

EIGHT

Functional Derivatives and Commutation Relations

In using path integrals it is possible to bring functional calculus to bear on quantum mechanics in a particularly convenient way.

First we define a functional derivative. Let $F[x(\tau)]$ be a functional. A “derivative” of F should say something about

$$F[x(\tau) + \eta(\tau)] - F[x(\tau)] \quad (8.1)$$

where $\eta(\tau)$ is a “small” function. If F were a function of N variables, say x_i , $i=1, \dots, N$ (with similar definition for η_i) then we could write (8.1) as

$$F(x_1 + \eta_1, x_2 + \eta_2, \dots) - F(x_1, x_2, \dots) = \sum_i \frac{\partial F}{\partial x_i} \eta_i \quad (8.2)$$

This leads to the definition of functional derivative $\delta F / \delta x(\sigma)$ as that function of σ for which, for “small” η ,

$$F[x(\tau) + \eta(\tau)] - F[x(\tau)] = \int \frac{\delta F}{\delta x(\sigma)} \eta(\sigma) d\sigma \quad (8.3)$$

Because (8.3) is merely a generalization of (8.2) the usual rules for differentiation of products, integration by parts, and so on, can be derived for functional derivatives.

Although $\exp[iS[x(\tau)]/\hbar]$ is not a real valued weight function it is still possible to use it to define a kind of “expectation value.” For a functional

F , let

$$\langle F \rangle_S = \int dx(\tau) F[x(\tau)] \exp\left[\frac{iS[x(\tau)]}{\hbar}\right] \quad (8.4)$$

In (8.4) we note that we can translate $x(\tau)$, and because $dx(\tau) = d[x(\tau) + \eta(\tau)]$ the value of the integral remains the same. Thus

$$\begin{aligned} 0 &= \int dx(\tau) \{ F(x+\eta) e^{iS(x+\eta)/\hbar} - F(x) e^{iS(x)/\hbar} \} \\ &= \int dx(\tau) \int d\sigma \left[\frac{\delta F}{\delta x(\sigma)} + F \frac{i}{\hbar} \frac{\delta S}{\delta x(\sigma)} \right] e^{iS/\hbar} \eta(\sigma) + O(\eta^2) \end{aligned} \quad (8.5)$$

It follows from the arbitrariness of η that

$$\left\langle \frac{\delta F}{\delta x(\sigma)} \right\rangle_S = -\frac{i}{\hbar} \left\langle F \frac{\delta S}{\delta x(\sigma)} \right\rangle_S, \quad \text{for all } \sigma \quad (8.6)$$

This important result can also be written in discrete form, where $x(\tau)$ is the broken line connecting x_1, \dots, x_N , and the limit $N \rightarrow \infty$ in the definition of the path integral has not yet been taken. We have

$$\left\langle \frac{\partial F}{\partial x_k} \right\rangle_S = -\frac{i}{\hbar} \left\langle F \frac{\partial S}{\partial x_k} \right\rangle_S \quad (8.7)$$

Note that the expectation value—the path integral—will now involve only a finite number of integrations. Writing

$$S = \int \left[\frac{1}{2} m \dot{x}^2 - V(x) \right] d\tau \rightarrow \sum_{k=1}^N \left[\frac{1}{2} \frac{mN}{t} (x_{k+1} - x_k)^2 - \frac{V(x_k)t}{N} \right] \quad (8.8)$$

Equation 8.7 becomes ($\epsilon = t/N$)

$$\left\langle \frac{\partial F}{\partial x_k} \right\rangle_S = \frac{i\epsilon}{\hbar} \left\langle F \left\{ m \left[\frac{x_{k+1} - 2x_k + x_{k-1}}{\epsilon^2} \right] + \frac{\partial V}{\partial x}(x_k) \right\} \right\rangle_S \quad (8.9)$$

A number of interesting results can be obtained by making various choices for F . Let $F \equiv 1$. The left side of (8.9) vanishes and we obtain (returning to continuum notation)

$$\langle m\ddot{x} \rangle_S = - \left\langle \frac{\partial V}{\partial x} \right\rangle_S \quad (8.10)$$

for all times (since k is arbitrary). This is a version of the Ehrenfest theorem.

Exercise: In comparing (8.10) to the standard quantum mechanical result, what sense can you make of \ddot{x} ? Can you justify the relation between the expression $\langle (x_{k+1} - x_k)/\epsilon \rangle_S$ and the equation $\dot{x} = i[H, x]/\hbar$?

HINT: Recall that $\langle x_k \rangle_S = \langle x(t_k) \rangle_S = \langle x_{\text{final}} | \exp[-i(t-t_k)H/\hbar] x_{\text{operator}} \times \exp[-it_k H/\hbar] | x_{\text{initial}} \rangle$.

Now let F be x_k for some particular k . Then (8.9) implies

$$\langle 1 \rangle_S = \frac{i}{\hbar} \left\langle mx_k \left[\frac{x_{k+1} - x_k}{\epsilon} - \frac{x_k - x_{k-1}}{\epsilon} \right] + \epsilon x_k V'(x_k) \right\rangle_S \quad (8.11)$$

For $\epsilon \rightarrow 0$ the term involving V' vanishes, and we have the result that the expectation value

$$m \left\langle x_k \frac{(x_{k+1} - x_k)}{\epsilon} \right\rangle_S \quad (8.12)$$

is different from

$$m \left\langle x_k \frac{(x_k - x_{k-1})}{\epsilon} \right\rangle_S \quad (8.13)$$

They differ only in the times at which x and $m\Delta x/\epsilon = m(x_{k+1} - x_k)/\epsilon$ are to be evaluated. Furthermore, the fact that they differ by 1 suggests that $m(x_{k+1} - x_k)/\epsilon$ be identified with the momentum operator and that (8.11) be interpreted as a commutation relation. If operators are ordered so that that with the earliest time argument operates first, then (8.11) is the familiar relation $-i\hbar = [p, x]$.

The calculational rules for working with this "momentum operator" can be tricky, as illustrated by the following example. We expect kinetic energy to be given by

$$\left\langle \frac{p^2}{2m} \right\rangle_S \quad (8.14)$$

However, it will not do to evaluate

$$\frac{1}{2}m \left\langle \left(\frac{x_{k+1} - x_k}{\epsilon} \right)^2 \right\rangle_S \quad (8.15)$$

We already have experience with such integrals and know that $\langle (x_{k+1} - x_k)^2 \rangle_S$ will give an ϵ , so that dividing by ϵ^2 in (8.15) will give an infinite result. The trick is to identify kinetic energy with

$$\lim_{\epsilon \downarrow 0} \frac{1}{2m} \langle p(t+\epsilon)p(t) \rangle_S \quad (8.16)$$

This will lead to consideration of

$$\frac{1}{2}m \left\langle \left(\frac{x_{k+1} - x_k}{\epsilon} \right) \left(\frac{x_k - x_{k-1}}{\epsilon} \right) \right\rangle_S \quad (8.17)$$

which is in fact the correct form for kinetic energy.

Apropos of the present discussion it is worth mentioning that some people have felt that the Feynman path integral formalism will solve the ordering problem for operators. For example, given the classical quantity $p^5 x^3$ a number of quantum mechanical operators can be associated with it. But one can turn to the path integral and observe that because $p^5 x^3$ is a well defined classical quantity, when it is put into the path integral some definite choice of operators will be made. Various schemes of this sort have been proposed but since they all founder on the same basic point, there is no harm done if we look at a particularly naive proposal. Thus let us try

$$\langle p^5 x^3 \rangle_S \quad (8.18)$$

and ask if this is a unique object obtained from the classical mechanics. In fact, we know this is not unique, since we have seen that

$$\lim_{\epsilon \downarrow 0} \langle p(t+\epsilon)x(t) \rangle_S \neq \lim_{\epsilon \downarrow 0} \langle x(t+\epsilon)p(t) \rangle_S \quad (8.19)$$

Moreover, the example of kinetic energy shows the arguments in (8.18) cannot all be taken at the same time. Therefore the particular choice that is made for the time sequencing of the p 's and x 's will determine the operator; different choices of sequence will lead to different operators. In the notes to Sections 27 and 31 are references on the use of path integrals in the operator ordering problem.