

15

Functional Derivatives

15.1 Functionals

A **functional** $G[f]$ is a map from a space of functions to a set of numbers. For instance, the **action** functional $S[q]$ for a particle in one dimension maps the coordinate $q(t)$, which is a function of the time t , into a number—the action of the process. If the particle has mass m and is moving slowly and freely, then for the interval (t_1, t_2) its action is

$$S_0[q] = \int_{t_1}^{t_2} dt \frac{m}{2} \left(\frac{dq(t)}{dt} \right)^2. \quad (15.1)$$

If the particle is moving in a potential $V(q(t))$, then its action is

$$S[q] = \int_{t_1}^{t_2} dt \left[\frac{m}{2} \left(\frac{dq(t)}{dt} \right)^2 - V(q(t)) \right]. \quad (15.2)$$

15.2 Functional Derivatives

A **functional derivative** is a functional

$$\delta G[f][h] = \left. \frac{d}{d\epsilon} G[f + \epsilon h] \right|_{\epsilon=0} \quad (15.3)$$

of a functional. For instance, if $G_n[f]$ is the functional

$$G_n[f] = \int dx f^n(x) \quad (15.4)$$

then its functional derivative is the functional that maps the pair of functions f, h to the number

$$\begin{aligned}\delta G_n[f][h] &= \left. \frac{d}{d\epsilon} G_n[f + \epsilon h] \right|_{\epsilon=0} = \left. \frac{d}{d\epsilon} \int dx (f(x) + \epsilon h(x))^n \right|_{\epsilon=0} \\ &= \int dx n f^{n-1}(x) h(x).\end{aligned}\quad (15.5)$$

Physicists often use the less elaborate notation

$$\frac{\delta G[f]}{\delta f(y)} = \delta G[f][\delta_y] \quad (15.6)$$

in which the function $h(x)$ is $\delta_y(x) = \delta(x-y)$. Thus in the preceding example

$$\frac{\delta G[f]}{\delta f(y)} = \int dx n f^{n-1}(x) \delta(x-y) = n f^{n-1}(y). \quad (15.7)$$

Functional derivatives of functionals that involve powers of derivatives also are easily dealt with. Suppose that the functional involves the square of the derivative $f'(x)$

$$G[f] = \int dx (f'(x))^2. \quad (15.8)$$

Then its functional derivative is

$$\begin{aligned}\delta G[f][h] &= \left. \frac{d}{d\epsilon} G[f + \epsilon h] \right|_{\epsilon=0} = \left. \frac{d}{d\epsilon} \int dx (f'(x) + \epsilon h'(x))^2 \right|_{\epsilon=0} \\ &= \int dx 2f'(x)h'(x) = -2 \int dx f''(x)h(x)\end{aligned}\quad (15.9)$$

in which we have integrated by parts and used suitable boundary conditions on $h(x)$ to drop the surface terms. In physics notation, $h(x) = \delta(x-y)$, and

$$\frac{\delta G[f]}{\delta f(y)} = -2 \int dx f''(x) \delta(x-y) = -2f''(y). \quad (15.10)$$

Let's now compute the functional derivative of the action (15.2), which in-

volves the square of the time-derivative $\dot{q}(t)$ and the potential energy $V(q(t))$

$$\begin{aligned}\delta S[q][h] &= \left. \frac{d}{d\epsilon} S[q + \epsilon h] \right|_{\epsilon=0} \\ &= \left. \frac{d}{d\epsilon} \int dt \left[\frac{m}{2} (\dot{q}(t) + \epsilon \dot{h}(t))^2 - V(q(t) + \epsilon h(t)) \right] \right|_{\epsilon=0} \\ &= \int dt [m\dot{q}(t)\dot{h}(t) - V'(q(t))h(t)] \\ &= \int dt [-m\ddot{q}(t) - V'(q(t))] h(t)\end{aligned}\quad (15.11)$$

where we once again have integrated by parts and used suitable boundary conditions to drop the surface terms. In physics notation, this is

$$\frac{\delta S[q]}{\delta q(t)} = \int dt' [-m\ddot{q}(t') - V'(q(t'))] \delta(t' - t) = -m\ddot{q}(t) - V'(q(t)). \quad (15.12)$$

In these terms, the stationarity of the action $S[q]$ is the vanishing of its functional derivative either in the form

$$\delta S[q][h] = 0 \quad (15.13)$$

for arbitrary functions $h(t)$ (that **vanish at the end points of the interval**) or equivalently in the form

$$\frac{\delta S[q]}{\delta q(t)} = 0 \quad (15.14)$$

which is Lagrange's equation of motion

$$m\ddot{q}(t) = -V'(q(t)). \quad (15.15)$$

Physicists also use the compact notation

$$\frac{\delta^2 Z[j]}{\delta j(y)\delta j(z)} \equiv \left. \frac{\partial^2 Z[j + \epsilon\delta_y + \epsilon'\delta_z]}{\partial\epsilon\partial\epsilon'} \right|_{\epsilon=\epsilon'=0} \quad (15.16)$$

in which $\delta_y(x) = \delta(x - y)$ and $\delta_z(x) = \delta(x - z)$.

Example 15.1 (Shortest Path is a Straight Line). On a plane, the length of the path $(x, y(x))$ from (x_0, y_0) to (x_1, y_1) is

$$L[y] = \int_{x_0}^{x_1} \sqrt{dx^2 + dy^2} = \int_{x_0}^{x_1} \sqrt{1 + y'^2} dx. \quad (15.17)$$

The shortest path $y(x)$ minimizes this length $L[y]$, so

$$\begin{aligned}\delta L[y][h] &= \left. \frac{d}{d\epsilon} L[y + \epsilon h] \right|_{\epsilon=0} = \left. \frac{d}{d\epsilon} \int_{x_0}^{x_1} \sqrt{1 + (y' + \epsilon h')^2} dx \right|_{\epsilon=0} \\ &= \int_{x_0}^{x_1} \frac{y' h'}{\sqrt{1 + y'^2}} dx = - \int_{x_0}^{x_1} h \frac{d}{dx} \frac{y'}{\sqrt{1 + y'^2}} dx = 0\end{aligned}\quad (15.18)$$

since $h(x_0) = h(x_1) = 0$. This can vanish for arbitrary $h(x)$ only if

$$\frac{d}{dx} \frac{y'}{\sqrt{1 + y'^2}} = 0 \quad (15.19)$$

which implies $y'' = 0$. Thus $y(x)$ is a straight line, $y = mx + b$. \square

15.3 Higher-Order Functional Derivatives

The second functional derivative is

$$\delta^2 G[f][h] = \left. \frac{d^2}{d\epsilon^2} G[f + \epsilon h] \right|_{\epsilon=0}. \quad (15.20)$$

So if $G_N[f]$ is the functional

$$G_N[f] = \int f^N(x) dx \quad (15.21)$$

then

$$\begin{aligned}\delta^2 G_N[f][h] &= \left. \frac{d^2}{d\epsilon^2} G_N[f + \epsilon h] \right|_{\epsilon=0} = \left. \frac{d^2}{d\epsilon^2} \int (f(x) + \epsilon h(x))^N dx \right|_{\epsilon=0} \\ &= \left. \frac{d^2}{d\epsilon^2} \int \binom{N}{2} \epsilon^2 h^2(x) f^{N-2}(x) dx \right|_{\epsilon=0} \\ &= N(N-1) \int f^{N-2}(x) h^2(x) dx.\end{aligned}\quad (15.22)$$

Example 15.2 ($\delta^2 S_0$). The second functional derivative of the action $S_0[q]$ (15.1) is

$$\begin{aligned}\delta^2 S_0[q][h] &= \left. \frac{d^2}{d\epsilon^2} \int_{t_1}^{t_2} dt \frac{m}{2} \left(\frac{dq(t)}{dt} + \epsilon \frac{dh(t)}{dt} \right)^2 \right|_{\epsilon=0} \\ &= \int_{t_1}^{t_2} dt m \left(\frac{dh(t)}{dt} \right)^2 \geq 0\end{aligned}\quad (15.23)$$

and is positive for all functions $h(t)$. Thus the stationary classical trajectory

$$q(t) = \frac{t - t_1}{t_2 - t_1} q(t_2) + \frac{t_2 - t}{t_2 - t_1} q(t_1) \quad (15.24)$$

is a **minimum** of the action $S_0[q]$. \square

The second functional derivative of the action $S[q]$ (15.2) is

$$\begin{aligned}\delta^2 S[q][h] &= \frac{d^2}{d\epsilon^2} \int_{t_1}^{t_2} dt \left[\frac{m}{2} \left(\frac{dq(t)}{dt} + \epsilon \frac{dh(t)}{dt} \right)^2 - V(q(t) + \epsilon h(t)) \right] \Big|_{\epsilon=0} \\ &= \int_{t_1}^{t_2} dt \left[m \left(\frac{dh(t)}{dt} \right)^2 - \frac{\partial^2 V(q(t))}{\partial q^2(t)} h^2(t) \right]\end{aligned}\quad (15.25)$$

and it can be positive, zero, or negative. Chaos sometimes arises in systems of several particles when the second variation of $S[q]$ about a stationary path is negative, $\delta^2 S[q][h] < 0$ while $\delta S[q][h] = 0$.

The n th functional derivative is defined as

$$\delta^n G[f][h] = \frac{d^n}{d\epsilon^n} G[f + \epsilon h] \Big|_{\epsilon=0}. \quad (15.26)$$

The n th functional derivative of the functional (15.21) is

$$\delta^n G_N[f][h] = \frac{N!}{(N-n)!} \int f^{N-n}(x) h^n(x) dx. \quad (15.27)$$

15.4 Functional Taylor Series

It follows from the Taylor-series theorem (4.6) that

$$e^\delta G[f][h] = \sum_{n=0}^{\infty} \frac{\delta^n}{n!} G[f][h] = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{d^n}{d\epsilon^n} G[f + \epsilon h] \Big|_{\epsilon=0} = G[f + h] \quad (15.28)$$

which illustrates an advantage of the present mathematical notation.

The functional $S_0[q]$ of Eq.(15.1) provides a simple example of the functional Taylor series (15.28):

$$\begin{aligned}e^\delta S_0[q][h] &= \left(1 + \frac{d}{d\epsilon} + \frac{1}{2} \frac{d^2}{d\epsilon^2} \right) S_0[q + \epsilon h] \Big|_{\epsilon=0} \\ &= \frac{m}{2} \int_{t_1}^{t_2} \left(1 + \frac{d}{d\epsilon} + \frac{1}{2} \frac{d^2}{d\epsilon^2} \right) \left(\dot{q}(t) + \epsilon \dot{h}(t) \right)^2 dt \Big|_{\epsilon=0} \\ &= \frac{m}{2} \int_{t_1}^{t_2} \left(\dot{q}^2(t) + 2\dot{q}(t)\dot{h}(t) + \dot{h}^2(t) \right) dt \\ &= \frac{m}{2} \int_{t_1}^{t_2} \left(\dot{q}(t) + \dot{h}(t) \right)^2 dt = S_0[q + h].\end{aligned}\quad (15.29)$$

If the function $q(t)$ makes the action $S_0[q]$ stationary, and if $h(t)$ is smooth and vanishes at the endpoints of the time interval, then

$$S_0[q+h] = S_0[q] + S_0[h]. \quad (15.30)$$

More generally, if $q(t)$ makes the action $S[q]$ stationary, and $h(t)$ is any loop from and to the origin, then

$$S[q+h] = e^\delta S[q][h] = S[q] + \sum_{n=2}^{\infty} \frac{1}{n!} \frac{d^n}{d\epsilon^n} S[q+\epsilon h]|_{\epsilon=0}. \quad (15.31)$$

If $S_2[q]$ also is quadratic in q and \dot{q} , then

$$S_2[q+h] = S_2[q] + S_2[h]. \quad (15.32)$$

15.5 Functional Differential Equations

In inner products like $\langle q'|f\rangle$, we represent the momentum operator as

$$p = \frac{\hbar}{i} \frac{d}{dq'} \quad (15.33)$$

because then

$$\langle q'|p q|f\rangle = \frac{\hbar}{i} \frac{d}{dq'} \langle q'|q|f\rangle = \frac{\hbar}{i} \frac{d}{dq'} (q' \langle q'|f\rangle) = \left(\frac{\hbar}{i} + q' \frac{\hbar}{i} \frac{d}{dq'} \right) \langle q'|f\rangle \quad (15.34)$$

which respects the commutation relation $[q, p] = i\hbar$.

So too in inner products $\langle \phi'|f\rangle$ of eigenstates $|\phi'\rangle$ of $\phi(\mathbf{x}, t)$

$$\phi(\mathbf{x}, t)|\phi'\rangle = \phi'(\mathbf{x})|\phi'\rangle \quad (15.35)$$

we can represent the momentum $\pi(\mathbf{x}, t)$ canonically conjugate to the field $\phi(\mathbf{x}, t)$ as the functional derivative

$$\pi(\mathbf{x}, t) = \frac{\hbar}{i} \frac{\delta}{\delta \phi'(\mathbf{x})} \quad (15.36)$$

because then

$$\begin{aligned}
 \langle \phi' | \pi(\mathbf{x}', t) \phi(\mathbf{x}, t) | f \rangle &= \frac{\hbar}{i} \frac{\delta \langle \phi' | \phi(\mathbf{x}, t) | f \rangle}{\delta \phi'(\mathbf{x}')} = \frac{\hbar}{i} \frac{\delta(\phi'(\mathbf{x}) \langle \phi' | f \rangle)}{\delta \phi'(\mathbf{x}')} \\
 &= \frac{\hbar}{i} \frac{\delta}{\delta \phi'(\mathbf{x}')} \left(\int \delta(\mathbf{x} - \mathbf{x}') \phi'(\mathbf{x}') d^3 x' \langle \phi' | f \rangle \right) \\
 &= \frac{\hbar}{i} \left(\delta(\mathbf{x} - \mathbf{x}') + \phi'(\mathbf{x}) \frac{\delta}{\delta \phi'(\mathbf{x}')} \right) \langle \phi' | f \rangle \\
 &= \langle \phi' | -i\hbar \delta(\mathbf{x} - \mathbf{x}') + \phi(\mathbf{x}, t) \pi(\mathbf{x}', t) | f \rangle
 \end{aligned} \tag{15.37}$$

which respects the equal-time commutation relation

$$[\phi(\mathbf{x}, t), \pi(\mathbf{x}', t)] = i\hbar \delta(\mathbf{x} - \mathbf{x}'). \tag{15.38}$$

We can use the representation (15.36) for $\pi(x)$ to find the wave function of the ground state $|0\rangle$ of the hamiltonian

$$H = \frac{1}{2} \int [\pi^2 + (\nabla\phi)^2 + m^2\phi^2] d^3x \tag{15.39}$$

where we have set $\hbar = c = 1$. We will use the trick we used in section 2.11 to find the ground state $|0\rangle$ of the harmonic-oscillator hamiltonian

$$H_0 = \frac{p^2}{2m} + \frac{m\omega^2 q^2}{2}. \tag{15.40}$$

In that trick, one writes

$$\begin{aligned}
 H_0 &= \frac{1}{2m} (m\omega q - ip)(m\omega q + ip) + \frac{i\omega}{2} [p, q] \\
 &= \frac{1}{2m} (m\omega q - ip)(m\omega q + ip) + \frac{1}{2} \hbar\omega
 \end{aligned} \tag{15.41}$$

and seeks a state $|0\rangle$ that is annihilated by $m\omega q + ip$

$$\langle q' | m\omega q + ip | 0 \rangle = \left(m\omega q' + \hbar \frac{d}{dq'} \right) \langle q' | 0 \rangle = 0. \tag{15.42}$$

The solution to this differential equation

$$\frac{d}{dq'} \langle q' | 0 \rangle = -\frac{m\omega q'}{\hbar} \langle q' | 0 \rangle \tag{15.43}$$

is

$$\langle q' | 0 \rangle = \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} \exp\left(-\frac{m\omega q'^2}{2\hbar} \right) \tag{15.44}$$

in which the prefactor is a constant of normalization.

Extending that trick to the hamiltonian (15.39), we factor H

$$H = \frac{1}{2} \int \left[\sqrt{-\nabla^2 + m^2} \phi - i\pi \right] \left[\sqrt{-\nabla^2 + m^2} \phi + i\pi \right] d^3x + C \quad (15.45)$$

in which C is the (infinite) constant

$$C = \frac{i}{2} \int \left[\pi, \sqrt{-\Delta + m^2} \phi \right] d^3x. \quad (15.46)$$

The ground state $|0\rangle$ of H therefore must satisfy the functional differential equation $\langle \phi' | \sqrt{-\nabla^2 + m^2} \phi + i\pi | 0 \rangle = 0$ or

$$\frac{\delta \langle \phi' | 0 \rangle}{\delta \phi'(\mathbf{x})} = -\sqrt{-\nabla^2 + m^2} \phi'(\mathbf{x}) \langle \phi' | 0 \rangle. \quad (15.47)$$

The solution to this equation is

$$\langle \phi | 0 \rangle = N \exp \left(-\frac{1}{2} \int \phi(\mathbf{x}) \sqrt{-\nabla^2 + m^2} \phi(\mathbf{x}) d^3x \right) \quad (15.48)$$

in which N is a normalization constant. To see that this functional does satisfy equation (15.47), we compute the derivative

$$\frac{d \langle \phi + \epsilon h | 0 \rangle}{d\epsilon} = N \frac{d}{d\epsilon} \exp \left[-\frac{1}{2} \int (\phi + \epsilon h) \sqrt{-\nabla^2 + m^2} (\phi + \epsilon h) d^3x \right] \quad (15.49)$$

which at $\epsilon = 0$ is

$$\begin{aligned} \left. \frac{d \langle \phi + \epsilon h | 0 \rangle}{d\epsilon} \right|_{\epsilon=0} &= -\frac{1}{2} \left[\int h(\mathbf{x}) \sqrt{-\nabla^2 + m^2} \phi(\mathbf{x}) d^3x \right. \\ &\quad \left. + \int \phi(\mathbf{x}) \sqrt{-\nabla^2 + m^2} h(\mathbf{x}) d^3x \right] \langle \phi | 0 \rangle. \end{aligned} \quad (15.50)$$

We integrate the second term by parts and drop the surface terms because the smooth function h goes to zero quickly as its arguments go to infinity. We then have

$$\left. \frac{d \langle \phi + \epsilon h | 0 \rangle}{d\epsilon} \right|_{\epsilon=0} = - \int h(\mathbf{x}') \sqrt{-\nabla^2 + m^2} \phi(\mathbf{x}') d^3x' \langle \phi | 0 \rangle. \quad (15.51)$$

Letting $h(\mathbf{x}') = \delta^{(3)}(\mathbf{x}' - \mathbf{x})$, we arrive at (15.47).

Since $\phi(x)$ is real, its spatial Fourier transform

$$\tilde{\phi}(\mathbf{p}) = \int e^{-i\mathbf{p}\cdot\mathbf{x}} \phi(\mathbf{x}) \frac{d^3x}{(2\pi)^{3/2}} \quad (15.52)$$

satisfies $\tilde{\phi}(-\mathbf{p}) = \tilde{\phi}^*(\mathbf{p})$. In terms of it, the ground-state wave function is

$$\langle \phi | 0 \rangle = N \exp \left(-\frac{1}{2} \int |\tilde{\phi}(\mathbf{p})|^2 \sqrt{\mathbf{p}^2 + m^2} d^3p \right). \quad (15.53)$$

Example 15.3 (Other theories, other vacua). We can find exact ground states for interacting theories with hamiltonians like

$$H = \frac{1}{2} \int \left[\sqrt{-\nabla^2 + m^2} \phi - ic_n \phi^n - i\pi \right] \left[\sqrt{-\nabla^2 + m^2} \phi + ic_n \phi^n + i\pi \right] d^3x. \quad (15.54)$$

The state $|\Omega\rangle$ will be an eigenstate of H with eigenvalue zero if

$$\frac{\delta \langle \phi | \Omega \rangle}{\delta \phi(\mathbf{x})} = - \left[\sqrt{-\nabla^2 + m^2} \phi(\mathbf{x}) + ic_n \phi^n \right] \langle \phi | \Omega \rangle. \quad (15.55)$$

By extending the argument of equations (15.45–15.51), one may show (exercise 15.4) that the wave functional of the vacuum is

$$\langle \phi | \Omega \rangle = N \exp \left[- \int \left(\frac{1}{2} \phi \sqrt{-\nabla^2 + m^2} \phi + \frac{ic_n}{n+1} \phi^{n+1} \right) d^3x \right]. \quad (15.56)$$

□

Exercises

- 15.1 Compute the action $S_0[q]$ (15.1) for the classical path (15.24).
- 15.2 Use (15.25) to find a formula for the second functional derivative of the action (15.2) of the harmonic oscillator for which $V(q) = m\omega^2 q^2/2$.
- 15.3 Derive (15.53) from equations (15.48 & 15.52).
- 15.4 Show that (15.56) satisfies (15.55).