Chapter I.2

Path Integral Formulation of Quantum Physics

The professor's nightmare: a wise guy in the class

As I noted in the preface, I know perfectly well that you are eager to dive into quantum field theory, but first we have to review the path integral formalism of quantum mechanics. This formalism is not universally taught in introductory courses on quantum mechanics, but even if you have been exposed to it, this chapter will serve as a useful review. The reason I start with the path integral formalism is that it offers a particularly convenient way of going from quantum mechanics to quantum field theory. I will first give a heuristic discussion, to be followed by a more formal mathematical treatment.

Perhaps the best way to introduce the path integral formalism is by telling a story, certainly apocryphal as many physics stories are. Long ago, in a quantum mechanics class, the professor droned on and on about the double-slit experiment, giving the standard treatment. A particle emitted from a source S (Fig. I.2.1) at time $t = 0$ passes through one or the other of two holes, A_1 and A_2, drilled in a screen and is detected at time $t = T$ by a detector located at O. The amplitude for detection is given by a fundamental postulate of quantum mechanics, the superposition principle, as the sum of the amplitude for the particle to propagate from the source S through the hole A_1 and then onward to the point O and the amplitude for the particle to propagate from the source S through the hole A_2 and then onward to the point O.

Suddenly, a very bright student, let us call him Feynman, asked, "Professor, what if we drill a third hole in the screen?" The professor replied, "Clearly, the amplitude for the particle to be detected at the point O is now given by the sum of three amplitudes, the amplitude for the particle to propagate from the source S through the hole A_1 and then onward to the point O, the amplitude for the particle to propagate from the source S through the hole A_2 and then onward to the point O, and the amplitude for the particle to propagate from the source S through the hole A_3 and then onward to the point O."

The professor was just about ready to continue when Feynman interjected again, "What if I drill a fourth and a fifth hole in the screen?" Now the professor is visibly

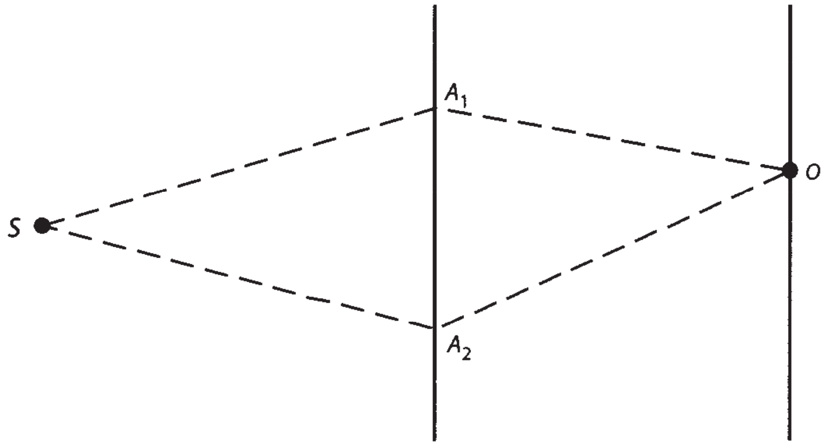

Figure I.2.1

losing his patience: "All right, wise guy, I think it is obvious to the whole class that we just sum over all the holes."

To make what the professor said precise, denote the amplitude for the particle to propagate from the source S through the hole A_i and then onward to the point O as $\mathcal{A}(S \to A_i \to O)$. Then the amplitude for the particle to be detected at the point O is

$$\mathcal{A}(\text{detected at } O) = \sum_i \mathcal{A}(S \to A_i \to O) \tag{1}$$

But Feynman persisted, "What if we now add another screen (Fig. I.2.2) with some holes drilled in it?" The professor was really losing his patience: "Look, can't you see that you just take the amplitude to go from the source S to the hole A_i in the first screen, then to the hole B_j in the second screen, then to the detector at O, and then sum over all i and j?"

Feynman continued to pester, "What if I put in a third screen, a fourth screen, eh? What if I put in a screen and drill an infinite number of holes in it so that the

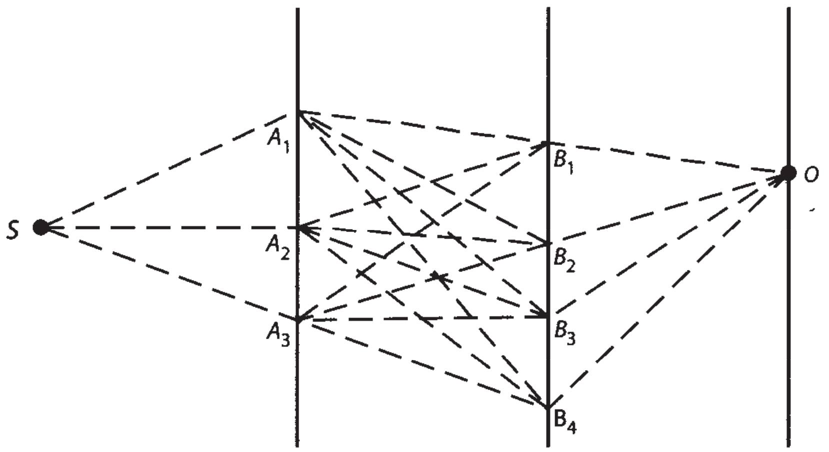

Figure I.2.2

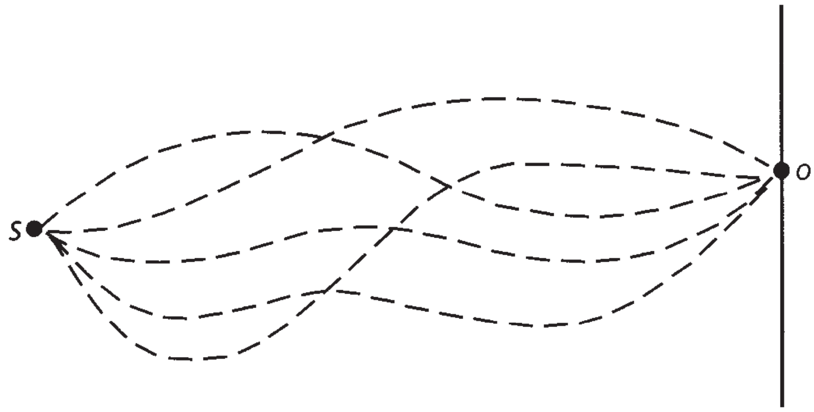

Figure I.2.3

screen is no longer there?" The professor sighed, "Let's move on; there is a lot of material to cover in this course."

But dear reader, surely you see what that wise guy Feynman was driving at. I especially enjoy his observation that if you put in a screen and drill an infinite number of holes in it, then that screen is not really there. Very Zen! What Feynman showed is that even if there were just empty space between the source and the detector, the amplitude for the particle to propagate from the source to the detector is the sum of the amplitudes for the particle to go through each one of the holes in each one of the (nonexistent) screens. In other words, we have to sum over the amplitude for the particle to propagate from the source to the detector following all possible paths between the source and the detector (Fig. I.2.3).

$$\mathcal{A}(\text{particle to go from } S \text{ to } O \text{ in time } T) =$$

$$\sum_{(\text{paths})} \mathcal{A}\left(\text{particle to go from } S \text{ to } O \text{ in time } T \text{ following a particular path}\right) \quad (2)$$

Now the mathematically rigorous will surely get anxious over how $\sum_{(\text{paths})}$ is to be defined. Feynman followed Newton and Leibniz: Take a path (Fig. I.2.4), approximate it by straight line segments, and let the segments go to zero. You can see that this is just like filling up a space with screens spaced infinitesimally close to each other, with an infinite number of holes drilled in each screen.

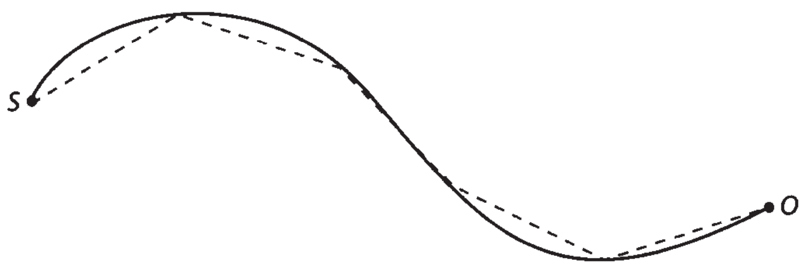

Figure I.2.4

Fine, but how to construct the amplitude $\mathcal{A}$(particle to go from S to O in time T following a particular path)? Well, we can use the unitarity of quantum mechanics: If we know the amplitude for each infinitesimal segment, then we just multiply them together to get the amplitude of the whole path.

In quantum mechanics, the amplitude to propagate from a point q_I to a point q_F in time T is governed by the unitary operator e^{-iHT}, where H is the Hamiltonian. More precisely, denoting by $|q\rangle$ the state in which the particle is at q, the amplitude in question is just $\langle q_F| e^{-iHT} |q_I\rangle$. Here we are using the Dirac bra and ket notation. Of course, philosophically, you can argue that to say the amplitude is $\langle q_F| e^{-iHT} |q_I\rangle$ amounts to a postulate and a definition of H. It is then up to experimentalists to discover that H is hermitean, has the form of the classical Hamiltonian, et cetera.

Indeed, the whole path integral formalism could be written down mathematically starting with the quantity $\langle q_F| e^{-iHT} |q_I\rangle$, without any of Feynman's jive about screens with an infinite number of holes. Many physicists would prefer a mathematical treatment without the talk. As a matter of fact, the path integral formalism was invented by Dirac precisely in this way, long before Feynman.

A necessary word about notation even though it interrupts the narrative flow: We denote the coordinates transverse to the axis connecting the source to the detector by q, rather than x, for a reason which will emerge in a later chapter. For notational simplicity, we will think of q as 1-dimensional and suppress the coordinate along the axis connecting the source to the detector.

Dirac's formulation

Let us divide the time T into N segments each lasting $\delta t = T/N$. Then we write

$$\langle q_F| e^{-iHT} |q_I\rangle = \langle q_F| e^{-iH\delta t} e^{-iH\delta t} \cdots e^{-iH\delta t} |q_I\rangle$$

Now use the fact that $|q\rangle$ forms a complete set of states so that $\int dq\, |q\rangle\langle q| = 1$. Insert 1 between all these factors of $e^{-iH\delta t}$ and write

$$\begin{aligned} &\langle q_F| e^{-iHT} |q_I\rangle \\ &= \left(\prod_{j=1}^{N-1} \int dq_j\right) \langle q_F| e^{-iH\delta t} |q_{N-1}\rangle \langle q_{N-1}| e^{-iH\delta t} |q_{N-2}\rangle \cdots \\ &\cdots \langle q_2| e^{-iH\delta t} |q_1\rangle \langle q_1| e^{-iH\delta t} |q_I\rangle \end{aligned} \tag{3}$$

Focus on an individual factor $\langle q_{j+1}| e^{-iH\delta t} |q_j\rangle$. Let us take the baby step of first evaluating it just for the free-particle case in which $H = \hat{p}^2/2m$. The hat on $\hat{p}$ reminds us that it is an operator. Denote by $|p\rangle$ the eigenstate of $\hat{p}$, namely $\hat{p}\,|p\rangle = p\,|p\rangle$. Do you remember from your course in quantum mechanics that $\langle q|p\rangle = e^{ipq}$? Sure you do. This just says that the momentum eigenstate is a plane wave in the coordinate representation. (The normalization is such that $\int (dp/2\pi)\,|p\rangle\langle p| = 1$.) So again inserting a complete set of states, we write

$$\langle q_{j+1}| e^{-i\delta t(\hat{p}^2/2m)} |q_j\rangle = \int \frac{dp}{2\pi} \langle q_{j+1}| e^{-i\delta t(\hat{p}^2/2m)} |p\rangle\langle p|q_j\rangle$$

$$= \int \frac{dp}{2\pi} e^{-i\delta t(p^2/2m)} \langle q_{j+1}|p\rangle\langle p|q_j\rangle$$

$$= \int \frac{dp}{2\pi} e^{-i\delta t(p^2/2m)} e^{ip(q_{j+1}-q_j)}$$

Note that we removed the hat from the momentum operator in the exponential: Since the momentum operator is acting on an eigenstate, it can be replaced by its eigenvalue.

The integral over p is known as a Gaussian integral, with which you may already be familiar. If not, turn to Appendix 1 to this chapter.

Doing the integral over p, we get

$$\langle q_{j+1}| e^{-i\delta t(\hat{p}^2/2m)} |q_j\rangle = \left(\frac{-i2\pi m}{\delta t}\right)^{\frac{1}{2}} e^{[im(q_{j+1}-q_j)^2]/2\delta t}$$

$$= \left(\frac{-i2\pi m}{\delta t}\right)^{\frac{1}{2}} e^{i\delta t(m/2)[(q_{j+1}-q_j)/\delta t]^2}$$

Putting this into (3) yields

$$\langle q_F| e^{-iHT} |q_I\rangle = \left(\frac{-i2\pi m}{\delta t}\right)^{\frac{N}{2}} \prod_{j=0}^{N-1} \int dq_j e^{i\delta t(m/2)\Sigma_{j=0}^{N-1}[(q_{j+1}-q_j)/\delta t]^2}$$

with $q_0 \equiv q_I$ and $q_N \equiv q_F$.

We can now go to the continuum limit $\delta t \to 0$. Newton and Leibniz taught us to replace $[(q_{j+1} - q_j)/\delta t]^2$ by $\dot{q}^2$, and $\delta t \sum_{j=0}^{N-1}$ by $\int_0^T dt$. Finally, we define the integral over paths as

$$\int Dq(t) = \lim_{N\to\infty} \left(\frac{-i2\pi m}{\delta t}\right)^{\frac{N}{2}} \prod_{j=0}^{N-1} \int dq_j.$$

We thus obtain the path integral representation

$$\langle q_F| e^{-iHT} |q_I\rangle = \int Dq(t)\, e^{i\int_0^T dt \frac{1}{2}m\dot{q}^2} \tag{4}$$

This fundamental result tells us that to obtain $\langle q_F| e^{-iHT} |q_I\rangle$ we simply integrate over all possible paths $q(t)$ such that $q(0) = q_I$ and $q(T) = q_F$.

As an exercise you should convince yourself that had we started with the Hamiltonian for a particle in a potential $H = \hat{p}^2/2m + V(\hat{q})$ (again the hat on $\hat{q}$ indicates an operator) the final result would have been

$$\langle q_F| e^{-iHT} |q_I\rangle = \int Dq(t)\, e^{i\int_0^T dt[\frac{1}{2}m\dot{q}^2 - V(q)]} \tag{5}$$

We recognize the quantity $\frac{1}{2}m\dot{q}^2 - V(q)$ as just the Lagrangian $L(\dot{q}, q)$. The Lagrangian has emerged naturally from the Hamiltonian. In general, we have

$$\langle q_F| e^{-iHT} |q_I\rangle = \int Dq(t)\, e^{i\int_0^T dt L(\dot{q},q)} \tag{6}$$

To avoid potential confusion, let me be clear that t appears as an integration variable in the exponential on the right-hand side. The appearance of t in the path integral measure $Dq(t)$ is simply to remind us that q is a function of t (as if we need reminding). Indeed, this measure will often be abbreviated to Dq. You might recall that $\int_0^T dt L(\dot{q}, q)$ is called the action $S(q)$ in classical mechanics. The action S is a functional of the function $q(t)$.

Often, instead of specifying that the particle starts at an initial position q_I and ends at a final position q_F, we prefer to specify that the particle starts in some initial state I and ends in some final state F. Then we are interested in calculating $\langle F| e^{-iHT} |I\rangle$, which upon inserting complete sets of states can be written as

$$\int dq_F \int dq_I \langle F|q_F\rangle\langle q_F| e^{-iHT} |q_I\rangle\langle q_I|I\rangle,$$

which mixing Schrödinger and Dirac notation we can write as

$$\int dq_F \int dq_I \Psi_F(q_F)^* \langle q_F| e^{-iHT} |q_I\rangle \Psi_I(q_I).$$

In most cases we are interested in taking $|I\rangle$ and $|F\rangle$ as the ground state, which we will denote by $|0\rangle$. It is conventional to give the amplitude $\langle 0| e^{-iHT} |0\rangle$ the name Z.

At the level of mathematical rigor we are working with, we count on the path integral $\int Dq(t)\, e^{i\int_0^T dt[\frac{1}{2}m\dot{q}^2 - V(q)]}$ to converge because the oscillatory phase factors from different paths tend to cancel out. It is somewhat more rigorous to perform a so-called Wick rotation to Euclidean time. This amounts to substituting $t \to -it$ and rotating the integration contour in the complex t plane so that the integral becomes

$$Z = \int Dq(t)\, e^{-\int_0^T dt[\frac{1}{2}m\dot{q}^2 + V(q)]}, \tag{7}$$

known as the Euclidean path integral. As is done in Appendix 1 to this chapter with ordinary integrals we will always assume that we can make this type of substitution with impunity.

One particularly nice feature of the path integral formalism is that the classical limit of quantum mechanics can be recovered easily. We simply restore Planck's constant $\hbar$ in (6):

$$\langle q_F| e^{-(i/\hbar)HT} |q_I\rangle = \int Dq(t)\, e^{(i/\hbar)\int_0^T dt L(\dot{q},q)}$$

and take the $\hbar \to 0$ limit. Applying the stationary phase or steepest descent method (if you don't know it see Appendix 2 to this chapter) we obtain $e^{(i/\hbar)\int_0^T dt L(\dot{q}_c, q_c)}$, where $q_c(t)$ is the "classical path" determined by solving the Euler-Lagrange equation $(d/dt)(\delta L/\delta \dot{q}) - (\delta L/\delta q) = 0$ with appropriate boundary conditions.

Appendix 1

I will now show you how to do the integral $G \equiv \int_{-\infty}^{+\infty} dx e^{-\frac{1}{2}x^2}$. The trick is to square the integral, call the dummy integration variable in one of the integrals y, and then pass to polar coordinates:

$$G^2 = \int_{-\infty}^{+\infty} dx\, e^{-\frac{1}{2}x^2} \int_{-\infty}^{+\infty} dy\, e^{-\frac{1}{2}y^2} = 2\pi \int_0^{+\infty} dr\, r e^{-\frac{1}{2}r^2}$$
$$= 2\pi \int_0^{+\infty} dw\, e^{-w} = 2\pi$$

Thus, we obtain

$$\int_{-\infty}^{+\infty} dx\, e^{-\frac{1}{2}x^2} = \sqrt{2\pi} \tag{8}$$

Believe it or not, a significant fraction of the theoretical physics literature consists of performing variations and elaborations of this basic Gaussian integral. The simplest extension is almost immediate:

$$\int_{-\infty}^{+\infty} dx\, e^{-\frac{1}{2}ax^2} = \left(\frac{2\pi}{a}\right)^{\frac{1}{2}} \tag{9}$$

as can be seen by scaling $x \to x/\sqrt{a}$.

Acting on this repeatedly with $-2(d/da)$ we obtain

$$\langle x^{2n} \rangle \equiv \frac{\int_{-\infty}^{+\infty} dx\, e^{-\frac{1}{2}ax^2} x^{2n}}{\int_{-\infty}^{+\infty} dx\, e^{-\frac{1}{2}ax^2}} = \frac{1}{a^n}(2n-1)(2n-3)\cdots 5\cdot 3\cdot 1 \tag{10}$$

The factor $1/a^n$ follows from dimensional analysis. To remember the factor $(2n-1)!! \equiv (2n-1)(2n-3)\cdots 5\cdot 3\cdot 1$ imagine $2n$ points and connect them in pairs. The first point can be connected to one of $(2n-1)$ points, the second point can now be connected to one of the remaining $(2n-3)$ points, and so on. This clever observation, due to Gian Carlo Wick, is known as Wick's theorem in the field theory literature. Incidentally, field theorists use the following graphical mnemonic in calculating, for example, $\langle x^6 \rangle$: Write $\langle x^6 \rangle$ as $\langle xxxxxx \rangle$ and connect the x's, for example

$$\langle xxxxxx \rangle$$


The pattern of connection is known as a Wick contraction. In this simple example, since the six x's are identical, any one of the distinct Wick contractions gives the same value

a^{-3} and the final result for $\langle x^6 \rangle$ is just a^{-3} times the number of distinct Wick contractions, namely $5 \cdot 3 \cdot 1 = 15$. We will soon come to a less trivial example, in which we have distinct x's, in which case distinct Wick contraction gives distinct values.

An important variant is the integral

$$\int_{-\infty}^{+\infty} dx\, e^{-\frac{1}{2}ax^2+Jx} = \left(\frac{2\pi}{a}\right)^{\frac{1}{2}} e^{J^2/2a} \tag{11}$$

To see this, take the expression in the exponent and "complete the square": $-ax^2/2 + Jx = -(a/2)(x^2 - 2Jx/a) = -(a/2)(x - J/a)^2 + J^2/2a$. The x integral can now be done by shifting $x \to x + J/a$, giving the factor of $(2\pi/a)^{\frac{1}{2}}$. Check that we can also obtain (10) by differentiating with respect to J repeatedly and then setting $J = 0$.

Another important variant is obtained by replacing J by iJ:

$$\int_{-\infty}^{+\infty} dx\, e^{-\frac{1}{2}ax^2+iJx} = \left(\frac{2\pi}{a}\right)^{\frac{1}{2}} e^{-J^2/2a} \tag{12}$$

To get yet another variant, replace a by $-ia$:

$$\int_{-\infty}^{+\infty} dx\, e^{\frac{1}{2}iax^2+iJx} = \left(\frac{2\pi i}{a}\right)^{\frac{1}{2}} e^{-iJ^2/2a} \tag{13}$$

Let us promote a to a real symmetric N by N matrix A_{ij} and x to a vector x_i $(i, j = 1, \cdots, N)$. Then (11) generalizes to

$$\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\cdots\int_{-\infty}^{+\infty} dx_1 dx_2 \cdots dx_N\, e^{-\frac{1}{2}x\cdot A\cdot x + J\cdot x} = \left(\frac{(2\pi)^N}{\det[A]}\right)^{\frac{1}{2}} e^{\frac{1}{2}J\cdot A^{-1}\cdot J} \tag{14}$$

where $x \cdot A \cdot x = x_i A_{ij} x_j$ and $J \cdot x = J_i x_i$ (with repeated indices summed.) To see this, diagonalize A by an orthogonal transformation O: $A = O^{-1} \cdot D \cdot O$ where D is a diagonal matrix. Call $y_i = O_{ij} x_j$. In other words, we rotate the coordinates in the N dimensional Euclidean space over which we are integrating. Using

$$\int_{-\infty}^{+\infty}\cdots\int_{-\infty}^{+\infty} dx_1 \cdots dx_N = \int_{-\infty}^{+\infty}\cdots\int_{-\infty}^{+\infty} dy_1 \cdots dy_N$$

we factorize the left-hand side of (14) into a product of N integrals of the form in (11). The result can then be expressed in terms of D^{-1}, which we write as $O \cdot A^{-1} \cdot O^{-1}$. (To make sure you got it, try this explicitly for $N = 2$.)

Putting in some i's $(A \to -iA,\ J \to iJ)$, we find the generalization of (13)

$$\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\cdots\int_{-\infty}^{+\infty} dx_1 dx_2 \cdots dx_N\, e^{(i/2)x\cdot A\cdot x + iJ\cdot x}$$

$$= \left(\frac{(2\pi i)^N}{\det[A]}\right)^{\frac{1}{2}} e^{-(i/2)J\cdot A^{-1}\cdot J} \tag{15}$$

The generalization of (10) is also easy to obtain. We differentiate (14) with respect to J repeatedly and then setting $J \to 0$. We find

$$\langle x_i x_j \cdots x_k x_l \rangle = \sum_{\text{Wick}} (A^{-1})_{ab} \cdots (A^{-1})_{cd} \tag{16}$$

where we have defined

$$\langle x_i x_j \cdots x_k x_l \rangle = \frac{\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\cdots\int_{-\infty}^{+\infty} dx_1 dx_2 \cdots dx_N \, e^{-\frac{1}{2}x\cdot A\cdot x} x_i x_j \cdots x_k x_l}{\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\cdots\int_{-\infty}^{+\infty} dx_1 dx_2 \cdots dx_N \, e^{-\frac{1}{2}x\cdot A\cdot x}} \tag{17}$$

and where the set of indices $\{a, b, \cdots, c, d\}$ represent a permutation of the set of indices $\{i, j, \cdots, k, l\}$. The sum in (16) is over all such permutations or Wick contractions. It is easiest to explain (16) for a simple example $\langle x_i x_j x_k x_l \rangle$. We connect the x's in pairs (Wick contraction) and write a factor $(A^{-1})_{ab}$ if we connect x_a to x_b. Thus,

$$\langle x_i x_j x_k x_l \rangle = (A^{-1})_{ij}(A^{-1})_{kl} + (A^{-1})_{il}(A^{-1})_{jk} + (A^{-1})_{ik}(A^{-1})_{jl} \tag{18}$$

(Recall that A and thus A^{-1} are symmetric.) Note that since $\langle x_i x_j \rangle = (A^{-1})_{ij}$, the right-hand side of (16) can also be written in terms of objects such as $\langle x_i x_j \rangle$. Please work out $\langle x_i x_j x_k x_l x_m x_n \rangle$; you will become an expert on Wick contractions. Of course, (16) reduces to (10) for $N = 1$.

Perhaps you are like me and do not like to memorize anything, but some of these formulas might be worth memorizing as they appear again and again in theoretical physics (and in this book).

Appendix 2

To do an exponential integral of the form $I = \int_{-\infty}^{+\infty} dq e^{-(1/\hbar)f(q)}$ we often have to resort to the steepest-descent approximation, which I will now review for your convenience. In the limit of $\hbar$ small, the integral is dominated by the minimum of $f(q)$. Expanding $f(q) = f(a) + \frac{1}{2}f''(a)(q-a)^2 + O[(q-a)^3]$ and applying (9) we obtain

$$I = e^{-(1/\hbar)f(a)} \left(\frac{2\pi\hbar}{f''(a)}\right)^{\frac{1}{2}} e^{-O(\hbar^{\frac{1}{2}})} \tag{19}$$

For $f(q)$ a function of many variables $q_1, \ldots, q_N$ and with a minimum at $q_j = a_j$, we generalize immediately to

$$I = e^{-(1/\hbar)f(a)} \left(\frac{2\pi\hbar}{\det f''(a)}\right)^{\frac{1}{2}} e^{-O(\hbar^{\frac{1}{2}})} \tag{20}$$

Here $f''(a)$ denotes the N by N matrix with entries $[f''(a)]_{ij} \equiv (\partial^2 f/\partial q_i \partial q_j)|_{q=a}$. In many situations, we do not even need the factor involving the determinant in (20). If you can derive (20) you are well on your way to becoming a quantum field theorist!

Exercises

I.2.1. Verify (5).

I.2.2. Derive (16).