derived for the mechanical action, with $L = L(q, \dot{q}, t)$, *mutatis mutandis.* Thus, the equation of motion is

$$\frac{d}{dx}\left(\frac{\partial L}{\partial y'}\right) = \frac{\partial L}{\partial y} \ , \tag{5.24}$$

which is a second order ODE for $y(x)$. Rather than treat the second order equation, though, we can integrate once to obtain a first order equation, by noticing that

$$\begin{aligned} \frac{d}{dx}\left[y'\,\frac{\partial L}{\partial y'} - L\right] &= y''\,\frac{\partial L}{\partial y'} + y'\,\frac{d}{dx}\left(\frac{\partial L}{\partial y'}\right) - \frac{\partial L}{\partial y'}\,y'' - \frac{\partial L}{\partial y}y' - \frac{\partial L}{\partial x} \\ &= y'\left[\frac{d}{dx}\left(\frac{\partial L}{\partial y'}\right) - \frac{\partial L}{\partial y}\right] - \frac{\partial L}{\partial x} \ . \end{aligned} \tag{5.25}$$

In the second line above, the term in square brackets vanishes, thus

$$\mathcal{J} = y'\,\frac{\partial L}{\partial y'} - L \quad \Rightarrow \quad \frac{d\mathcal{J}}{dx} = -\frac{\partial L}{\partial x} \ , \tag{5.26}$$

and when L has no explicit x-dependence, $\mathcal{J}$ is conserved. One finds

$$\mathcal{J} = 2\pi y \cdot \frac{y'^2}{\sqrt{1+y'^2}} - 2\pi y\,\sqrt{1+y'^2} = -\frac{2\pi y}{\sqrt{1+y'^2}} \ . \tag{5.27}$$

Solving for y',

$$\frac{dy}{dx} = \pm\sqrt{\left(\frac{2\pi y}{\mathcal{J}}\right)^2 - 1} \ , \tag{5.28}$$

which may be integrated with the substitution $y = \frac{\mathcal{J}}{2\pi}\cosh\chi$, yielding

$$y(x) = b\,\cosh\left(\frac{x-a}{b}\right) \ , \tag{5.29}$$

where a and $b = \frac{\mathcal{J}}{2\pi}$ are constants of integration. Note there are two such constants, as the original equation was second order. This shape is called a *catenary.* As we shall later find, it is also the shape of a uniformly dense rope hanging between two supports, under the influence of gravity. To fix the constants a and b, we invoke the boundary conditions $y(x_1) = y_1$ and $y(x_2) = y_2$.

Consider the case where $-x_1 = x_2 \equiv x_0$ and $y_1 = y_2 \equiv y_0$. Then clearly $a = 0$, and we have

$$y_0 = b\,\cosh\left(\frac{x_0}{b}\right) \quad \Rightarrow \quad \gamma = \kappa^{-1}\,\cosh\kappa \ , \tag{5.30}$$

with $\gamma \equiv y_0/x_0$ and $\kappa \equiv x_0/b$. One finds that for any $\gamma > 1.5089$ there are two solutions, one of which is a global minimum and one of which is a local minimum or saddle of $A[y(x)]$.

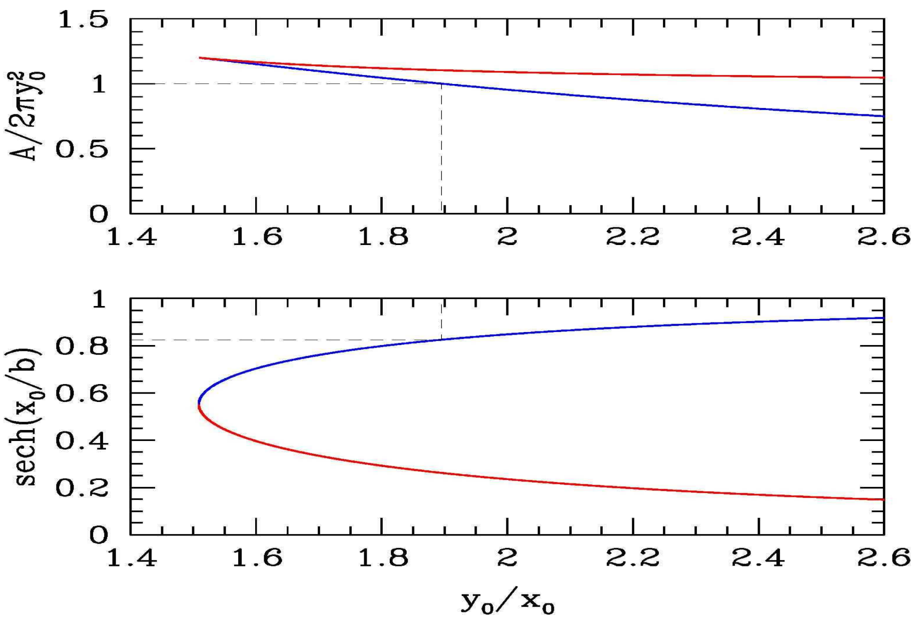

Figure 5.4: Minimal surface solution, with $y(x) = b\cosh(x/b)$ and $y(x_0) = y_0$. Top panel: $A/2\pi y_0^2$ *vs.* y_0/x_0. Bottom panel: $\mathrm{sech}(x_0/b)$ *vs.* y_0/x_0. The blue curve corresponds to a global minimum of $A[y(x)]$, and the red curve to a local minimum or saddle point.

The solution with the smaller value of κ (*i.e.* the larger value of $\mathrm{sech}\,\kappa$) yields the smaller value of A, as shown in Fig. 5.4. Note that

$$\frac{y}{y_0} = \frac{\cosh(x/b)}{\cosh(x_0/b)} , \tag{5.31}$$

so $y(x=0) = y_0\,\mathrm{sech}(x_0/b)$.

When extremizing functions that are defined over a finite or semi-infinite interval, one must take care to evaluate the function at the boundary, for it may be that the boundary yields a global extremum even though the derivative may not vanish there. Similarly, when extremizing functionals, one must investigate the functions at the boundary of function space. In this case, such a function would be the discontinuous solution, with

$$y(x) = \begin{cases} y_1 & \text{if } x = x_1 \\ \\ 0 & \text{if } x_1 < x < x_2 \\ \\ y_2 & \text{if } x = x_2 \ . \end{cases} \tag{5.32}$$

This solution corresponds to a surface consisting of two discs of radii y_1 and y_2, joined by an infinitesimally thin thread. The area functional evaluated for this particular $y(x)$ is clearly $A = \pi(y_1^2 + y_2^2)$. In Fig. 5.4, we plot $A/2\pi y_0^2$ *versus* the parameter $\gamma = y_0/x_0$.

For $\gamma > \gamma_c \approx 1.564$, one of the catenary solutions is the global minimum. For $\gamma < \gamma_c$, the minimum area is achieved by the discontinuous solution.

Note that the functional derivative,

$$K_1(x) = \frac{\delta A}{\delta y(x)} = \left\{ \frac{\partial L}{\partial y} - \frac{d}{dx}\left(\frac{\partial L}{\partial y'}\right) \right\} = \frac{2\pi\big(1 + y'^2 - yy''\big)}{(1 + y'^2)^{3/2}} \ , \tag{5.33}$$

indeed vanishes for the catenary solutions, but does not vanish for the discontinuous solution, where $K_1(x) = 2\pi$ throughout the interval $(-x_0, x_0)$. Since $y = 0$ on this interval, y cannot be decreased. The fact that $K_1(x) > 0$ means that increasing y will result in an increase in A, so the boundary value for A, which is $2\pi y_0^2$, is indeed a local minimum.

We furthermore see in Fig. 5.4 that for $\gamma < \gamma_* \approx 1.5089$ the local minimum and saddle are no longer present. This is the familiar saddle-node bifurcation, here in function space. Thus, for $\gamma \in [0, \gamma_*)$ there are no extrema of $A[y(x)]$, and the minimum area occurs for the discontinuous $y(x)$ lying at the boundary of function space. For $\gamma \in (\gamma_*, \gamma_c)$, two extrema exist, one of which is a local minimum and the other a saddle point. Still, the area is minimized for the discontinuous solution. For $\gamma \in (\gamma_c, \infty)$, the local minimum is the global minimum, and has smaller area than for the discontinuous solution.

5.3.2 Example 2 : geodesic on a surface of revolution

We use cylindrical coordinates (ρ, ϕ, z) on the surface $z = z(\rho)$. Thus,

$$\begin{aligned} ds^2 &= d\rho^2 + \rho^2\, d\phi^2 + dx^2 \\ &= \Big\{ 1 + \big[z'(\rho)\big]^2 \Big\}\, d\rho + \rho^2\, d\phi^2 \ , \end{aligned} \tag{5.34}$$

and the distance functional $D\big[\phi(\rho)\big]$ is

$$D\big[\phi(\rho)\big] = \int\limits_{\rho_1}^{\rho_2} \! d\rho\, L(\phi, \phi', \rho) \ , \tag{5.35}$$

where

$$L(\phi, \phi', \rho) = \sqrt{1 + z'^2(\rho) + \rho^2\, \phi'^2(\rho)} \ . \tag{5.36}$$

The Euler-Lagrange equation is

$$\frac{\partial L}{\partial \phi} - \frac{d}{d\rho}\left(\frac{\partial L}{\partial \phi'}\right) = 0 \quad \Rightarrow \quad \frac{\partial L}{\partial \phi'} = \text{const.} \tag{5.37}$$

Thus,

$$\frac{\partial L}{\partial \phi'} = \frac{\rho^2\, \phi'}{\sqrt{1 + z'^2 + \rho^2\, \phi'^2}} = a \ , \tag{5.38}$$

where a is a constant. Solving for ϕ', we obtain

$$d\phi = \frac{a\sqrt{1+\big[z'(\rho)\big]^2}}{\rho\sqrt{\rho^2 - a^2}}\,d\rho \ , \tag{5.39}$$

which we must integrate to find $\phi(\rho)$, subject to boundary conditions $\phi(\rho_i) = \phi_i$, with $i = 1, 2$.

On a cone, $z(\rho) = \lambda\rho$, and we have

$$d\phi = a\sqrt{1+\lambda^2}\,\frac{d\rho}{\rho\sqrt{\rho^2 - a^2}} = \sqrt{1+\lambda^2}\,d\tan^{-1}\sqrt{\frac{\rho^2}{a^2} - 1} \ , \tag{5.40}$$

which yields

$$\phi(\rho) = \beta + \sqrt{1+\lambda^2}\,\tan^{-1}\sqrt{\frac{\rho^2}{a^2} - 1} \ , \tag{5.41}$$

which is equivalent to

$$\rho\,\cos\bigg(\frac{\phi - \beta}{\sqrt{1+\lambda^2}}\bigg) = a \ . \tag{5.42}$$

The constants β and a are determined from $\phi(\rho_i) = \phi_i$.

5.3.3 Example 3 : brachistochrone

Problem: find the path between (x_1, y_1) and (x_2, y_2) which a particle sliding frictionlessly and under constant gravitational acceleration will traverse in the shortest time. To solve this we first must invoke some elementary mechanics. Assuming the particle is released from (x_1, y_1) at rest, energy conservation says

$$\tfrac{1}{2}mv^2 - mgy = mgy_1 \ . \tag{5.43}$$

Then the time, which is a functional of the curve $y(x)$, is

$$\begin{aligned} T\big[y(x)\big] &= \int\limits_{x_1}^{x_2} \frac{ds}{v} = \frac{1}{\sqrt{2g}} \int\limits_{x_1}^{x_2} dx\,\sqrt{\frac{1+y'^2}{y_1 - y}} \\ &\equiv \int\limits_{x_1}^{x_2} dx\,L(y, y', x) \ , \end{aligned} \tag{5.44}$$

with

$$L(y, y', x) = \sqrt{\frac{1+y'^2}{2g(y_1 - y)}} \ . \tag{5.45}$$

Since L is independent of x, eqn. 5.25, we have that

$$\mathcal{J} = y'\,\frac{\partial L}{\partial y'} - L = -\Big[2g\,(y_1 - y)\,\big(1 + y'^2\big)\Big]^{-1/2} \tag{5.46}$$

is conserved. This yields

$$dx = -\sqrt{\frac{y_1 - y}{2a - y_1 + y}}\, dy \ , \tag{5.47}$$

with $a = (4g\mathcal{J}^2)^{-1}$. This may be integrated parametrically, writing

$$y_1 - y = 2a \sin^2(\tfrac{1}{2}\theta) \quad \Rightarrow \quad dx = 2a \sin^2(\tfrac{1}{2}\theta)\, d\theta \ , \tag{5.48}$$

which results in the parametric equations

$$x - x_1 = a\,\big(\theta - \sin\theta\big) \tag{5.49}$$

$$y - y_1 = -a\,(1 - \cos\theta) \ . \tag{5.50}$$

This curve is known as a *cycloid.*

5.3.4 Ocean waves

Surface waves in fluids propagate with a definite relation between their angular frequency ω and their wavevector $k = 2\pi/\lambda$, where λ is the wavelength. The *dispersion relation* is a function $\omega = \omega(k)$. The *group velocity* of the waves is then $v(k) = d\omega/dk$.

In a fluid with a flat bottom at depth h, the dispersion relation turns out to be

$$\omega(k) = \sqrt{gk\,\tanh kh} \approx \begin{cases} \sqrt{gh}\,k & \text{shallow } (kh \ll 1) \\ \\ \sqrt{gk} & \text{deep } (kh \gg 1) \ . \end{cases} \tag{5.51}$$

Suppose we are in the shallow case, where the wavelength λ is significantly greater than the depth h of the fluid. This is the case for ocean waves which break at the shore. The phase velocity and group velocity are then identical, and equal to $v(h) = \sqrt{gh}$. The waves propagate more slowly as they approach the shore.

Let us choose the following coordinate system: x represents the distance parallel to the shoreline, y the distance perpendicular to the shore (which lies at $y = 0$), and $h(y)$ is the depth profile of the bottom. We assume $h(y)$ to be a slowly varying function of y which satisfies $h(0) = 0$. Suppose a disturbance in the ocean at position (x_2, y_2) propagates until it reaches the shore at $(x_1, y_1 = 0)$. The time of propagation is

$$T\big[y(x)\big] = \int \frac{ds}{v} = \int\limits_{x_1}^{x_2} dx\,\sqrt{\frac{1 + y'^2}{g\,h(y)}} \ . \tag{5.52}$$

We thus identify the integrand

$$L(y, y', x) = \sqrt{\frac{1 + y'^2}{g\,h(y)}} \ . \tag{5.53}$$

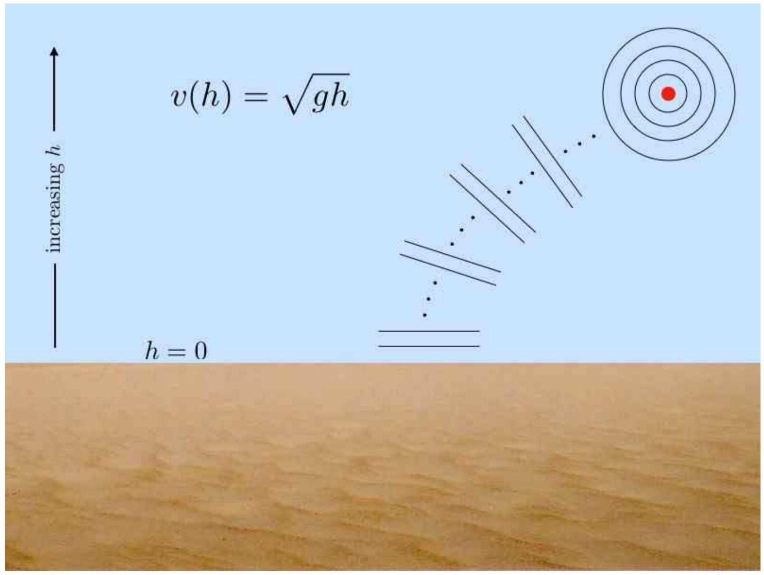

Figure 5.5: For shallow water waves, $v = \sqrt{gh}$. To minimize the propagation time from a source to the shore, the waves break parallel to the shoreline.

As with the brachistochrone problem, to which this bears an obvious resemblance, L is cyclic in the independent variable x, hence

$$\mathcal{J} = y'\,\frac{\partial L}{\partial y'} - L = -\Big[g\,h(y)\left(1+y'^2\right)\Big]^{-1/2} \tag{5.54}$$

is constant. Solving for $y'(x)$, we have

$$\tan\theta = \frac{dy}{dx} = \sqrt{\frac{a}{h(y)} - 1}\ , \tag{5.55}$$

where $a = (g\mathcal{J})^{-1}$ is a constant, and where θ is the local slope of the function $y(x)$. Thus, we conclude that near $y = 0$, where $h(y) \to 0$, the waves come in *parallel to the shoreline.* If $h(y) = \alpha y$ has a linear profile, the solution is again a cycloid, with

$$x(\theta) = b\,(\theta - \sin\theta) \tag{5.56}$$

$$y(\theta) = b\,(1 - \cos\theta)\ , \tag{5.57}$$

where $b = 2a/\alpha$ and where the shore lies at $\theta = 0$. Expanding in a Taylor series in θ for small θ, we may eliminate θ and obtain $y(x)$ as

$$y(x) = \left(\tfrac{9}{2}\right)^{1/3} b^{1/3}\, x^{2/3} + \ldots\ . \tag{5.58}$$

A *tsunami* is a shallow water wave that manages propagates in deep water. This requires $\lambda > h$, as we've seen, which means the disturbance must have a very long spatial extent out in the open ocean, where $h \sim 10\,\text{km}$. An undersea earthquake is the only possible source;

the characteristic length of earthquake fault lines can be hundreds of kilometers. If we take $h = 10\,\mathrm{km}$, we obtain $v = \sqrt{gh} \approx 310\,\mathrm{m/s}$ or $1100\,\mathrm{km/hr}$. At these speeds, a tsunami can cross the Pacific Ocean in less than a day.

As the wave approaches the shore, it must slow down, since $v = \sqrt{gh}$ is diminishing. But energy is conserved, which means that the amplitude must concomitantly rise. In extreme cases, the water level rise at shore may be 20 meters or more.

5.4 Appendix : More on Functionals

We remarked in section 5.2 that a function f is an animal which gets fed a real number x and excretes a real number $f(x)$. We say f maps the reals to the reals, or

$$f\colon \mathbf{R} \to \mathbf{R} \tag{5.59}$$

Of course we also have functions $g\colon \mathbf{C} \to \mathbf{C}$ which eat and excrete complex numbers, multivariable functions $h\colon \mathbf{R}^N \to \mathbf{R}$ which eat N-tuples of numbers and excrete a single number, *etc.*

A *functional* $F[f(x)]$ eats entire functions (!) and excretes numbers. That is,

$$F\colon \Big\{ f(x) \;\Big|\; x \in \mathbf{R} \Big\} \to \mathbf{R} \tag{5.60}$$

This says that F operates on the set of real-valued functions of a single real variable, yielding a real number. Some examples:

$$F[f(x)] = \tfrac{1}{2}\int\limits_{-\infty}^{\infty} \!dx\, \big[f(x)\big]^2 \tag{5.61}$$

$$F[f(x)] = \tfrac{1}{2}\int\limits_{-\infty}^{\infty} \!dx \int\limits_{-\infty}^{\infty}\! dx'\, K(x,x')\, f(x)\, f(x') \tag{5.62}$$

$$F[f(x)] = \int\limits_{-\infty}^{\infty}\! dx\, \bigg\{ \tfrac{1}{2} A\, f^2(x) + \tfrac{1}{2} B \left(\frac{df}{dx}\right)^{\!2} \bigg\} \ . \tag{5.63}$$

In classical mechanics, the action S is a functional of the path $q(t)$:

$$S[q(t)] = \int\limits_{t_\mathrm{a}}^{t_\mathrm{b}}\! dt\, \Big\{ \tfrac{1}{2} m \dot{q}^2 - U(q) \Big\} \ . \tag{5.64}$$

We can also have functionals which feed on functions of more than one independent variable, such as

$$S[y(x,t)] = \int\limits_{t_\mathrm{a}}^{t_\mathrm{b}}\! dt \int\limits_{x_\mathrm{a}}^{x_\mathrm{b}}\! dx\, \bigg\{ \tfrac{1}{2}\mu \bigg(\frac{\partial y}{\partial t}\bigg)^{\!2} - \tfrac{1}{2}\tau \bigg(\frac{\partial y}{\partial x}\bigg)^{\!2} \bigg\} \ , \tag{5.65}$$

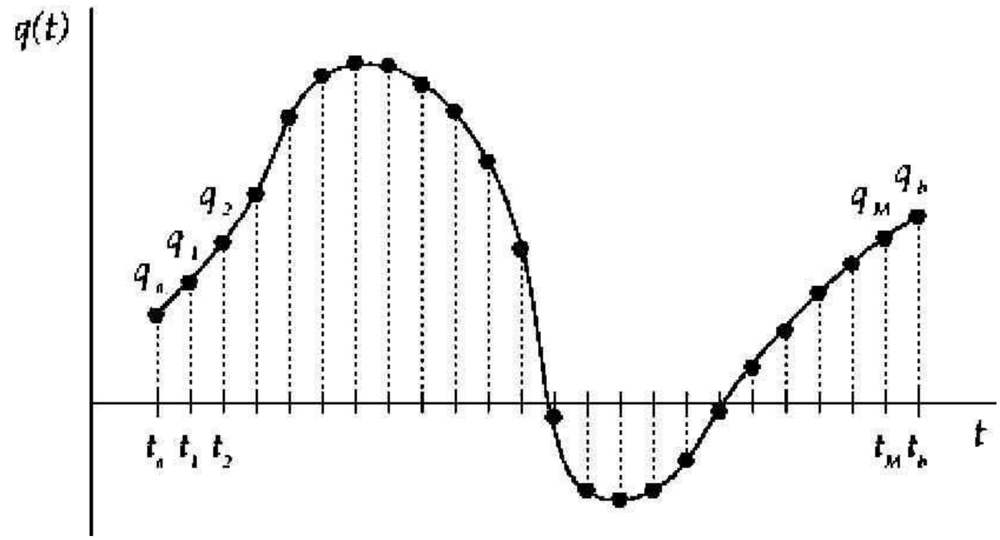

Figure 5.6: A functional $S[q(t)]$ is the continuum limit of a function of a large number of variables, $S(q_1, \ldots, q_M)$.

which happens to be the functional for a string of mass density μ under uniform tension τ. Another example comes from electrodynamics:

$$S[A^\mu(\boldsymbol{x},t)] = -\int\! d^3\!x \int\! dt \left\{ \frac{1}{16\pi} F_{\mu\nu}\, F^{\mu\nu} + \frac{1}{c} j_\mu\, A^\mu \right\} , \tag{5.66}$$

which is a functional of the four fields $\{A^0, A^1, A^2, A^3\}$, where $A^0 = c\phi$. These are the components of the 4-potential, each of which is itself a function of four independent variables (x^0, x^1, x^2, x^3), with $x^0 = ct$. The field strength tensor is written in terms of derivatives of the A^μ: $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$, where we use a metric $g_{\mu\nu} = \mathrm{diag}(+,-,-,-)$ to raise and lower indices. The 4-potential couples linearly to the source term J_μ, which is the electric 4-current $(c\rho, \boldsymbol{J})$.

We extremize functions by sending the independent variable x to $x + dx$ and demanding that the variation $df = 0$ to first order in dx. That is,

$$f(x + dx) = f(x) + f'(x)\, dx + \tfrac{1}{2} f''(x)(dx)^2 + \ldots\ , \tag{5.67}$$

whence $df = f'(x)\, dx + \mathcal{O}\big((dx)^2\big)$ and thus

$$f'(x^*) = 0 \quad \Longleftrightarrow \quad x^* \text{ an extremum.} \tag{5.68}$$

We extremize *functionals* by sending

$$f(x) \to f(x) + \delta f(x) \tag{5.69}$$

and demanding that the variation δF in the functional $F[f(x)]$ vanish to first order in $\delta f(x)$. The variation $\delta f(x)$ must sometimes satisfy certain boundary conditions. For example, if

$F[f(x)]$ only operates on functions which vanish at a pair of endpoints, *i.e.* $f(x_a) = f(x_b) = 0$, then when we extremize the functional F we must do so *within the space of allowed functions*. Thus, we would in this case require $\delta f(x_a) = \delta f(x_b) = 0$. We may expand the functional $F[f + \delta f]$ in a *functional Taylor series*,

$$\begin{aligned} F[f+\delta f] = F[f] &+ \int dx_1\, K_1(x_1)\, \delta f(x_1) + \tfrac{1}{2!}\int dx_1 \int dx_2\, K_2(x_1,x_2)\, \delta f(x_1)\, \delta f(x_2) \\ &+ \tfrac{1}{3!}\int dx_1 \int dx_2 \int dx_3\, K_3(x_1,x_2,x_3)\, \delta f(x_1)\, \delta f(x_2)\, \delta f(x_3) + \ldots \end{aligned} \tag{5.70}$$

and we write

$$K_n(x_1,\ldots,x_n) \equiv \frac{\delta^n F}{\delta f(x_1) \cdots \delta f(x_n)} \ . \tag{5.71}$$

In a more general case, $F = F[\{f_i(\boldsymbol{x})\}$ is a functional of several functions, each of which is a function of several independent variables.[1] We then write

$$\begin{aligned} F[\{f_i + \delta f_i\}] = F[\{f_i\}] &+ \int d\boldsymbol{x}_1\, K_1^i(\boldsymbol{x}_1)\, \delta f_i(\boldsymbol{x}_1) \\ &+ \tfrac{1}{2!}\int d\boldsymbol{x}_1 \int d\boldsymbol{x}_2\, K_2^{ij}(\boldsymbol{x}_1,\boldsymbol{x}_2)\, \delta f_i(\boldsymbol{x}_1)\, \delta f_j(\boldsymbol{x}_2) \\ &+ \tfrac{1}{3!}\int d\boldsymbol{x}_1 \int d\boldsymbol{x}_2 \int dx_3\ K_3^{ijk}(\boldsymbol{x}_1,\boldsymbol{x}_2,x_3)\, \delta f_i(\boldsymbol{x}_1)\, \delta f_j(\boldsymbol{x}_2)\, \delta f_k(\boldsymbol{x}_3) + \ldots\ , \end{aligned} \tag{5.72}$$

with

$$K_n^{i_1 i_2 \cdots i_n}(\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n) = \frac{\delta^n F}{\delta f_{i_1}(\boldsymbol{x}_1)\, \delta f_{i_2}(\boldsymbol{x}_2)\, \delta f_{i_n}(\boldsymbol{x}_n)} \ . \tag{5.73}$$

Another way to compute functional derivatives is to send

$$f(x) \to f(x) + \epsilon_1\, \delta(x - x_1) + \ldots + \epsilon_n\, \delta(x - x_n) \tag{5.74}$$

and then differentiate n times with respect to ϵ_1 through ϵ_n. That is,

$$\frac{\delta^n F}{\delta f(x_1) \cdots \delta f(x_n)} = \frac{\partial^n}{\partial\epsilon_1 \cdots \partial\epsilon_n}\bigg|_{\epsilon_1=\epsilon_2=\cdots\epsilon_n=0} F\big[f(x) + \epsilon_1\, \delta(x - x_1) + \ldots + \epsilon_n\, \delta(x - x_n)\big] \ . \tag{5.75}$$

Let's see how this works. As an example, we'll take the action functional from classical mechanics,

$$S[q(t)] = \int\limits_{t_a}^{t_b} dt\, \Big\{ \tfrac{1}{2} m\dot{q}^2 - U(q) \Big\} \ . \tag{5.76}$$

[1] It may be also be that different functions depend on a different number of independent variables. *E.g.* $F = F[f(x),\, g(x,y),\, h(x,y,z)]$.

To compute the first functional derivative, we replace the function $q(t)$ with $q(t)+\epsilon\,\delta(t-t_1)$, and expand in powers of ϵ:

$$\begin{aligned} S\big[q(t)+\epsilon\delta(t-t_1)\big] &= S[q(t)] + \epsilon \int\limits_{t_a}^{t_b}\! dt\, \Big\{ m\,\dot q\,\delta'(t-t_1) - U'(q)\,\delta(t-t_1)\Big\} \\ &= -\epsilon\,\Big\{ m\,\ddot q(t_1) + U'\big(q(t_1)\big)\Big\}\ , \end{aligned} \tag{5.77}$$

hence

$$\frac{\delta S}{\delta q(t)} = -\Big\{ m\,\ddot q(t) + U'\big(q(t)\big)\Big\} \tag{5.78}$$

and setting the first functional derivative to zero yields Newton's Second Law, $m\ddot q = -U'(q)$, for all $t \in [t_a, t_b]$. Note that we have used the result

$$\int\limits_{-\infty}^{\infty}\! dt\,\delta'(t-t_1)\,h(t) = -h'(t_1)\ , \tag{5.79}$$

which is easily established upon integration by parts.

To compute the second functional derivative, we replace

$$q(t) \longrightarrow q(t) + \epsilon_1\,\delta(t-t_1) + \epsilon_2\,\delta(t-t_2) \tag{5.80}$$

and extract the term of order $\epsilon_1\,\epsilon_2$ in the double Taylor expansion. One finds this term to be

$$\epsilon_1\,\epsilon_2 \int\limits_{t_a}^{t_b}\! dt\,\Big\{ m\,\delta'(t-t_1)\,\delta'(t-t_2) - U''(q)\,\delta(t-t_1)\,\delta(t-t_2)\Big\}\ . \tag{5.81}$$

Note that we needn't bother with terms proportional to ϵ_1^2 or ϵ_2^2 since the recipe is to differentiate once with respect to each of ϵ_1 and ϵ_2 and then to set $\epsilon_1 = \epsilon_2 = 0$. This procedure uniquely selects the term proportional to $\epsilon_1\,\epsilon_2$, and yields

$$\frac{\delta^2 S}{\delta q(t_1)\,\delta q(t_2)} = -\Big\{ m\,\delta''(t_1-t_2) + U''\big(q(t_1)\big)\,\delta(t_1-t_2)\Big\}\ . \tag{5.82}$$

In multivariable calculus, the stability of an extremum is assessed by computing the matrix of second derivatives at the extremal point, known as the Hessian matrix. One has

$$\frac{\partial f}{\partial x_i}\bigg|_{\boldsymbol{x}^*} = 0 \quad \forall\ i \qquad ; \qquad H_{ij} = \frac{\partial^2 f}{\partial x_i\,\partial x_j}\bigg|_{\boldsymbol{x}^*}\ . \tag{5.83}$$

The eigenvalues of the Hessian H_{ij} determine the stability of the extremum. Since H_{ij} is a symmetric matrix, its eigenvectors η^α may be chosen to be orthogonal. The associated eigenvalues λ_α, defined by the equation

$$H_{ij}\,\eta^\alpha_j = \lambda_\alpha\,\eta^\alpha_i\ , \tag{5.84}$$

are the respective curvatures in the directions η^α, where $\alpha \in \{1,\ldots,n\}$ where n is the number of variables. The extremum is a local minimum if all the eigenvalues λ_α are positive, a maximum if all are negative, and otherwise is a saddle point. Near a saddle point, there are some directions in which the function increases and some in which it decreases.

In the case of functionals, the second functional derivative $K_2(x_1,x_2)$ defines an eigenvalue problem for $\delta f(x)$:

$$\int\limits_{x_a}^{x_b} dx_2\, K_2(x_1,x_2)\,\delta f(x_2) = \lambda\, \delta f(x_1) \ . \tag{5.85}$$

In general there are an infinite number of solutions to this equation which form a basis in function space, subject to appropriate boundary conditions at $x_{\rm a}$ and $x_{\rm b}$. For example, in the case of the action functional from classical mechanics, the above eigenvalue equation becomes a differential equation,

$$-\bigg\{ m\,\frac{d^2}{dt^2} + U''\big(q^*(t)\big)\bigg\}\,\delta q(t) = \lambda\,\delta q(t) \ , \tag{5.86}$$

where $q^*(t)$ is the solution to the Euler-Lagrange equations. As with the case of ordinary multivariable functions, the functional extremum is a local minimum (in function space) if every eigenvalue λ_α is positive, a local maximum if every eigenvalue is negative, and a saddle point otherwise.

Consider the simple harmonic oscillator, for which $U(q) = \frac{1}{2}\, m\omega_0^2\, q^2$. Then $U''\big(q^*(t)\big) = m\,\omega_0^2$; note that we don't even need to know the solution $q^*(t)$ to obtain the second functional derivative in this special case. The eigenvectors obey $m(\delta\ddot{q} + \omega_0^2\,\delta q) = -\lambda\,\delta q$, hence

$$\delta q(t) = A\cos\Big(\sqrt{\omega_0^2 + (\lambda/m)}\; t + \varphi\Big) \ , \tag{5.87}$$

where A and φ are constants. Demanding $\delta q(t_{\rm a}) = \delta q(t_{\rm b}) = 0$ requires

$$\sqrt{\omega_0^2 + (\lambda/m)}\,\big(t_{\rm b} - t_{\rm a}\big) = n\pi \ , \tag{5.88}$$

where n is an integer. Thus, the eigenfunctions are

$$\delta q_n(t) = A\sin\bigg(n\pi\cdot\frac{t-t_{\rm a}}{t_{\rm b}-t_{\rm a}}\bigg) \ , \tag{5.89}$$

and the eigenvalues are

$$\lambda_n = m\Big(\frac{n\pi}{T}\Big)^2 - m\omega_0^2 \ , \tag{5.90}$$

where $T = t_{\rm b} - t_{\rm a}$. Thus, so long as $T > \pi/\omega_0$, there is at least one negative eigenvalue. Indeed, for $\frac{n\pi}{\omega_0} < T < \frac{(n+1)\pi}{\omega_0}$ there will be n negative eigenvalues. This means the action is generally not a minimum, but rather lies at a *saddle point* in the (infinite-dimensional) function space.

To test this explicitly, consider a harmonic oscillator with the boundary conditions $q(0) = 0$ and $q(T) = Q$. The equations of motion, $\ddot{q} + \omega_0^2\, q = 0$, along with the boundary conditions, determine the motion,

$$q^*(t) = \frac{Q\, \sin(\omega_0 t)}{\sin(\omega_0 T)} \ . \tag{5.91}$$

The action for this path is then

$$\begin{aligned} S[q^*(t)] &= \int\limits_0^T \! dt \left\{ \tfrac{1}{2} m\, \dot{q}^{*2} - \tfrac{1}{2} m\omega_0^2\, q^{*2} \right\} \\ &= \frac{m\, \omega_0^2\, Q^2}{2 \sin^2\!\omega_0 T} \int\limits_0^T \! dt \left\{ \cos^2\!\omega_0 t - \sin^2\!\omega_0 t \right\} \\ &= \tfrac{1}{2} m\omega_0\, Q^2\ \mathrm{ctn}\,(\omega_0 T) \ . \end{aligned} \tag{5.92}$$

Next consider the path $q(t) = Q\, t/T$ which satisfies the boundary conditions but does not satisfy the equations of motion (it proceeds with constant velocity). One finds the action for this path is

$$S[q(t)] = \tfrac{1}{2} m\omega_0\, Q^2 \left(\frac{1}{\omega_0 T} - \tfrac{1}{3}\omega_0 T \right) \ . \tag{5.93}$$

Thus, provided $\omega_0 T \neq n\pi$, in the limit $T \to \infty$ we find that the constant velocity path has lower action.

Finally, consider the general mechanical action,

$$S\big[q(t)\big] = \int\limits_{t_a}^{t_b} \! dt\, L(q, \dot{q}, t) \ . \tag{5.94}$$

We now evaluate the first few terms in the functional Taylor series:

$$\begin{aligned} S\big[q^*(t) + \delta q(t)\big] = \int\limits_{t_a}^{t_b} \! dt \Bigg\{ & L(q^*, \dot{q}^*, t) + \frac{\partial L}{\partial q_i}\bigg|_{q^*} \delta q_i + \frac{\partial L}{\partial \dot{q}_i}\bigg|_{q^*} \delta \dot{q}_i \\ & + \frac{1}{2}\, \frac{\partial^2 L}{\partial q_i\, \partial q_j}\bigg|_{q^*} \delta q_i\, \delta q_j + \frac{\partial^2 L}{\partial q_i\, \partial \dot{q}_j}\bigg|_{q^*} \delta q_i\, \delta \dot{q}_j + \frac{1}{2}\, \frac{\partial^2 L}{\partial \dot{q}_i\, \partial \dot{q}_j}\bigg|_{q^*} \delta \dot{q}_i\, \delta \dot{q}_j + \ldots \Bigg\} \ . \end{aligned} \tag{5.95}$$

To identify the functional derivatives, we integrate by parts. Let $\Phi_{\ldots}(t)$ be an arbitrary function of time. Then

$$\int_{t_a}^{t_b} dt\,\Phi_i(t)\,\delta\dot{q}_i(t) = -\int_{t_a}^{t_b} dt\,\dot{\Phi}_i(t)\,\delta q_i(t) \tag{5.96}$$

$$\begin{aligned}\int_{t_a}^{t_b} dt\,\Phi_{ij}(t)\,\delta q_i(t)\,\delta\dot{q}_j(t) &= \int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt'\,\Phi_{ij}(t)\,\delta(t-t')\,\frac{d}{dt'}\,\delta q_i(t)\,\delta q_j(t') \\ &= \int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt'\,\Phi_{ij}(t))\,\delta'(t-t')\,\delta q_i(t)\,\delta q_j(t')\end{aligned} \tag{5.97}$$

$$\begin{aligned}\int_{t_a}^{t_b} dt\,\Phi_{ij}(t)\,d\dot{q}_i(t)\,\delta\dot{q}_j(t) &= \int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt'\,\Phi_{ij}(t)\,\delta(t-t')\,\frac{d}{dt}\,\frac{d}{dt'}\,\delta q_i(t)\,\delta q_j(t') \\ &= -\int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt' \Big[\dot{\Phi}_{ij}(t)\,\delta'(t-t') + \Phi_{ij}(t)\,\delta''(t-t')\Big]\,\delta q_i(t)\,\delta q_j(t')\ .\end{aligned} \tag{5.98}$$

Thus,

$$\frac{\delta S}{\delta q_i(t)} = \left[\frac{\partial L}{\partial q_i} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right)\right]_{q^*(t)} \tag{5.99}$$

$$\begin{aligned}\frac{\delta^2 S}{\delta q_i(t)\,\delta q_j(t')} = \Bigg\{ &\frac{\partial^2 L}{\partial q_i\,\partial q_j}\bigg|_{q^*(t)} \delta(t-t') - \frac{\partial^2 L}{\partial \dot{q}_i\,\partial \dot{q}_j}\bigg|_{q^*(t)} \delta''(t-t') \\ &+ \left[2\,\frac{\partial^2 L}{\partial q_i\,\partial \dot{q}_j} - \frac{d}{dt}\left(\frac{\partial^2 L}{\partial \dot{q}_i\,\partial \dot{q}_j}\right)\right]_{q^*(t)} \delta'(t-t')\Bigg\}\ .\end{aligned} \tag{5.100}$$