19
Functional derivatives

19.1 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

$$S_0[q] = \int_{t_1}^{t_2} dt \, \frac{m}{2} \left(\frac{dq(t)}{dt} \right)^2 . \tag{19.1}$$

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

$$S[q] = \int_{t_1}^{t_2} dt \, \left[\frac{m}{2} \left(\frac{dq(t)}{dt} \right)^2 - V(q(t)) \right] . \tag{19.2}$$

19.2 Functional derivatives

A **functional derivative** is a functional

$$\delta G[f][h] = \frac{d}{d\epsilon} G[f + \epsilon h] \bigg|_{\epsilon=0} \tag{19.3}$$

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

$$G_n[f] = \int dx \, f^n(x) \tag{19.4}$$

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

$$\delta G_n[f][h] = \frac{d}{d\epsilon} G_n[f + \epsilon h]\bigg|_{\epsilon=0} = \frac{d}{d\epsilon} \int dx\, (f(x) + \epsilon h(x))^n \bigg|_{\epsilon=0}$$
$$= \int dx\, n f^{n-1}(x) h(x). \tag{19.5}$$

Physicists often use the less elaborate notation

$$\frac{\delta G[f]}{\delta f(y)} = \delta G[f][\delta_y] \tag{19.6}$$

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

$$\frac{\delta G[f]}{\delta f(y)} = \int dx\, n f^{n-1}(x) \delta(x-y) = n f^{n-1}(y). \tag{19.7}$$

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

$$G[f] = \int dx\, \left(f'(x)\right)^2 . \tag{19.8}$$

Then its functional derivative is

$$\delta G[f][h] = \frac{d}{d\epsilon} G[f + \epsilon h]\bigg|_{\epsilon=0} = \frac{d}{d\epsilon} \int dx\, \left(f'(x) + \epsilon h'(x)\right)^2 \bigg|_{\epsilon=0}$$
$$= \int dx\, 2 f'(x) h'(x) = -2 \int dx\, f''(x) h(x) \tag{19.9}$$

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

$$\frac{\delta G[f]}{\delta f(y)} = -2 \int dx\, f''(x) \delta(x-y) = -2 f''(y). \tag{19.10}$$

Let's now compute the functional derivative of the action (19.2), which involves the square of the time-derivative $\dot{q}(t)$ and the potential energy $V(q(t))$

$$\begin{aligned}\delta S[q][h] &= \frac{d}{d\epsilon} S[q+\epsilon h]\Big|_{\epsilon=0} \\ &= \frac{d}{d\epsilon}\int dt \left[\frac{m}{2}\left(\dot{q}(t)+\epsilon\dot{h}(t)\right)^2 - V(q(t)+\epsilon h(t))\right]\Bigg|_{\epsilon=0} \\ &= \int dt \left[m\dot{q}(t)\dot{h}(t) - V'(q(t))h(t)\right] \\ &= \int dt \left[-m\ddot{q}(t) - V'(q(t))\right] h(t) \end{aligned} \tag{19.11}$$

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

$$\frac{\delta S[q]}{\delta q(t)} = \int dt' \left[-m\ddot{q}(t') - V'(q(t'))\right] \delta(t'-t) = -m\ddot{q}(t) - V'(q(t)). \tag{19.12}$$

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

$$\delta S[q][h] = 0 \tag{19.13}$$

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

$$\frac{\delta S[q]}{\delta q(t)} = 0 \tag{19.14}$$

which is Lagrange's equation of motion

$$m\ddot{q}(t) = -V'(q(t)). \tag{19.15}$$

Physicists also use the compact notation

$$\frac{\delta^2 Z[j]}{\delta j(y)\delta j(z)} \equiv \frac{\partial^2 Z[j+\epsilon\delta_y+\epsilon'\delta_z]}{\partial\epsilon\,\partial\epsilon'}\Bigg|_{\epsilon=\epsilon'=0} \tag{19.16}$$

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

Example 19.1 (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

$$L[y] = \int_{x_0}^{x_1} \sqrt{dx^2+dy^2} = \int_{x_0}^{x_1} \sqrt{1+y'^2}\,dx. \tag{19.17}$$

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

$$\delta L[y][h] = \frac{d}{d\epsilon} L[y+\epsilon h]\bigg|_{\epsilon=0} = \frac{d}{d\epsilon}\int_{x_0}^{x_1} \sqrt{1+(y'+\epsilon h')^2}\,dx\bigg|_{\epsilon=0}$$
$$= \int_{x_0}^{x_1} \frac{y'h'}{\sqrt{1+y'^2}}\,dx = -\int_{x_0}^{x_1} h\frac{d}{dx}\frac{y'}{\sqrt{1+y'^2}}\,dx = 0 \quad (19.18)$$

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

$$\frac{d}{dx}\frac{y'}{\sqrt{1+y'^2}} = 0 \quad (19.19)$$

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

19.3 Higher-order functional derivatives

The second functional derivative is

$$\delta^2 G[f][h] = \frac{d^2}{d\epsilon^2}\, G[f+\epsilon h]|_{\epsilon=0}\,. \quad (19.20)$$

So if $G_n[f]$ is the functional

$$G_n[f] = \int f^n(x)dx \quad (19.21)$$

then

$$\delta^2 G_n[f][h] = \frac{d^2}{d\epsilon^2}\, G_n[f+\epsilon h]|_{\epsilon=0} = \frac{d^2}{d\epsilon^2}\int (f(x)+\epsilon h(x))^n\,dx\bigg|_{\epsilon=0}$$
$$= \frac{d^2}{d\epsilon^2}\int \binom{n}{2}\epsilon^2 h^2(x) f^{n-2}(x)\,dx\bigg|_{\epsilon=0}$$
$$= n(n-1)\int f^{n-2}(x)h^2(x)dx. \quad (19.22)$$

Example 19.2 ($\delta^2 S_0$) The second functional derivative of the action $S_0[q]$ (19.1) is

$$\delta^2 S_0[q][h] = \frac{d^2}{d\epsilon^2}\int_{t_1}^{t_2} dt\, \frac{m}{2}\left(\frac{dq(t)}{dt} + \epsilon\frac{dh(t)}{dt}\right)^2\bigg|_{\epsilon=0}$$
$$= \int_{t_1}^{t_2} dt\, m\left(\frac{dh(t)}{dt}\right)^2 \geq 0 \quad (19.23)$$

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

$$q(t) = \frac{t-t_1}{t_2-t_1}\,q(t_2) + \frac{t_2-t}{t_2-t_1}\,q(t_1) \quad (19.24)$$

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

The second functional derivative of the action $S[q]$ (19.2) is

$$\delta^2 S[q][h] = \frac{d^2}{d\epsilon^2} \int_{t_1}^{t_2} dt \left[\frac{m}{2} \left(\frac{dq(t)}{dt} + \epsilon \frac{dh(t)}{dt} \right)^2 - V(q(t) + \epsilon h(t)) \right] \Bigg|_{\epsilon=0}$$
$$= \int_{t_1}^{t_2} dt \left[m \left(\frac{dh(t)}{dt} \right)^2 - \frac{\partial^2 V(q(t))}{\partial q^2(t)} h^2(t) \right] \tag{19.25}$$

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 nth functional derivative is defined as

$$\delta^n G[f][h] = \frac{d^n}{d\epsilon^n} \, G[f + \epsilon h]\big|_{\epsilon=0} \, . \tag{19.26}$$

The nth functional derivative of the functional (19.21) is

$$\delta^n G_N[f][h] = \frac{N!}{(N-n)!} \int f^{N-n}(x) h^n(x) dx. \tag{19.27}$$

19.4 Functional Taylor series

It follows from the Taylor-series theorem (5.7) that

$$e^{\delta} G[f][h] = \sum_{n=0}^{\infty} \frac{\delta^n}{n!} G[f][h] = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{d^n}{d\epsilon^n} G[f + \epsilon h] \Bigg|_{\epsilon=0} = G[f + h] \tag{19.28}$$

which illustrates an advantage of the present mathematical notation.

The functional $S_0[q]$ of Eq.(19.1) provides a simple example of the functional Taylor series (19.28):

$$e^{\delta} S_0[q][h] = \left(1 + \frac{d}{d\epsilon} + \frac{1}{2} \frac{d^2}{d\epsilon^2} \right) S_0[q + \epsilon h] \Bigg|_{\epsilon=0}$$
$$= \frac{m}{2} \int_{t_1}^{t_2} \left(1 + \frac{d}{d\epsilon} + \frac{1}{2} \frac{d^2}{d\epsilon^2} \right) \left(\dot{q}(t) + \epsilon \dot{h}(t) \right)^2 dt \Bigg|_{\epsilon=0}$$
$$= \frac{m}{2} \int_{t_1}^{t_2} \left(\dot{q}^2(t) + 2\dot{q}(t)\dot{h}(t) + \dot{h}^2(t) \right) dt$$
$$= \frac{m}{2} \int_{t_1}^{t_2} \left(\dot{q}(t) + \dot{h}(t) \right)^2 dt = S_0[q + h]. \tag{19.29}$$

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

$$S_0[q+h] = S_0[q] + S_0[h]. \tag{19.30}$$

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

$$S[q+h] = e^{\delta} S[q][h] = S[q] + \sum_{n=2}^{\infty} \frac{1}{n!} \frac{d^n}{d\epsilon^n} \, S[q+\epsilon h]\big|_{\epsilon=0} . \tag{19.31}$$

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

$$S_2[q+h] = S_2[q] + S_2[h]. \tag{19.32}$$

19.5 Functional differential equations

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

$$p = \frac{\hbar}{i} \frac{d}{dq'} \tag{19.33}$$

because then

$$\langle q'|p\,q|f\rangle = \frac{\hbar}{i} \frac{d}{dq'} \langle q'|q|f\rangle = \frac{\hbar}{i} \frac{d}{dq'} \Big(q' \langle q'|f\rangle \Big) = \left(\frac{\hbar}{i} + q' \frac{\hbar}{i} \frac{d}{dq'} \right) \langle q'|f\rangle \tag{19.34}$$

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

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

$$\phi(\boldsymbol{x},t)|\phi'\rangle = \phi'(\boldsymbol{x})|\phi'\rangle \tag{19.35}$$

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

$$\pi(\boldsymbol{x},t) = \frac{\hbar}{i} \frac{\delta}{\delta\phi'(\boldsymbol{x})} \tag{19.36}$$

because then

$$\begin{aligned}
\langle\phi'|\pi(\boldsymbol{x'},t)\phi(\boldsymbol{x},t)|f\rangle &= \frac{\hbar}{i}\frac{\delta\langle\phi'|\phi(\boldsymbol{x},t)|f\rangle}{\delta\phi'(\boldsymbol{x'})} = \frac{\hbar}{i}\frac{\delta\big(\phi'(\boldsymbol{x})\langle\phi'|f\rangle\big)}{\delta\phi'(\boldsymbol{x'})} \\
&= \frac{\hbar}{i}\frac{\delta}{\delta\phi'(\boldsymbol{x'})}\left(\int \delta(\boldsymbol{x}-\boldsymbol{x'})\,\phi'(\boldsymbol{x'})\,d^3x'\,\langle\phi'|f\rangle\right) \\
&= \frac{\hbar}{i}\left(\delta(\boldsymbol{x}-\boldsymbol{x'}) + \phi'(\boldsymbol{x})\frac{\delta}{\delta\phi'(\boldsymbol{x'})}\right)\langle\phi'|f\rangle \\
&= \langle\phi'| - i\hbar\delta(\boldsymbol{x}-\boldsymbol{x'}) + \phi(\boldsymbol{x},t)\,\pi(\boldsymbol{x'},t)|f\rangle
\end{aligned} \tag{19.37}$$

which respects the equal-time commutation relation

$$[\phi(\boldsymbol{x},t),\pi(\boldsymbol{x'},t)] = i\,\hbar\,\delta(\boldsymbol{x}-\boldsymbol{x'}). \tag{19.38}$$

We can use the representation (19.36) for $\pi(x)$ to find the wave function of the ground state $|0\rangle$ of the hamiltonian

$$H = \frac{1}{2}\int \left[\pi^2 + (\nabla\phi)^2 + m^2\phi^2\right]\,d^3x \tag{19.39}$$

where we have set $\hbar = c = 1$. We will use the trick we used in section 18.1 to find the ground state $|0\rangle$ of the harmonic-oscillator hamiltonian

$$H_0 = \frac{p^2}{2m} + \frac{m\omega^2 q^2}{2}. \tag{19.40}$$

In that trick, one writes

$$\begin{aligned}
H_0 &= \frac{1}{2m}(m\omega q - ip)(m\omega q + ip) + \frac{i\omega}{2}[p,q] \\
&= \frac{1}{2m}(m\omega q - ip)(m\omega q + ip) + \frac{1}{2}\hbar\omega
\end{aligned} \tag{19.41}$$

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

$$\langle q'|m\omega q + ip|0\rangle = \left(m\omega q' + \hbar\frac{d}{dq'}\right)\langle q'|0\rangle = 0. \tag{19.42}$$

The solution to this differential equation

$$\frac{d}{dq'}\langle q'|0\rangle = -\frac{m\omega q'}{\hbar}\langle q'|0\rangle \tag{19.43}$$

is

$$\langle q'|0\rangle = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega q'^2}{2\hbar}\right) \tag{19.44}$$

in which the prefactor is a constant of normalization.

Extending that trick to the hamiltonian (19.39), we factor H

$$H = \frac{1}{2}\int \left[\sqrt{-\nabla^2 + m^2}\,\phi - i\pi\right]\left[\sqrt{-\nabla^2 + m^2}\,\phi + i\pi\right] d^3x + C \qquad (19.45)$$

in which C is the (infinite) constant

$$C = \frac{i}{2}\int \left[\pi, \sqrt{-\triangle + m^2}\,\phi\right] d^3x. \qquad (19.46)$$

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

$$\frac{\delta\langle\phi'|0\rangle}{\delta\phi'(\boldsymbol{x})} = -\sqrt{-\nabla^2 + m^2}\,\phi'(\boldsymbol{x})\,\langle\phi'|0\rangle. \qquad (19.47)$$

The solution to this equation is

$$\langle\phi|0\rangle = N\,\exp\left(-\frac{1}{2}\int \phi(\boldsymbol{x})\,\sqrt{-\nabla^2 + m^2}\,\phi(\boldsymbol{x})\,d^3x\right) \qquad (19.48)$$

in which N is a normalization constant. To see that this functional does satisfy equation (19.47), we compute the derivative

$$\frac{d\langle\phi + \epsilon h|0\rangle}{d\epsilon} = N\frac{d}{d\epsilon}\exp\left[-\tfrac{1}{2}\int (\phi + \epsilon h)\,\sqrt{-\nabla^2 + m^2}\,(\phi + \epsilon h)\,d^3x\right] \qquad (19.49)$$

which at $\epsilon = 0$ is

$$\begin{aligned}\left.\frac{d\langle\phi + \epsilon h|0\rangle}{d\epsilon}\right|_{\epsilon=0} = -\frac{1}{2}\Bigg[&\int h(\boldsymbol{x})\sqrt{-\nabla^2 + m^2}\,\phi(\boldsymbol{x})\,\delta^3x \\ &+ \int \phi(\boldsymbol{x})\sqrt{-\nabla^2 + m^2}\,h(\boldsymbol{x})\,d^3x\Bigg]\langle\phi|0\rangle.\end{aligned} \qquad (19.50)$$

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

$$\left.\frac{d\langle\phi + \epsilon h|0\rangle}{d\epsilon}\right|_{\epsilon=0} = -\int h(\boldsymbol{x'})\sqrt{-\nabla^2 + m^2}\,\phi(\boldsymbol{x'})\,d^3x'\,\langle\phi|0\rangle. \qquad (19.51)$$

Letting $h(\boldsymbol{x'}) = \delta^{(3)}(\boldsymbol{x'} - \boldsymbol{x})$, we arrive at (19.47).

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

$$\tilde{\phi}(\boldsymbol{p}) = \int e^{-i\boldsymbol{p}\cdot\boldsymbol{x}}\,\phi(\boldsymbol{x})\,\frac{d^3x}{(2\pi)^{3/2}} \qquad (19.52)$$

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

$$\langle\phi|0\rangle = N\,\exp\left(-\frac{1}{2}\int |\tilde{\phi}(\boldsymbol{p})|^2\,\sqrt{\boldsymbol{p}^2 + m^2}\,d^3p\right). \qquad (19.53)$$

Example 19.3 (Other theories, other vacua) We can find exact ground states for interacting theories with hamiltonians like

$$H = \frac{1}{2}\int \left[\sqrt{-\nabla^2 + m^2}\,\phi - ic_n\phi^n - i\pi\right]\left[\sqrt{-\nabla^2 + m^2}\,\phi + ic_n\phi^n + i\pi\right] d^3x. \tag{19.54}$$

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

$$\frac{\delta\langle\phi|\Omega\rangle}{\delta\phi(\boldsymbol{x})} = -\left[\sqrt{-\nabla^2 + m^2}\,\phi(\boldsymbol{x}) + ic_n\phi^n\right]\langle\phi|\Omega\rangle. \tag{19.55}$$

By extending the argument of equations (19.45–19.51), one may show (exercise 19.4) that the wave functional of the vacuum is

$$\langle\phi|\Omega\rangle = N\,\exp\left[-\int\left(\tfrac{1}{2}\phi\,\sqrt{-\nabla^2 + m^2}\,\phi + \frac{ic_n}{n+1}\phi^{n+1}\right) d^3x\right]. \tag{19.56}$$

□

Exercises

19.1 Compute the action $S_0[q]$ (19.1) for the classical path (19.24).

19.2 Use (19.25) to find a formula for the second functional derivative of the action (19.2) of the harmonic oscillator for which $V(q) = m\omega^2 q^2/2$.

19.3 Derive (19.53) from equations (19.48 & 19.52).

19.4 Show that (19.56) satisfies (19.55).