5

Path integrals and quantum mechanics

> Thirty-one years ago, Dick Feynman told me about his 'sum over histories' version of quantum mechanics. 'The electron does anything it likes', he said. 'It goes in any direction at any speed, forward or backward in time, however it likes, and then you add up the amplitudes and it gives you the wave-function.' I said to him, 'You're crazy'. But he wasn't.
>
> F.J. Dyson‡

A common type of calculation in particle physics is that of a scattering cross section for a particular process, for example electron–electron scattering $e^-e^- \to e^-e^-$. Under the inspiring guidance of Feynman, a short-hand way of expressing – and of thinking about – these quantities has been developed. Thus, in the particular case of e^-e^- scattering, to a first order approximation the process is represented by the 'Feynman diagram' of Fig. 1.14, and the crucial part of this diagram is the 'propagation' of the photon between the two electrons. There are 'Feynman rules' which allow one to associate with each diagram a scattering amplitude, and from the total amplitude (there may be more than one diagram for each process) one calculates the cross section in a straightforward way. In this chapter and the next one it will be shown how the Feynman rules arise, and, in particular, how to find an expression for the 'propagation' of the virtual particle. In this chapter it will be shown how quantum mechanics can be formulated so that scattering processes may be understood directly in these terms. In the next chapter we shall extend the treatment to scalar and spinor fields, and in Chapter 7 to gauge fields. In this chapter we retain Planck's constant $\hbar$ in the relevant formulae.

5.1 Path-integral formulation of quantum mechanics

In the usual formulation of quantum mechanics, the quantities q and p are replaced by operators which obey Heisenberg commutation relations. The mathematics one invokes is that of operators in Hilbert space. The *path-integral formulation* of quantum mechanics, on the other hand, is based directly on the notion of a *propagator* $K(q_f t_f; q_i t_i)$. Given a wave function $\psi(q_i, t_i)$ at

‡ In H. Woolf (ed.), *Some Strangeness in the Proportion*, Addison-Wesley, 1980, p. 376. Quoted with kind permission.

time t_i, the propagator gives the corresponding wave function at a later time t_f by an appeal to Huygens' principle:

$$\psi(q_f, t_f) = \int K(q_f t_f; q_i t_i)\psi(q_i t_i)\,\mathrm{d}q_i. \tag{5.1}$$

(For simplicity we consider only one spatial dimension.) This equation is quite general and merely expresses causality. According to the usual interpretation of quantum mechanics, $\psi(q_f, t_f)$ is the probability amplitude that the particle is at the point q_f at the time t_f, so $K(q_f t_f; q_i t_i)$ is the probability amplitude for a *transition* from q_i at time t_i to q_f at time t_f. The *probability* that it is observed at q_f at time t_f

$$P(q_f t_f; q_i t_i) = |K(q_f t_f; q_i t_i)|^2.$$

This is a fundamental principle of quantum mechanics, as every student knows.

Let us divide the time interval between t_i and t_f into two, with t as the intermediate time, and q the intermediate point in space, as shown in Fig. 5.1. Repeated application of (5.1) gives

$$\psi(q_f, t_f) = \int\int K(q_f t_f; qt)K(qt; q_i t_i)\psi(q_i, t_i)\,\mathrm{d}q_i\,\mathrm{d}q,$$

from which it follows that

$$K(q_f t_f; q_i t_i) = \int K(q_f t_f; qt)K(qt; q_i t_i)\,\mathrm{d}q, \tag{5.2}$$

so the transition from (q_i, t_i) to (q_f, t_f) may be regarded as the result of transition from (q_i, t_i) to *all available intermediate points* q followed by transition from (q, t) to (q_f, t_f).

As a simple and familiar illustration of this, consider the 2-slit experiment with electrons, shown in Fig. 5.2. Denote by $K(2A; 1)$ the probability amplitude that the electron passes from the source 1 to the hole $2A$, and by $K(3; 2A)$ the amplitude that it passes from the hole $2A$ to the detectors 3, and so on. Equation (5.2) then gives

$$K(3; 1) = K(3; 2A)K(2A; 1) + K(3; 2B)K(2B; 1)$$

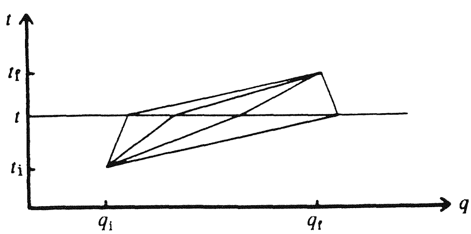


Fig. 5.1. Propagation of a particle from (q_i, t_i) to (q_f, t_f) via an intermediate position (q, t).

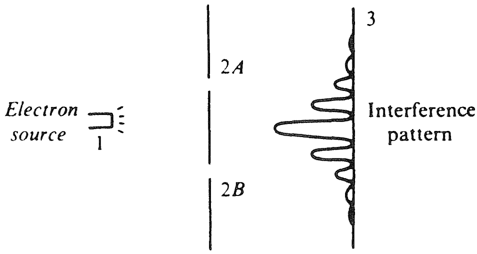


Fig. 5.2. The 2-slit experiment.

and the intensity pattern of the 'screen' 3 is given by the probability

$$P(3; 1) = |K(3; 1)|^2$$

which will clearly contain interference terms, characteristic of the quantum theory. Note that we cannot say 'the electron travelled either through hole A or hole B' – it travelled, in a sense, over *both paths* (if not detected at the slits).‡ This notion of *all possible paths* is important in the *path integral* formalism.

We may show that the propagator K is actually the more familiar quantity $\langle q_f t_f | q_i t_i \rangle$. To see this, note that the wave function $\psi(q, t)$ is

$$\psi(q, t) = \langle q | \psi t \rangle_S$$

where the state vector $|\psi t\rangle_S$ in the Schrödinger picture is related to that in the Heisenberg picture $|\psi\rangle_H$ by

$$|\psi t\rangle_S = e^{-iHt/\hbar} |\psi\rangle_H.$$

Let us define the vector

$$|qt\rangle = e^{iHt/\hbar} |q\rangle \tag{5.3}$$

which we may call, for obvious reasons, a 'moving frame'. We then have

$$\psi(q, t) = \langle qt | \psi \rangle_H. \tag{5.4}$$

Completeness of states enables us to write

$$\langle q_f t_f | \psi \rangle = \int \langle q_f t_f | q_i t_i \rangle \langle q_i t_i | \psi \rangle \, dq_i$$

which, with the help of (5.4), is

$$\psi(q_f, t_f) = \int \langle q_f t_f | q_i t_i \rangle \psi(q_i, t_i) \, dq_i.$$

‡ For an excellent discussion of the 2-slit experiment, see Feynman, Leighton & Sands (1965).

On comparison with (5.1) we see that

$$\langle q_f t_f | q_i t_i \rangle = K(q_f t_f; q_i t_i), \tag{5.5}$$

as claimed.

The propagator K summarises the quantum mechanics of the system. In the usual formulation of quantum mechanics, given an initial wave function, one can find the final wave function by solving the time-dependent Schrödinger equation. In this formulation, however, the propagator gives the solution directly. The idea now is to express $\langle q_f t_f | q_i t_i \rangle$ as a path integral.

Let us split the time interval between t_i and t_f into $(n+1)$ equal pieces τ, as in Fig. 5.3. Equation (5.2) now becomes

$$\langle q_f t_f | q_i t_i \rangle = \int \dots \int \mathrm{d}q_1 \, \mathrm{d}q_2 \dots \mathrm{d}q_n \langle q_f t_f | q_n t_n \rangle \langle q_n t_n | q_{n-1} t_{n-1} \rangle \dots \langle q_1 t_1 | q_i t_i \rangle \tag{5.6}$$

and the integral is taken over all possible 'trajectories'; they are not trajectories in the normal sense, since each segment $(q_j t_j; q_{j-1} t_{j-1})$ may be subdivided into smaller segments, so there is no derivative. The paths are really Markov chains.

Let us calculate the propagator over a small segment in the path integral. From (5.3) we have

$$\begin{aligned}
\langle q_{j+1} t_{j+1} | q_j t_j \rangle &= \langle q_{j+1} | \mathrm{e}^{-\mathrm{i} H \tau / \hbar} | q_j \rangle \\
&= \left\langle q_{j+1} \left| 1 - \frac{\mathrm{i}}{\hbar} H \tau + O(\tau^2) \right| q_j \right\rangle \\
&= \delta(q_{j+1} - q_j) - \frac{\mathrm{i}\tau}{\hbar} \langle q_{j+1} | H | q_j \rangle \\
&= \frac{1}{2\pi\hbar} \int \mathrm{d}p \exp\left[\frac{\mathrm{i}}{\hbar} p (q_{j+1} - q_j) \right] - \frac{\mathrm{i}\tau}{\hbar} \langle q_{j+1} | H | q_j \rangle .
\end{aligned} \tag{5.7}$$

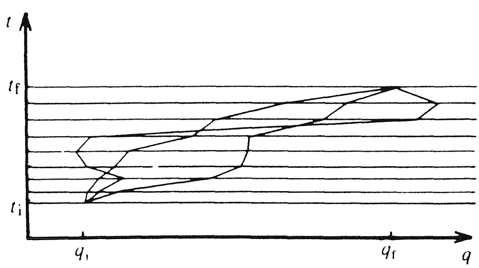


Fig. 5.3. Propagation over many paths from (q_i, t_i) to (q_f, t_f).

The Hamiltonian H is a function of the operators p and q. In the special case where H is of the form

$$H = \frac{p^2}{2m} + V(q) \tag{5.8}$$

(actually, H can be any function of p plus any function of q), the matrix element in (5.7) may easily be calculated. We have

$$\left\langle q_{j+1} \left| \frac{p^2}{2m} \right| q_j \right\rangle = \int \mathrm{d}p' \,\mathrm{d}p \langle q_{j+1}|p'\rangle \left\langle p' \left| \frac{p^2}{2m} \right| p \right\rangle \langle p|q_j\rangle,$$

and now substitute $\langle q_{j+1}|p'\rangle = (2\pi\hbar)^{-1/2} \exp(\mathrm{i}p'q_{j+1}/\hbar)$, giving

$$\begin{aligned} \left\langle q_{j+1} \left| \frac{p^2}{2m} \right| q_j \right\rangle &= \int \frac{\mathrm{d}p' \,\mathrm{d}p}{2\pi\hbar} \exp\left[\frac{\mathrm{i}}{\hbar}(p'q_{j+1} - pq_j)\right] \frac{p^2}{2m} \delta(p - p') \\ &= \int \frac{\mathrm{d}p}{h} \exp\left[\frac{\mathrm{i}}{\hbar} p(q_{j+1} - q_j)\right] \frac{p^2}{2m}. \end{aligned} \tag{5.9}$$

It is to be noted here that p^2 on the left-hand side of (5.9) is an *operator*, whereas on the right-hand side it is a *number*. We could (and perhaps should) have used a notation such as $\hat{p}$ to call attention to the operator nature of p on the left-hand side. But in any case, it is an important result that the formula we have on the right of (5.9) contains no operators. In a similar way,

$$\begin{aligned} \langle q_{j+1}|V(q)|q_j &= V\left(\frac{q_{j+1} + q_j}{2}\right) \langle q_{j+1}|q_j\rangle \\ &= V\left(\frac{q_{j+1} + q_j}{2}\right) \delta(q_{j+1} - q_j) \\ &= \int \frac{\mathrm{d}p}{h} \exp\left[\frac{\mathrm{i}}{\hbar} p(q_{j+1} - q_j)\right] V(\bar{q}_j), \end{aligned} \tag{5.10}$$

where $\bar{q}_j = \frac{1}{2}(q_j + q_{j-1})$, and $V(q)$ on the left is an operator expression, but the integral on the right contains no operators. Putting (5.9) and (5.10) together, we have

$$\langle q_{j+1}|H|q_j\rangle = \int \frac{\mathrm{d}p}{h} \exp\left[\frac{\mathrm{i}}{\hbar} p(q_{j+1} - q_j)\right] H(p, \bar{q}_j)$$

and, from (5.7),

$$\langle q_{j+1}t_{j+1}|q_j t_j\rangle = \frac{1}{h} \int \mathrm{d}p_j \exp\left\{\frac{\mathrm{i}}{\hbar}[p_j(q_{j+1} - q_j) - \tau H(p_j, \bar{q}_j]\right\} \tag{5.11}$$

where p_j is the momentum between t_j and t_{j+1}, or, equivalently, q_j and q_{j+1} – see Fig. 5.4. This gives the propagator over a segment of one possible path.

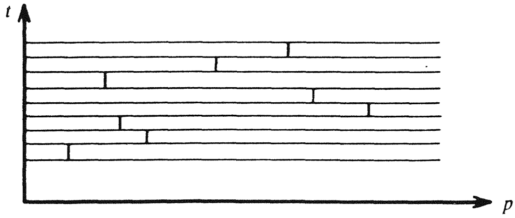


Fig. 5.4. Segments of the trajectory in momentum space.

The full propagator is got by substituting this into (5.6), giving, in the continuum limit (where p_j is the momentum along the path between q_j and q_{j+1}),

$$\langle q_f t_f | q_i t_i \rangle = \lim_{n\to\infty} \int \prod_{j=1}^{n} \mathrm{d}q_j \prod_{j=0}^{n} \frac{\mathrm{d}p_j}{h} \exp\left\{ \frac{\mathrm{i}}{\hbar} \sum_{j=0}^{n} [p_j(q_{j+1} - q_j) - \tau H(p_j, \bar{q}_j]\right\} \tag{5.12}$$

with $q_0 = q_i$, $q_{n+1} = q_f$. This may be written in the symbolic form

■ $$\langle q_f t_f | q_i t_i \rangle = \int \frac{\mathcal{D}q\mathcal{D}p}{h} \exp \frac{\mathrm{i}}{\hbar} \left[\int_{t_i}^{t_f} \mathrm{d}t[p\dot{q} - H(p, q)] \right] \tag{5.13}$$

with $q(t_i) = q_i$, $q(t_f) = q_f$. In the continuum limit q becomes a function of t, and the integral is a 'functional integral', an integral over all *functions*. It is infinite-dimensional. Expression (5.13) is the path integral expression for the transition amplitude from (q_i, t_i) to (q_f, t_f). Each function $q(t)$ and $p(t)$ defines a *path in phase space*. As mentioned above, the more usual approach to quantum mechanics is to solve the Schrödinger equation $\mathrm{i}\hbar(\mathrm{d}|\psi\rangle/\mathrm{d}t) = \hat{H}|\psi\rangle$ where $\hat{H}$ is an operator, subject to some boundary conditions. In the path-integral formulation we have an explicit expression for the transition amplitude, which is clearly very well suited to scattering problems. The quantities p and q occurring in the integral are *classical* quantities, *not* operators (c-numbers, not q-numbers). It is not obvious, however, that infinite-dimensional integrals of this type are well-defined mathematically, that is, whether they converge; in other words, exist! We shall assume that they do. The reader interested in the mathematical status of functional integrals is referred to Gel'fand & Yaglom (1960), Kac (1959), Keller & McLaughlin (1975), and Gudder (1979).

There is another form for the transition amplitude, which holds when H is of the form (5.8), since in that case we can perform the p-integration. Equation (5.12) becomes

$$\langle q_f t_f | q_i t_i \rangle = \lim_{n\to\infty} \int \prod_{1}^{n} \mathrm{d}q_j \prod_{0}^{n} \frac{\mathrm{d}p_j}{h} \exp\left\{ \frac{\mathrm{i}}{\hbar} \sum_{0}^{n} \left[p_j(q_{j+1} - q_j) - \frac{p_j^2}{2m}\tau - V(\bar{q}_j)\tau \right]\right\}.$$

As far as the p_j integration is concerned, this is of the same form as equation (5A.3) (see the appendix to this chapter), so we get

$$\langle q_f t_f | q_i t_i \rangle = \lim_{n\to\infty} \left(\frac{m}{\mathrm{i}\hbar\tau}\right)^{(n+1)/2} \int \prod_1^n \mathrm{d}q_j \exp\left\{\frac{\mathrm{i}\tau}{\hbar}\sum_0^n \left[\frac{m}{2}\left(\frac{q_{j+1}-q_j}{\tau}\right)^2 - V\right]\right\} \tag{5.14}$$

and hence, in the continuum limit

■ $$\langle q_f t_f | q_i t_i \rangle = N \int \mathscr{D}q \exp\left[\frac{\mathrm{i}}{\hbar}\int_{t_i}^{t_f} L(q, \dot{q})\,\mathrm{d}t\right] \tag{5.15}$$

where $L = T - V$, the classical Lagrangian. In the limit $n \to \infty$, N becomes infinite, but this does not matter, since we shall always deal with normalised transition amplitudes.

The integrand in (5.15) is the classical action $S = \int L\,\mathrm{d}t$. We have proved this equation from the postulates of quantum mechanics, and by assuming that the Hamiltonian is of the form (5.8). Feynman's original approach was to adopt (5.15) as a hypothesis and then prove the Schrödinger equation from it. The disadvantage of this approach is that (5.15) does not hold in general, since (5.8) does not. A counter example has been given by Lee & Yang (1962). If

$$L = \frac{\dot{q}^2}{2} f(q),$$

which describes a system with a velocity-dependent potential, then the momentum is

$$p = \frac{\partial L}{\partial \dot{q}} = \dot{q} f(q)$$

and the Hamiltonian is

$$H = p\dot{q} - L = \tfrac{1}{2}\dot{q}^2 f(q) = \tfrac{1}{2}\frac{p^2}{f(q)}$$

and this is not of the form (5.8). Substituting this into (5.13) and performing the p integrations gives, eventually,

$$\langle q_f t_f | q_i t_i \rangle = N \int \mathscr{D}q \exp\left(\frac{\mathrm{i}}{\hbar} S_{\text{eff}}\right)$$

where

$$S_{\text{eff}} = \int \mathrm{d}t \left[L(q, \dot{q}) - \frac{\mathrm{i}}{2}\delta(0) \ln f(q)\right].$$

Instead of (5.14), we have an *effective* action, which differs from $S = \int L\,\mathrm{d}t$.

In the case of field theories, similarly, the transition from an equation like (5.13) to one like (5.15) may not in general be made, and in particular this is true in the case of non-Abelian gauge-field theories. However, when we come to consider these theories, in Chapter 7, we shall for simplicity adopt a 'heuristic' approach to the derivation of the Feynman rules, and work from an equation analogous to (5.15).

5.2 Perturbation theory and the S matrix‡

It is our aim to illustrate how the path-integral method is used in the calculation of scattering processes, and we shall consider Rutherford scattering in particular, in §5.3 below. The scattering of one particle on another is described, non-relativistically, by interaction through a potential $V(x)$ (we change the notation, in this section, for the space co-ordinate, from q of x). Since the expression for the transition amplitude is not exactly calculable, we resort, as usual, to perturbation theory. This is valid when the potential $V(x)$ is small, or, more precisely, when the time integral of $V(x, t)$ is small compared with $\hbar$. In that case we may write

$$\exp\left[\frac{-\mathrm{i}}{\hbar}\int_{t_\mathrm{i}}^{t_\mathrm{f}} V(x,t)\,\mathrm{d}t\right] = 1 - \frac{\mathrm{i}}{\hbar}\int_{t_\mathrm{i}}^{t_\mathrm{f}} V(x,t)\,\mathrm{d}t - \frac{1}{2!\hbar^2}\left[\int_{t_\mathrm{i}}^{t_\mathrm{f}} V(x,t)\,\mathrm{d}t\right]^2 + \cdots. \tag{5.16}$$

This is the perturbation expansion. When substituted into the expression (5.15) for the propagator $K(x_\mathrm{f}t_\mathrm{f}; x_\mathrm{i}t_\mathrm{i})$ (see (5.5)) we get a series expansion

$$K = K_0 + K_1 + K_2 + \ldots, \tag{5.17}$$

the first term of which is the free propagator K_0:

$$K_0 = N\int\left[\exp\left(\frac{\mathrm{i}}{\hbar}S\right)\right]\mathscr{D}x$$

$$= N\int\left[\exp\left(\frac{\mathrm{i}}{\hbar}\int \tfrac{1}{2}m\dot{x}^2\,\mathrm{d}t\right)\right]\mathscr{D}x.$$

To evaluate this, we write it in the discrete form (see (5.14))

$$K_0 = \lim_{n\to\infty}\left(\frac{m}{\mathrm{i}\hbar\tau}\right)^{(n+1)/2}\int_{-\infty}^{\infty}\prod_{j=1}^{n}\mathrm{d}x_j \exp\left[\frac{\mathrm{i}m}{2\hbar\tau}\sum_{j=0}^{n}(x_{j+1}-x_j)^2\right].$$

‡ In this section and the following one I have drawn freely from M. Veltman, lectures at Basko-Polje School, 1974 (unpublished).

The value of this integral is known: see (5A.4),

$$\text{integral} = \frac{1}{(n+1)^{1/2}}\left(\frac{i\hbar\tau}{m}\right)^{n/2}\exp\left[\frac{im}{2\hbar(n+1)\tau}(x_f - x_i)^2\right],$$

so, putting $(n+1)\tau = t_f - t_i$, we have for the free particle propagator

$$K_0 x_f t_f; x_i t_i) = \left(\frac{m}{i\hbar(t_f - t_i}\right)^{1/2}\exp\left[\frac{im(x_f - x_i)^2}{2\hbar(t_f - t_i)}\right] \quad (t_f > t_i). \tag{5.18}$$

The condition $t_f > t_i$ is clearly crucial for the propagator, since it vanishes, by causality, if $t_f < t_i$, so we may properly put

$$K_0(x_f t_f; x_i t_i) = \theta(t_f - t_i)\left(\frac{m}{i\hbar(t_f - t_i)}\right)^{1/2}\exp\left[\frac{im(x_f - x_i)^2}{2\hbar(t_f - t_i)}\right]. \tag{5.19}$$

Let us now calculate K_1. From (5.14) and (5.16) we have

$$K_1 = \frac{-i}{\hbar}\lim_{n\to\infty} N^{(n+1)/2}\sum_{i=1}^{n}\tau\int\exp\left[\frac{im}{2\hbar\tau}\sum_{j=0}^{n}(x_{j+1} - x_j)^2\right]V(x_i, t_i)\,dx_1 \ldots dx_n,$$

where $N = m/i\hbar\tau$, and we have replaced integration over t by summation over t_i. Noting that V depends on x_i, we now split up the sum in the exponent into two, one going from $j = 0$ to $j = i - 1$, and the other from $j = i$ to $j = n$. We also separate out the integration over x_i, and get

$$K_1 = \lim_{n\to\infty}\frac{-i}{\hbar}\sum_{i=1}^{n}\tau\int dx_i\left\{N^{(n-i+1)/2}\int\exp\left[\frac{im}{2\hbar\tau}\sum_{j=i}^{n}(x_{j+1} - x_j)^2\right]dx_{i+1}\ldots dx_n\right\}$$
$$\times V(x_i, t_i)\left\{N^{i/2}\int\exp\left[\frac{im}{2\hbar\tau}\sum_{j=0}^{i-1}(x_{j+1} - x_j)^2\right]dx_1\ldots dx_{i-1}\right\}.$$

The two terms in curly brackets are $K_0(x_f t_f; xt)$ and $K_0(xt; x_i t_i)$, so, replacing $\sum_i \tau\int dx_i$ by $\int dx\,dt$, the above expression becomes

$$K_1(x_f t_f; x_i t_i) = -\frac{i}{\hbar}\int_{t_i}^{t_f}dt\int_{-\infty}^{\infty}K_0(x_f t_f; xt)V(x, t)K_0(xt; x_i t_i)\,dx. \tag{5.20}$$

Now $K_0(x_f t_f; xt)$ vanishes if $t > t_f$ and $K_0(xt; x_i t_i)$ vanishes if $t < t_i$, so the integration in (5.20) may be taken over all values of t, to give

$$K_1(x_f t_f; x_i t_i) = \frac{-i}{\hbar}\int_{-\infty}^{\infty}dt\int K_0(x_f t_f; xt)V(x, t)K_0(xt; x_i t_i)\,dx. \tag{5.21}$$

This is the first order correction to the free propagator. In a similar way, we may prove that the second order correction is

$$K_2(x_f t_f; x_i t_i) = \left(\frac{-i}{\hbar}\right)^2 \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 K_0(x_f t_f; x_2 t_2) V(x_2, t_2)$$
$$\times K_0(x_2 t_2; x_1 t_1) V(x_1, t_1) K_0(x_1 t_1; x_i t_i). \tag{5.22}$$

Analogous expressions hold for all K_n in the expansion (5.17), so we write

$$K(x_f t_f; x_i t_i) = K_0(x_f t_f; x_i t_i) - \frac{i}{\hbar} \int K_0(x_f t_f; x_1 t_1) V(x_1, t_1) K_0(x_1 t_1; x_i t_i) \, dx_1 \, dt_1$$
$$- \frac{1}{\hbar^2} \int K_0(x_f t_f; x_1 t_1) V(x_1, t_1) K_0(x_1 t_1; x_2 t_2) V(x_2 t_2)$$
$$\times K_0(x_2 t_2; x_i t_i) \, dx_1 \, dx_2 \, dt_1 \, dt_2 + \dots . \tag{5.23}$$

This is the solution to the perturbation series in K, and is called the *Born series*. It may be visualised as in Fig. 5.5. K_0 describes the free propagation of the wave function from $x_i t_i$ to $x_f t_f$; K_1 describes propagation with one interaction with the potential V; and so on.

A noteworthy feature of (5.22) is that it does not include the factor 1/2! present in (5.16). The reason for this is as follows. The two interactions with V occur at different times but are indistinguishable, so we write

$$\frac{1}{2!} \int V(t') V(t'') \, dt' \, dt'' = \frac{1}{2!} \int [\theta(t' - t'') V(t') V(t'')$$
$$+ \theta(t'' - t') V(t') V(t'')] \, dt' \, dt''$$
$$= \int \theta(t_1 - t_2) V(t_1) V(t_2) \, dt_1 \, dt_2. \tag{5.24}$$

In a similar way, there is no factor $1/n!$ in the expression for K_n. We shall now

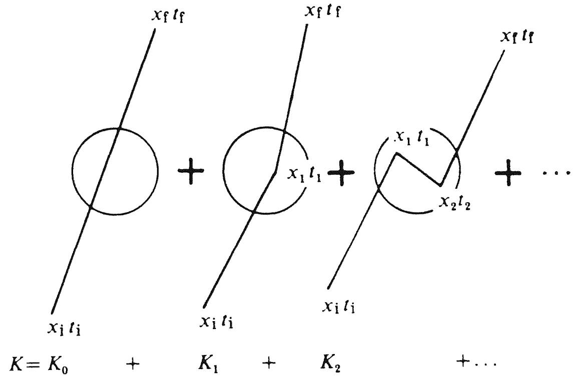


Fig. 5.5. The Born series.

show that the free propagator K_0 is simply the Green's function for the Schrödinger equation. To see this, substitute the Born series (5.23) into (5.1), giving

$$\begin{aligned}\psi(\mathrm{x}_\mathrm{f}t_\mathrm{f}) &= \int K(\mathrm{x}_\mathrm{f}t_\mathrm{f};\, \mathrm{x}_\mathrm{i}t_\mathrm{i})\psi(\mathrm{x}_\mathrm{i}t_\mathrm{i})\,\mathrm{d}\mathrm{x}_\mathrm{i} \\ &= \int K_0(\mathrm{x}_\mathrm{f}t_\mathrm{f};\, \mathrm{x}_\mathrm{i}t_\mathrm{i})\psi(\mathrm{x}_\mathrm{i}t_\mathrm{i})\,\mathrm{d}\mathrm{x}_\mathrm{i} \\ &\quad - \frac{\mathrm{i}}{\hbar}\int K_0(\mathrm{x}_\mathrm{f}t_\mathrm{f};\, \mathrm{x}t)V(\mathrm{x},\, t)K_0(\mathrm{x}t;\, \mathrm{x}_\mathrm{i}t_\mathrm{i})\psi(\mathrm{x}_\mathrm{i}t_\mathrm{i})\,\mathrm{d}t\,\mathrm{d}\mathrm{x}\,\mathrm{d}\mathrm{x}_\mathrm{i} \\ &\quad + \ldots . \end{aligned} \tag{5.25}$$

Here we have changed from one space dimension to three. Assuming the series above converges, the effect of the unwritten terms is to modify the last K_0 to the full propagator K, so that

$$\psi(\mathrm{x}_\mathrm{f}t_\mathrm{f}) = \int K_0(\mathrm{x}_\mathrm{f}t_\mathrm{f};\, \mathrm{x}_\mathrm{i}t_\mathrm{i})\psi(\mathrm{x}_\mathrm{i}t_\mathrm{i})\,\mathrm{d}\mathrm{x}_\mathrm{i} - \frac{\mathrm{i}}{\hbar}\int K_0(\mathrm{x}_\mathrm{f}t_\mathrm{f};\, \mathrm{x}t)V(\mathrm{x},\, t)\psi(\mathrm{x}t)\,\mathrm{d}\mathrm{x}\,\mathrm{d}t. \tag{5.26}$$

This equation is exact, and is an integral equation for ψ. Now assume that in the distant past, $t_\mathrm{i} \to -\infty$, ψ becomes free – a plane wave ϕ – then the first term on the right-hand side of (5.26) is also a plane wave, since it results from the free propagation of $\psi(\mathrm{x}_\mathrm{i}t_\mathrm{i})$, and we may write

$$\psi(\mathrm{x}_\mathrm{f}t_\mathrm{f}) = \phi(\mathrm{x}_\mathrm{f}t_\mathrm{f}) - \frac{\mathrm{i}}{\hbar}\int K_0(\mathrm{x}_\mathrm{f}t_\mathrm{f};\, \mathrm{x}t)V(\mathrm{x},\, t)\psi(\mathrm{x}t)\,\mathrm{d}\mathrm{x}\,\mathrm{d}t. \tag{5.27}$$

Now $\psi(\mathrm{x}_\mathrm{f}t_\mathrm{f})$ obeys the Schrödinger equation

$$\frac{\hbar^2}{2m}\nabla^2_{\mathrm{x}_\mathrm{f}}\psi(\mathrm{x}_\mathrm{f}t_\mathrm{f}) + \mathrm{i}\hbar\frac{\partial\psi(\mathrm{x}_\mathrm{f}t_\mathrm{f})}{\partial t_\mathrm{f}} = V(\mathrm{x}_\mathrm{f}t_\mathrm{f})\psi(\mathrm{x}_\mathrm{f}t_\mathrm{f}). \tag{5.28}$$

Since $\phi(\mathrm{x}_\mathrm{f}t_\mathrm{f})$ obeys the free-particle equation (with $V = 0$), then K_0 must obey

$$\frac{\hbar^2}{2m}\nabla^2_{\mathrm{x}_\mathrm{f}}K_0(\mathrm{x}_\mathrm{f}t_\mathrm{f};\, \mathrm{x}t) + \mathrm{i}\hbar\frac{\partial}{\partial t_\mathrm{f}}K_0(\mathrm{x}_\mathrm{f}t_\mathrm{f};\, \mathrm{x}t) = \mathrm{i}\hbar\delta(\mathrm{x}_\mathrm{f} - \mathrm{x})\delta(t_\mathrm{f} - t) \tag{5.29}$$

which is the equation for the Green's function of (5.28). Note that the presence of the $\delta(t_\mathrm{f} - t)$ is to be expected from the $\theta(t_\mathrm{f} - t)$ occurring in the definition (5.19) of K_0. The propagator K_0 is then simply the Green's function of the Schrödinger equation, as claimed.

We pass now to the calculation of the scattering amplitude. In the measurement of a scattering process, the experimental conditions are that a particle is free at $t = -\infty$, then scatters, and is free again at $t = +\infty$. This is a source of difficulty, however, because a free particle (that is, one with a definite energy and momentum) is described by a plane wave, which spreads out over all space and time, *including* the centre of the interaction potential $V(\mathbf{x})$, so the particle can never be free! To get round this problem the *adiabatic hypothesis* is invoked; the potential V is switched on and off again slowly, so that $V = 0$ at $t = \pm\infty$ and the particle is free. V must not be switched on and off too quickly; this would imply, through Fourier transformation, that the time dependence of V results in the scattering centre emitting or absorbing energy, which must not happen.

Returning to the scattering problem, the initial condition is that ψ is a plane wave:

$$\psi_{\text{in}}(\mathbf{x}_i t_i) \quad \text{plane wave.}$$

We assume that $V \to 0$ for large negative t, and that t_i is even further in the past. Taking the first Born approximation in (5.25) gives

$$\begin{aligned}\psi^{(+)}(\mathbf{x}_f t_f) &= \int K_0(\mathbf{x}_f t_f; \mathbf{x}_i t_i)\psi_{\text{in}}(\mathbf{x}_i t_i)\,d\mathbf{x}_i \\ &\quad - \frac{i}{\hbar}\int K_0(\mathbf{x}_f t_f; \mathbf{x}t)V(\mathbf{x}, t)K_0(\mathbf{x}t; \mathbf{x}_i t_i)\psi_{\text{in}}(\mathbf{x}_i t_i)\,d\mathbf{x}\,d\mathbf{x}_i\,dt. \qquad (5.30)\end{aligned}$$

The superscript on $\psi^{(+)}(\mathbf{x}_f t_f)$ denotes that it corresponds to a wave which was free at $t = -\infty$, and thus involves the 'retarded' propagator $K_0(\mathbf{x}t; \mathbf{x}'t')$, which vanishes for $t' > t$. It is equally acceptable to write a solution $\psi^{(-)}(x_1 t_1)$ consisting of a wave which becomes free at $t = \infty(\psi_{\text{out}})$, and an 'advanced' propagator $K_0(\mathbf{x}t; \mathbf{x}'t')$ which vanishes when $t' < t$.

We are interested in the amplitude for detecting a final particle with definite momentum, i.e. a plane wave ψ_{out}. This is called the *scattering amplitude S*, and is the overlap of the wave functions

$$\begin{aligned}S &= \int \psi^*_{\text{out}}(\mathbf{x}_f t_f)\psi^{(+)}(\mathbf{x}_f t_f)\,d\mathbf{x}_f \\ &= \int \psi^*_{\text{out}}(\mathbf{x}_f t_f)K_0(\mathbf{x}_f t_f; \mathbf{x}_i t_i)\psi_{\text{in}}(\mathbf{x}_i t_i)\,d\mathbf{x}_i\,d\mathbf{x}_f \\ &\quad - \frac{i}{\hbar}\int \psi^*_{\text{out}}(\mathbf{x}_f t_f)K_0(\mathbf{x}_f t_f; \mathbf{x}t)V(\mathbf{x}, t)K_0(\mathbf{x}t; \mathbf{x}_i t_i)\psi_{\text{in}}(\mathbf{x}_i t_i)\,d\mathbf{x}_f\,d\mathbf{x}\,d\mathbf{x}_i\,dt \\ &= \int \psi^*_{\text{out}}(\mathbf{x}_f t_f)\phi(\mathbf{x}_f t_f)\,d\mathbf{x}_f - \frac{i}{\hbar}\int \psi^*_{\text{out}}(\mathbf{x}_f t_f)K_0(\mathbf{x}_f t_f; \mathbf{x}t) \\ &\quad \times V(\mathbf{x}, t)K_0(\mathbf{x}t; \mathbf{x}_i t_i)\psi_{\text{in}}(\mathbf{x}_i t_i)\,d\mathbf{x}_f\,d\mathbf{x}\,d\mathbf{x}_i\,dt \qquad (5.31)\end{aligned}$$

where $\phi(\mathbf{x}_f t_f)$, just like $\psi_{in}(\mathbf{x}_i t_i)$, is a plane wave. If the initial and final momenta are $\mathbf{p}_i = \hbar\mathbf{k}_i$, $\mathbf{p}_f = \hbar\mathbf{k}_f$, we have, with box normalisation,

$$\psi_{in}(\mathbf{x}t) = \frac{1}{\sqrt{\tau}} \exp\left[\frac{i}{\hbar}(\mathbf{p}_i \cdot \mathbf{x} - E_i t)\right],$$
$$\psi_{out}(\mathbf{x}t) = \frac{1}{\sqrt{\tau}} \exp\left[\frac{i}{\hbar}(\mathbf{p}_f \cdot \mathbf{x} - E_f t)\right] \tag{5.32}$$

where $E = p^2/2m$ and τ is the volume of the box, which of course is arbitrary. Substituting (5.32) into the first term of (5.31), using

$$\int e^{i\mathbf{q}\cdot\mathbf{x}}\, d\mathbf{x} = (2\pi)^3 \delta(\mathbf{q}),$$

and putting, for convenience, $\tau = (2\pi)^3$, we get

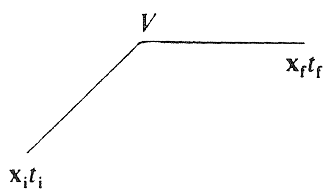
$$S_{fi} = \delta(\mathbf{k}_i - \mathbf{k}_f) - \frac{i}{\hbar}\int \psi^*_{out}(\mathbf{x}_f t_f) K_0(\mathbf{x}_f t_f; \mathbf{x}t) V(\mathbf{x}, t)$$
$$\times K_0(\mathbf{x}t; \mathbf{x}_i t_i)\psi_{in}(\mathbf{x}_i t_i)\, d\mathbf{x}_f\, d\mathbf{x}\, d\mathbf{x}_i\, dt. \tag{5.33}$$

The scattering amplitude is then seen to be one element of a matrix S, whose (fi) element appears above; this is the *scattering matrix* or *S matrix*. The first term corresponds to no interaction giving momentum conservation and a unit S matrix. Genuine interactions are represented by the second term in (5.33), and the amplitude that a particular 'out' state results from a particular 'in' state is

$$A = -\frac{i}{\hbar}\int \psi^*_{out}(\mathbf{x}_f t_f) K_0(\mathbf{x}_f t_f; \mathbf{x}t) V(\mathbf{x}, t) K_0(\mathbf{x}t; \mathbf{x}_i t_i)\psi_{in}(\mathbf{x}_i t_i)\, d\mathbf{x}_f\, d\mathbf{x}\, d\mathbf{x}_i\, dt. \tag{5.34}$$

We now have an expression for the scattering amplitude in terms of the free propagator K_0 and the interaction potential V. Equation (5.34) may be translated into a set of simple rules for the scattering amplitude; these rules are known as the *Feynman rules*.

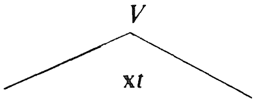
We may represent amplitude (5.34) (which is a first order approximation), by the diagram



(5.35)

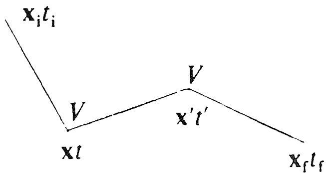
It is clear that the rules for translating this diagram into the expression for the scattering amplitude may be summarised by making the correspondence

$K_0(\mathbf{x}_2 t_2; \mathbf{x}_1 t_1)$ (5.36)



$-\dfrac{\mathrm{i}}{\hbar} V(\mathbf{x}t)$; integration over x and t

In addition, we multiply by ψ_{in} and ψ^*_{out} at the ends of the diagram and integrate over the two relevant spatial variables. Thus, the amplitude for the second order process



(5.37)

is

$$A^{(2)} = \left(\frac{-\mathrm{i}}{\hbar}\right)^2 \int \psi^*_{\text{out}}(\mathbf{x}_f t_f) K_0(\mathbf{x}_f t_f; \mathbf{x}'t') V(\mathbf{x}', t') K_0(\mathbf{x}'t'; \mathbf{x}t) V(\mathbf{x}, t) \times K_0(\mathbf{x}t; \mathbf{x}_i t_i) \psi_{\text{in}}(\mathbf{x}_i t_i)\, \mathrm{d}\mathbf{x}_i\, \mathrm{d}\mathbf{x}\, \mathrm{d}t\, \mathrm{d}\mathbf{x}'\, \mathrm{d}t'\, \mathrm{d}\mathbf{x}_f.$$

The rules (5.36) are called the Feynman rules. In the non-relativistic quantum mechanics we are dealing with at present, these rules are hardly necessary to do calculations, but in quantum field theory, to be considered in the next chapter, they are a great aid to calculation.

The rules (5.36) are written in co-ordinate space. In many calculations, however, it is more convenient to work in momentum space, and in the remainder of this section we will derive the corresponding Feynman rules in momentum space. Let $\mathcal{K}(\mathbf{p}_1, t_1; \mathbf{p}_0 t_0)$ be the amplitude that a particle with momentum $\mathbf{p}_0$ at time t_0 be later observed to have momentum $\mathbf{p}_1$ at time t_1. It is given by

$$\mathcal{K}(\mathbf{p}_1, t_1; \mathbf{p}_0 t_0) = \int \exp\left(-\frac{\mathrm{i}}{\hbar}\mathbf{p}_1 \cdot \mathbf{x}_1\right) K(\mathbf{x}_1 t_1; \mathbf{x}_0 t_0) \exp\left(\frac{\mathrm{i}}{\hbar}\mathbf{p}_0 \cdot \mathbf{x}_0\right) \mathrm{d}\mathbf{x}_0\, \mathrm{d}\mathbf{x}_1. \quad (5.38)$$

The free propagator $K_0(\mathbf{x}_1 t_1; \mathbf{x}_0 t_0)$ is given by the 3-dimensional generalisation of (5.19), i.e.

$$K_0(\mathbf{x}_1 t_1; \mathbf{x}_0 t_0) = \theta(t_1 - t_0)\left[\frac{m}{\mathrm{i}h(t_1 - t_0)}\right]^{3/2} \exp\left[\frac{\mathrm{i}m}{2\hbar}\frac{(\mathbf{x}_0 - \mathbf{x}_1)^2}{(t_1 - t_0)}\right]. \quad (5.39)$$

$\mathcal{K}_0$ is then

$$\mathcal{K}_0(\mathbf{p}_1 t_1; \mathbf{p}_0 t_0) = \theta(t_1 - t_0)\left(\frac{m}{\mathrm{i}h(t_1 - t_0)}\right)^{3/2} \int \exp\left[\frac{\mathrm{i}}{\hbar}(\mathbf{p}_0 \cdot \mathbf{x}_0 - \mathbf{p}_1 \cdot \mathbf{x}_1)\right] \times \exp\left[\frac{\mathrm{i}m}{2\hbar}\frac{(\mathbf{x}_0 - \mathbf{x}_1)^2}{(t_1 - t_0)}\right] \mathrm{d}\mathbf{x}_0\, \mathrm{d}\mathbf{x}_1.$$

To evaluate this integral we introduce the variables

$$\mathbf{x} = \mathbf{x}_0 - \mathbf{x}_1, \quad \mathbf{X} = \mathbf{x}_0 + \mathbf{x}_1, \quad \mathbf{p} = \mathbf{p}_0 - \mathbf{p}_1, \quad \mathbf{P} = \mathbf{p}_0 + \mathbf{p}_1$$

so that

$$2(\mathbf{p}_0 \cdot \mathbf{x}_0 - \mathbf{p}_1 \cdot \mathbf{x}_1) = \mathbf{P} \cdot \mathbf{x} + \mathbf{p} \cdot \mathbf{X}.$$

The Jacobian of the transformation is $(\frac{1}{2})^3 = \frac{1}{8}$, so we have

$$\mathcal{K}_0(\mathbf{p}_1, t_1 \colon \mathbf{p}_0, t_0) = \theta(t_1 - t_0)\left(\frac{2\alpha}{\mathrm{i}}\right)^{3/2}\frac{1}{8}\int \exp\left(\frac{\mathrm{i}}{2\hbar}\mathbf{p} \cdot \mathbf{X}\right) \mathrm{d}\mathbf{X}$$
$$\times \int \exp\left(\frac{\mathrm{i}}{2\hbar}\mathbf{P} \cdot \mathbf{x}\right) \mathrm{e}^{\mathrm{i}\alpha \mathbf{x}^2}\, \mathrm{d}\mathbf{x}$$

where $\alpha = m/2\hbar(t_1 - t_0)$. The first integral is $8(2\pi\hbar)^3\delta\mathbf{p} = 8(2\pi\hbar)^3\delta(\mathbf{p}_0 - \mathbf{p}_1)$, so

$$\mathcal{K}_0(\mathbf{p}_1 t_1; \mathbf{p}_0 t_0) = (2\pi\hbar)^3\theta(t_1 - t_0)\delta(\mathbf{p}_0 - \mathbf{p}_1)\left(\frac{2\alpha}{\mathrm{i}}\right)^{3/2}\int \exp\left(\frac{\mathrm{i}}{2\hbar}\mathbf{P} \cdot \mathbf{x} + \mathrm{i}\alpha \mathbf{x}^2\right) \mathrm{d}\mathbf{x}.$$

The integral may be evaluated by appealing to equation (5A.3) giving

$$\mathcal{K}_0(\mathbf{p}_1 t_1; \mathbf{p}_0 t_0) = (2\pi\hbar)^3\theta(t_1 - t_0)\delta(\mathbf{p}_0 - \mathbf{p}_1)\exp\left[\frac{-\mathrm{i}\mathbf{P}^2(t_1 - t_0)}{8m\hbar}\right].$$

Note that the delta function implies that $\mathbf{p}_1 = \mathbf{p}_0$, and there is only propagation when momentum is conserved. Moreover, we then have $\mathbf{P}^2 = 4\mathbf{p}_0^2$, so finally

$$\mathcal{K}_0(\mathbf{p}_1 t_1; \mathbf{p}_0 t_0) = (2\pi\hbar)^3\theta(t_1 - t_0)\delta(\mathbf{p}_0 - \mathbf{p}_1)\exp\left[\frac{\mathrm{i}\mathbf{p}_0^2(t_1 - t_0)}{2m\hbar}\right]. \tag{5.40}$$

This propagator, as already noted, gives the amplitude for observing a particle with momentum $\mathbf{p}_1$ at time t_1, if one has been observed with momentum $\mathbf{p}_0$ at time t_0. The Fourier transform of this quantity is, of course, $\mathcal{K}_0(\mathbf{x}_1 t_1; \mathbf{x}_0 t_0)$, given by the inverse of (5.38), which yields, on substituting (5.40),

$$K_0(\mathbf{x}_1 t_1; \mathbf{x}_0 t_0) = \frac{1}{(2\pi\hbar)^6}\int \exp\left(\frac{\mathrm{i}}{\hbar}\mathbf{p}_1 \cdot \mathbf{x}_1\right)\mathcal{K}_0(\mathbf{p}_1 t_1; \mathbf{p}_0 t_0)\exp\left(-\frac{\mathrm{i}}{\hbar}\mathbf{p}_0 \cdot \mathbf{x}_0\right) \mathrm{d}\mathbf{p}_1\, \mathrm{d}\mathbf{p}_0$$
$$= \theta(t_1 - t_0)\frac{1}{(2\pi\hbar)^3}\int \exp\left\{\frac{\mathrm{i}}{\hbar}\left[\mathbf{q} \cdot (\mathbf{x}_1 - \mathbf{x}_0) - \frac{\mathbf{q}^2}{2m}(t_1 - t_0)\right]\right\} \mathrm{d}\mathbf{q}. \tag{5.41}$$

We shall use this expression in the calculation of Coulomb scattering in the next section.

Finally, let us take the Fourier transform of the t dependence, so as to treat time and space in a symmetric manner. This is necessary for relativistic examples. The propagator we require is then

$$k_0(\mathbf{p}_1 E_1; \mathbf{p}_0 E_0) = \int \exp\left(\frac{i}{\hbar} E_1 t_1\right) \mathcal{K}_0(\mathbf{p}_1 t_1; \mathbf{p}_0 t_0) \exp\left(-\frac{i}{\hbar} E_0 t_0\right) dt_0\, dt_1$$
$$= (2\pi\hbar)^3 \delta(\mathbf{p}_0 - \mathbf{p}_1) \int \theta(\tau) \exp\left(\frac{-ip_1^2}{2m\hbar}\tau\right)$$
$$\times \exp\left[\frac{i}{\hbar}(E_1 t_1 - E_0 t_0)\right] dt_0\, dt_1 \qquad (5.42)$$

where $\tau = t_1 - t_0$. Regarding τ and t_0 as the independent variables, this gives

$$\mathcal{K}_0(\mathbf{p}_1 E_1; \mathbf{p}_0 E_0) = (2\pi\hbar)^3 \delta(\mathbf{p}_0 - \mathbf{p}_1) \int_{-\infty}^{\infty} \exp\left[\frac{i}{\hbar}(E_1 - E_0) t_0\right] dt_0$$
$$\times \int_{-\infty}^{\infty} \theta(\tau) \exp\left[\frac{i}{\hbar}\left(E_1 - \frac{p_1^2}{2m}\right)\tau\right] d\tau.$$

The first of these integrals is $(2\pi\hbar)\delta(E_1 - E_0)$. The presence of the $\theta(\tau)$ function in the second integral means that it is of the form

$$\int_0^{\infty} e^{i\omega\tau}\, d\tau$$

which, if ω is real, does not converge. To make it converge, ω must be replaced by $\omega + i\varepsilon$, where ε is small and positive. The value of the integral is then $i/(\omega + i\varepsilon)$.‡ Substituting for ω, we have finally

$$k_0(\mathbf{p}_1 E_1; \mathbf{p}_0 E_0) = (2\pi\hbar)^4 \delta(\mathbf{p}_0 - \mathbf{p}_1) \delta(E_0 - E_1) \frac{i\hbar}{E_1 - \dfrac{p_1^2}{2m} + i\varepsilon}. \qquad (5.43)$$

As may have been anticipated, this propagator yields energy conservation as well as momentum conservation. The limit $\varepsilon \to 0$ should be understood in equation (5.43). An important observation to make is that the energy E is not necessarily $p^2/2m$ for a particle described by wave mechanics. E and p are independent variables (used to define Fourier transforms from t and x space). It is only for a classical point particle, described in quantum theory by a wave packet of vanishing size, that $E = p^2/2m$. In this limiting case, the propagator above has a pole. Propagation takes place in general, however, for any value of E and p.

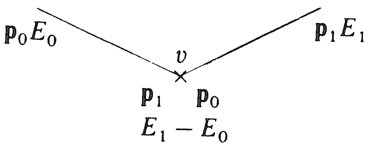
It is now straightforward, if tedious, to show that if we introduce the Fourier transform of the potential $V(\mathbf{x}, t)$ by

$$V(\mathbf{x}, t) = \int \exp\left[\frac{i}{\hbar}(\mathbf{q}\cdot\mathbf{x} - Wt)\right] v(\mathbf{q}, W)\, d\mathbf{q}\, dW \qquad (5.44)$$

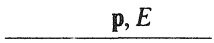
‡ Equivalently, the Fourier transform of $\theta(t)$ is given by

$$\theta(t) = \lim_{\varepsilon \to 0^+} \frac{1}{2\pi} \int e^{i\omega t} \frac{1}{\omega - i\varepsilon} d\omega$$

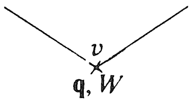
then the amplitude (5.34) may be expressed in terms of k_0 and v, and summarised by the momentum–space diagram



whose meaning is given by the *Feynman rules*



$$\frac{1}{(2\pi\hbar)^4}\frac{\mathrm{i}\hbar}{E - \dfrac{p^2}{2m} + \mathrm{i}\varepsilon}, \tag{5.45}$$



$$\frac{-\mathrm{i}}{\hbar}(2\pi\hbar)^4 v(\mathbf{q}, W).$$

with energy and momentum conservation.

These are the Feynman rules in momentum space. The expression for the scattering amplitude A contains ψ^*_{out}, ψ_{in} and integration over relevant variables.

5.3 Coulomb scattering

Let us now apply the theory developed above to the well-known problem of the scattering of charged spinless particles in a Coulomb field (Rutherford scattering). The scattering amplitude in the first Born approximation is given by (5.34)

$$A = \frac{-\mathrm{i}}{\hbar}\int \psi^*_{\text{out}}(\mathbf{x}_1 t_1) K_0(\mathbf{x}_1 t_1; \mathbf{x}t) V(\mathbf{x}, t) K_0(\mathbf{x}t; \mathbf{x}_0 t_0)\psi_{\text{in}}(\mathbf{x}_0 t_0)\, \mathrm{d}\mathbf{x}_1\, \mathrm{d}\mathbf{x}\, \mathrm{d}\mathbf{x}_0\, \mathrm{d}t$$

where $V(\mathbf{x}, t)$ represents the Coulomb potential. Now substitute for K_0 from (5.41), and for ψ_{out} and ψ_{in} from (5.32), giving

$$\begin{aligned} A = {} & \frac{-\mathrm{i}}{\hbar\tau}\frac{1}{(2\pi\hbar)^6}\int \exp\left[\frac{-\mathrm{i}}{\hbar}\left(\mathbf{p}_{\mathrm{f}}\cdot\mathbf{x}_1 - \frac{p_{\mathrm{f}}^2}{2m}t_1\right)\right]\theta(t_1 - t) \\ & \times \exp\left\{\frac{\mathrm{i}}{\hbar}\left[\mathbf{q}\cdot(\mathbf{x}_1 - \mathbf{x}) - \frac{q^2}{2m}(t_1 - t)\right]\right\} \\ & \times V(\mathbf{x}, t)\exp\left\{\frac{\mathrm{i}}{\hbar}\left[\mathbf{q}'\cdot(\mathbf{x} - \mathbf{x}_0) - \frac{q'^2}{2m}(t - t_0)\right]\right\}\theta(t - t_0) \\ & \times \exp\left[\frac{\mathrm{i}}{\hbar}\left(\mathbf{p}_{\mathrm{i}}\cdot\mathbf{x}_0 - \frac{p_i^2}{2m}t_0\right)\right]\mathrm{d}\mathbf{x}_1\, \mathrm{d}\mathbf{x}\, \mathrm{d}\mathbf{x}_0\, \mathrm{d}t\, \mathrm{d}\mathbf{q}\, \mathrm{d}\mathbf{q}'. \end{aligned}$$

Integration over $\mathbf{x}_1$ and $\mathbf{x}_0$ gives the delta functions

$$(2\pi\hbar)^3\delta(\mathbf{p}_f - \mathbf{q}) \quad \text{and} \quad (2\pi\hbar)^3\delta(\mathbf{q}' - \mathbf{p}_i).$$

Integration over $\mathbf{q}$ and $\mathbf{q}'$ then eliminates the terms in t_1 and t_0. Taking the limits $t_0 \to -\infty$, $t_1 \to \infty$ to eliminate the θ functions then gives

$$A = \frac{-i}{\hbar\tau}\int \exp\left\{\frac{i}{\hbar}[(\mathbf{p}_i - \mathbf{p}_f)\cdot\mathbf{x} - (E_i - E_f)t]\right\} V(\mathbf{x}, t)\,d\mathbf{x}\,dt$$

with $E_{i,f} = p_{i,f}^2/2m$. For the Coulomb potential $V = Ze^2/4\pi\varepsilon_0 r$ and integration over t then gives

$$A = \frac{-i}{\hbar}2\pi\delta\left(\frac{E_i - E_f}{\hbar}\right)\frac{Ze^2}{4\pi\varepsilon_0}\int \exp\left[\frac{i}{\hbar}(\mathbf{p}_i - \mathbf{p}_f)\cdot\mathbf{x}\right]\frac{1}{r}\,d\mathbf{x}.$$

The last integral does not converge at infinity, so a factor e^{-ar} is introduced, and, on letting $a \to 0$, the value of the integral is $4\pi\hbar^2/q^2$, where $\mathbf{q} = \mathbf{p}_i - \mathbf{p}_f$, so

$$A = \frac{-i}{\hbar\tau}\frac{2\pi Ze^2\hbar^2}{\varepsilon_0 q^2}\delta\left(\frac{E_i - E_f}{\hbar}\right). \tag{5.46}$$

This is the scattering amplitude, from which we want to calculate the scattering cross section σ. $|A|^2$ gives the probability that a particle emerges with momentum p_f. Assuming a box normalisation volume τ, then

$$|A|^2\frac{\tau\,d\mathbf{p}_f}{(2\pi\hbar)^3}$$

gives the probability that a particle emerges with momentum between $\mathbf{p}_f$ and $\mathbf{p}_f + d\mathbf{p}_f$. If the interaction lasts an effective time T, then

$$\frac{|A|^2}{T}\tau\frac{d\mathbf{p}_f}{(2\pi\hbar)^3}$$

is the number of particles per second emerging in this momentum range. To get the cross section, we divide by the incident flux and integrate over $\mathbf{p}_f$. The incident particles travel with speed p_i/m and there are $1/\tau$ of them per unit volume, so the flux is $p_i/\tau m$ particle per second per unit area. The cross section is then

$$\sigma = \int\frac{|A|^2}{T}\frac{\tau m}{p_i}\frac{\tau\,d\mathbf{p}_f}{(2\pi\hbar)^3}. \tag{5.47}$$

$|A|^2$ involves $|\delta(E_i - E_f/\hbar)|^2$. What is this? We appeal to the definition of $\delta(x)$:

$$\begin{aligned}\left|\delta\left(\frac{E_i - E_f}{\hbar}\right)\right|^2 &= \lim_{T\to\infty}\left|\frac{1}{2\pi}\int_{-T/2}^{T/2}\exp\left[i(E_i - E_f)t/\hbar\right]dt\right|^2 \\ &= \lim_{T\to\infty}\left|\frac{\sin\left[(E_i - E_f)T/2\hbar\right]}{\pi(E_i - E_f)/\hbar}\right|^2 \\ &= \frac{T}{2\pi}\delta\left(\frac{E_i - E_f}{\hbar}\right) \\ &= \frac{T\hbar}{2\pi}\delta(E_i - E_f) \end{aligned} \quad (5.48)$$

where we have used the formula $\lim_{\alpha\to\infty}(\sin^2\alpha x/\alpha x^2) = \pi\delta(x)$. Collecting together equations (5.46–8) gives

$$\begin{aligned}\sigma &= \frac{mZ^2e^4}{4\pi^2\varepsilon_0^2}\int\frac{1}{p_i}\frac{1}{q^4}\delta(E_f - E_i)\,d^3p_f \\ &= \frac{mZ^2e^4}{4\pi^2\varepsilon_0^2}\int\frac{1}{p_i}\frac{1}{q^4}p_f^2\,dp_f\delta(E_f - E_i)\,d\Omega.\end{aligned}$$

Now use $E = p^2/2m$ to put $p_i = (2mE_i)^{1/2}$ and $p_f^2\,dp_f = (2m^3E_f)^{1/2}\,dE_f$, and integrate over E_f to give

$$\sigma = \frac{m^2Z^2e^4}{4\pi^2\varepsilon_0^2}\int\frac{1}{q^4}\,d\Omega$$

where, because of the delta function, $p_i = p_f = p$. Hence $q^2 = 4p^2\sin^2(\theta/2)$ where θ is the angle between $\mathbf{p}_i$ and $\mathbf{p}_f$. Finally, putting $p = mv$ we have the differential cross section

$$\frac{d\sigma}{d\Omega} = \left(\frac{Ze^2}{8\pi\varepsilon_0 mv^2}\right)^2\frac{1}{\sin^4(\theta/2)} \quad (5.49)$$

which is the Rutherford formula.

5.4 Functional calculus: differentiation

Quantities like the propagator

$$\langle x_f t_f | x_i t_i\rangle = \int \mathcal{D}x\exp\left[\frac{i}{\hbar}\int_{t_i}^{t_f}L(x,\dot{x})\,dt\right]$$

are *functional integrals*: the integration is taken over all functions $x(t)$. The left-hand side is a number, so the integral associates with each *function* $x(t)$, a *number*. The integral is called a *functional*, and clearly depends on *the value of* *the function $x(t)$ at all points*. We may write this in short hand:

$$\text{functional: function} \longrightarrow \text{number}. \tag{5.50}$$

A *function*, for example $f(t) = t^2 + 2t$, has a value (a *number*) for each value of the independent parameter, which is also a number. Given a value for t, we calculate the value of f. In short hand:

$$\text{function: number} \longrightarrow \text{number}. \tag{5.51}$$

In mathematical notation, numbers belong to the space of *reals* $\mathbb{R}$, so a function defines a mapping

$$\text{function: } \mathbb{R} \longrightarrow \mathbb{R}. \tag{5.52}$$

Sometimes, of course, a function may be a vector quantity, like an electric field **E**, and therefore belong to $\mathbb{R}^3$; and it associates this electric field with every point of 3-dimensional space, and so is a mapping $\mathbb{R}^3 \rightarrow \mathbb{R}^3$. On the other hand, a scalar function $\phi(\mathrm{x})$ clearly defines a mapping $\mathbb{R}^3 \rightarrow \mathbb{R}$. In general, then, we have the definition

$$\text{function: } \mathbb{R}^n \longrightarrow \mathbb{R}^m. \tag{5.53}$$

Functions are continuous – to be precise, they are n-times differentiable. In physics, we generally concern ourselves with functions which are infinitely differentiable. The underlying co-ordinate space is a *manifold* M (for example $\mathbb{R}$, or $\mathbb{R}^3$ for 3-dimensional Euclidean space), and a function is denoted $C^n(M)$; and in the case of infinitely differentiable functions, $C^\infty(M)$. A functional, then, from (5.50), defines a mapping

$$\text{functional: } C^\infty(M) \longrightarrow \mathbb{R}. \tag{5.54}$$

It should by now be obvious, but nonetheless important to note, that a functional is *not* a function of a function, which is, of course, a function. It is common to denote a functional F of a function f by using square brackets, $F[f]$.

We now define functional differentiation. By analogy with ordinary differentiation, the derivative of the functional $F[f]$ with respect to the function $f(y)$ is defined by

$$\frac{\delta F[f(x)]}{\delta f(y)} = \lim_{\varepsilon \to 0} \frac{F[f(x) + \varepsilon\delta(x-y)] - F[f(x)]}{\varepsilon}. \tag{5.55}$$

Let us take a specific example. Consider the functional

$$F[f] = \int f(x)\,\mathrm{d}x. \tag{5.56}$$

Then

$$\frac{\delta F[f]}{\delta f(y)} = \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\left\{\int [f(x) + \varepsilon\delta(x - y)]\,dx - \int f(x)\,dx\right\}$$

$$= \int \delta(x - y)\,dx = 1. \tag{5.57}$$

As a second example, consider

$$F_x[f] = \int G(x, y) f(y)\,dy. \tag{5.58}$$

Here, x on the left-hand side is to be regarded as a parameter. Then

$$\frac{\delta F_x[f]}{\delta f(z)} = \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\left(\int \{G(x, y)[f(y) + \varepsilon\delta(y - z)]\}\,dy - \int G(x, y) f(y)\,dy\right)$$

$$= \int G(x, y)\delta(y - z)\,dy$$

$$= G(x, z). \tag{5.59}$$

5.5 Further properties of path integrals

We have shown that the transition amplitude from $q_i t_i$ to $q_f t_f$ is given by

$$\langle q_f t_f | q_i t_i\rangle = N\int \mathcal{D}q \exp\left[\frac{i}{\hbar}\int_{t_i}^{t_f} dt L(q, \dot{q})\right]$$

in the case where $H = (p^2/2m) + V(q)$, which is sufficiently general for the present purposes, and the boundary conditions of the problem are

$$q(t_f) = q_f, \quad q(t_i) = q_i.$$

This type of boundary condition may be appropriate in the motion of classical particles, but it is not what we meet in field theory. Its analogue there would be, for example, $\psi(t_i) = \psi_i$, $\psi(t_f) = \psi_f$. But what really happens is that particles are *created* (for example, by collision), they interact, and are *destroyed* by observation (i.e. by detection). For example, in measuring the differential cross section $d\sigma/d\Omega$ for πN scattering, the pion is created by an NN collision, and it is destroyed when it is detected.

The act of creation may be represented as a source, and that of destruction by a sink, which is, in a manner of speaking, a source. The boundary conditions of the problem may then be represented as in Fig. 5.6; the vacuum at $t = -\infty$ evolves into the vacuum at $t \to \infty$, via the creation, interaction and destruction of a particle, through the agency of a source. We want to know the *vacuum-to-vacuum transition amplitude in the presence of a source*. This

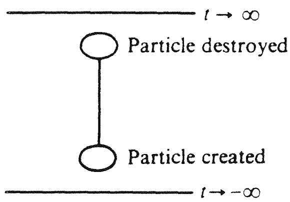


Fig. 5.6. Representation of the vacuum–vacuum transition amplitude in the presence of a source.

formulation, using the language of sources, is due to Schwinger (1969). The source $J(t)$ is represented by modifying the Lagrangian

$$L \to L + \hbar J(t)q(t). \tag{5.60}$$

If $|0, t\rangle^J$ is the ground state (vacuum) vector (in the moving frame) in the presence of the source, i.e. for a system described by (5.60), then the transition amplitude is

$$Z[J] \propto \langle 0, \infty|0, -\infty\rangle^J \tag{5.61}$$

where a proportionality factor has been omitted. The source $J(t)$ plays a role analogous to that of an electromagnetic current, which acts as a 'source' of the electromagnetic field. The charged scalar field ϕ, for example, has the Lagrangian (3.65) and its interaction with the electromagnetic field A^μ is given by the Lagrangian (3.73), of the form $J_\mu A^\mu$. The current J_μ acts as a source of the electromagnetic field, and this idea is generalised by Schwinger in the above formulation: any field ϕ may be 'created' by an appropriate source J. $Z[J]$ is a functional of J, and we now derive an expression for it, i.e. for the transition amplitude up to a constant factor. The salient feature is the presence of the ground state; how do we arrive at it?

The situation is represented by looking at the time axis in Fig. 5.7. What follows leans heavily on Abers & Lee (1973). The source $J(t)$ is non-zero only between times t and $t'(t < t')$. T is an earlier time than t, and T' a later time than t', so the transition amplitude is

$$\langle Q'T'|QT\rangle^J = N\int \mathfrak{D}q \exp\left[\frac{\mathrm{i}}{\hbar}\int_T^{T'} \mathrm{d}t(L + \hbar Jq)\right]. \tag{5.62}$$

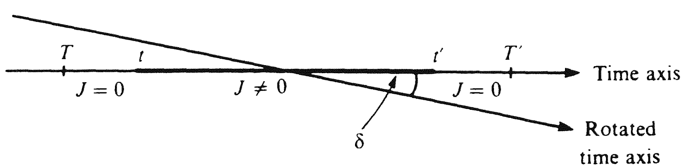


Fig. 5.7. Rotation of the time axis in calculating the vacuum–vacuum transition amplitude.

We may write

$$\langle Q'T'|QT\rangle^J = \int \mathrm{d}q'\,\mathrm{d}q \langle Q'T'|q't'\rangle\langle q't'|qt\rangle^J\langle qt|QT\rangle. \qquad (5.63)$$

Referring to (5.3) we then have

$$\begin{aligned}\langle Q'T'|q't'\rangle &= \left\langle Q'\left|\exp\left(-\frac{\mathrm{i}}{\hbar}HT'\right)\exp\left(\frac{\mathrm{i}}{\hbar}Ht'\right)\right|q'\right\rangle \\ &= \sum_m \phi_m(Q')\phi_m^*(q')\exp\left[\frac{\mathrm{i}}{\hbar}E_m(t'-T')\right], \end{aligned} \qquad (5.64)$$

where $\phi_m(q)$ are a complete set of energy eigenstates, Similarly,

$$\langle qt|QT\rangle = \sum_n \phi_n(q)\phi_n^*(Q)\exp\left[-\frac{\mathrm{i}}{\hbar}E_n(t-T)\right]. \qquad (5.65)$$

Now substitute these equations into (5.63). By taking the limit $T' \to \infty\,\mathrm{e}^{-\mathrm{i}\delta}$, $T \to -\infty\,\mathrm{e}^{-\mathrm{i}\delta}$, with δ an arbitrary angle $\leqslant \pi/2$ (see Fig. 5.7), we see that, since the imaginary part of T is $\mathrm{i}|T|\sin\delta$, the term $(\mathrm{i}/\hbar)E_nT$ contains a real part $-(1/\hbar)|T|\sin\delta$ which gives a damping factor $\exp\{-(1/\hbar)E_n|T|\sin\delta\}$. In the summation in (5.65), then, all the terms are damped but, the larger E_n is, the more they are damped. Hence the term which suffers the least damping is the one with the *smallest* E_n, that is E_0, the lowest energy stage, or vacuum. Hence in the summation *only the ground state (vacuum) contribution survives*. This is the feature we want. We then have

$$\begin{aligned}\lim_{\substack{T'\to\infty \mathrm{e}^{-\mathrm{i}\delta}\\ T\to-\infty \mathrm{e}^{-\mathrm{i}\delta}}} \langle Q'T'|QT\rangle^J &= \phi_0^*(Q)\phi_0(Q')\exp\left[-\frac{\mathrm{i}}{\hbar}E_0(T'-T)\right] \\ &\quad\times \int \mathrm{d}q'\,\mathrm{d}q\,\phi_0^*(q',t')\langle q't'|qt\rangle^J\phi_0(q,t)\end{aligned}$$

or

$$\begin{aligned}&\int \mathrm{d}q'\,\mathrm{d}q\,\phi_0^*(q',t')\langle q't'|qt\rangle^J\phi_0(q,t) \\ &\qquad = \lim_{\substack{T'\to\infty \mathrm{e}^{-\mathrm{i}\delta}\\ T\to-\infty \mathrm{e}^{-\mathrm{i}\delta}}} \frac{\langle Q'T'|QT\rangle^J}{\phi_0^*(Q)\phi_0(Q')\exp\left[-\frac{\mathrm{i}}{\hbar}E_0(T'-T)\right]}. \end{aligned} \qquad (5.66)$$

The left-hand side is the ground state expectation value of the transition amplitude. The times t' and $-t$ may be taken as large as one likes, so the left-hand side becomes $\langle 0,\infty|0,-\infty\rangle^J$. The denominator on the right-hand side is simply a numerical factor, so we have

$$\langle 0,\infty|0,-\infty\rangle^J \propto \lim_{\substack{T'\to\infty e^{-i\delta}\\ T\to-\infty e^{-i\delta}}} \langle Q'T'|QT\rangle^J \tag{5.67}$$

with

$$\langle Q'T'|QT\rangle^J = N\int \mathfrak{D}Q \exp\left\{\frac{i}{\hbar}\int_T^{T'} dt[L(Q,\dot{Q}) + \hbar JQ]\right\}.$$

Finally, instead of rotating the time axis as we have done, the ground state contribution may be isolated by adding a small negative imaginary part to the Hamiltonian in (5.64) and (5.65); adding $-\frac{1}{2}i\varepsilon q^2$ will achieve the result. This is equivalent to adding $+\frac{1}{2}i\varepsilon q^2$ to L, so we finally define $Z[J]$ in (5.61) by

■ $$Z[J] = \int \mathfrak{D}q \exp\left[\frac{i}{\hbar}\int_{-\infty}^{\infty} dt(L + \hbar Jq + \tfrac{1}{2}i\varepsilon q^2)\right] \propto \langle 0,\infty|0,-\infty\rangle^J. \tag{5.68}$$

This expression for the transition amplitude will be taken over when we consider field theory, in the next chapter. Meanwhile, we shall prove one more relation, involving the functional derivatives of Z with respect to $J(t)$.

To begin, instead of $\langle q_f t_f|q_i t_i\rangle$, consider $\langle q_f t_f|q(t_{n_1})|q_i t_i\rangle$, where $t_f > t_{n_1} > t_i$, and it should be remembered that $q(t_{n_1})$ is an operator. Consider equation (5.6), and choose t_{n_1} to be one of the times $t_1, \ldots, t_n$. Then

$$\langle q_f t_f|q(t_{n_1})|q_i t_i\rangle = \int dq_1 \ldots dq_n \langle q_f t_f|q_n t_n\rangle\langle q_n t_n|q_{n-1} t_{n-1}\rangle$$
$$\ldots \langle q_{n_1} t_{n_1}|q(t_{n_1})|q_{n_1-1} t_{n_1-1}\rangle \ldots \langle q_1 t_1|q_i t_i\rangle.$$

The expression $\langle q_{n_1} t_{n_1}|q(t_{n_1})|\langle q_{n_1-1} t_{n_1-1}\rangle$ may clearly be replaced by $q(t_{n_1})\langle q_{n_1} t_{n_1}|\langle q_{n_1-1} t_{n_1-1}\rangle$, where this time $q(t_{n_1})$ is a scalar. The rest of the argument is analogous to that leading from (5.6) to (5.13), so we have, finally,

$$\langle q_f t_f|q(t_1)|q_i t_i\rangle = \int \frac{\mathfrak{D}q\mathfrak{D}p}{h} q(t_1) \exp\left\{\frac{i}{\hbar}\int_{t_i}^{t_f}[p\dot{q} - H(p,q)]\,dt\right\}. \tag{5.69}$$

Next, we suppose we want to find

$$\langle q_f t_f|q(t_{n_1})q(t_{n_2})|q_i t_i\rangle.$$

If $t_{n_1} > t_{n_2}$ we have

$$\langle q_f t_f|q(t_{n_1})q(t_{n_2})|q_i t_i\rangle = \int dq_1 \ldots dq_n \langle q_f t_f|q_n t_n\rangle \ldots \langle q_{n_1} t_{n_1}|q(t_{n_1})|q_{n_1-1} t_{n_1-1}\rangle$$
$$\ldots \langle q_{n_2} t_{n_2}|q(t_{n_2})|q_{n_2-1} t_{n_2-1}\rangle \ldots \langle q_1 t_1|q_i t_i\rangle,$$

giving, finally,

$$\langle q_f t_f|q(t_1)q(t_2)|q_i t_i\rangle = \int \frac{\mathfrak{D}q\mathfrak{D}p}{h} q(t_1)q(t_2) \exp\left[\frac{i}{\hbar}\int_{t_i}^{t_f}(p\dot{q} - H)\,dt\right] \tag{5.70}$$

if $t_1 > t_2$. If, on the other hand, $t_2 > t_1$, this is not true; in that case, the right-hand side of (5.70) is equal to

$$\langle q_f t_f | q(t_2) q(t_1) | q_i t_i \rangle.$$

In general, then, the right-hand side of (5.70) is equal to

$$\langle q_f t_f | T[q(t_1) q(t_2)] | q_i t_i \rangle$$

where the *time ordering operator* T has the definition

$$T[A(t_1)B(t_2)] = \begin{cases} A(t_1)B(t_2) & \text{if } t_1 > t_2, \\ B(t_2)A(t_1) & \text{if } t_2 > t_1. \end{cases} \tag{5.71}$$

T has the effect of putting earlier times to the right. The result we have found generalises to

$$\langle q_f t_f | T[q(t_1) q(t_2) \ldots q(t_n)] | q_i t_i \rangle = \int \frac{\mathscr{D}q \mathscr{D}p}{h} q(t_1) q(t_2) \ldots q(t_n) \times \exp\left\{ \frac{i}{\hbar} \int_{t_i}^{t_f} [p\dot{q} - H(p, q)] \, dt \right\}. \tag{5.72}$$

In the case where H is of the form (5.8), this becomes

$$\langle q_f t_f | T[q(t_1) q(t_2) \ldots q(t_n)] | q_i t_i \rangle = N \int \mathscr{D}q \, q(t_1) q(t_2) \ldots q(t_n) \times \exp\left(\frac{i}{\hbar} \int_{t_i}^{t_f} L \, dt \right). \tag{5.73}$$

However, from the definition of $Z[J]$ in (5.68), its functional derivative with respect to J is

$$\frac{\delta Z[J]}{\delta J(t_1)} = i \int \mathscr{D}q \, q(t_1) \exp\left[\frac{i}{\hbar} \int_{-\infty}^{\infty} dt (L + \hbar J q + \tfrac{1}{2} i \varepsilon q^2) \right]$$

and hence

$$\frac{\delta^n Z[J]}{\delta J(t_1) \ldots \delta J(t_n)} = i^n \int \mathscr{D}q \, q(t_1) \ldots q(t_n) \exp\left[\frac{i}{\hbar} \int_{-\infty}^{\infty} dt (L + \hbar J q + \tfrac{1}{2} i \varepsilon q^2) \right] \tag{5.74}$$

which gives, on putting $J = 0$,

$$\left. \frac{\delta^n Z[J]}{\delta J(t_1) \ldots \delta J(t_n)} \right|_{J=0} = i^n \int \mathscr{D}q \, q(t_1) \ldots q(t_n) \exp\left[\frac{i}{\hbar} \int_{-\infty}^{\infty} dt (L + \tfrac{1}{2} i \varepsilon q^2) \right]. \tag{5.75}$$

Comparing the right-hand side of this equation with that of (5.73) above, we note that the difference lies in the $\frac{1}{2}i\varepsilon q^2$ term; but we know, from what was said above, that it is this term that has the effect of isolating the ground state contribution, so we finish up with the vacuum expectation value of the time-ordered product:

■
$$\left.\frac{\delta^n Z[J]}{\delta J(t_1)\ldots\delta J(t_n)}\right|_{J=0} \propto i^n\langle 0,\infty|T[q(t_1)\ldots q(t_n)]|0,-\infty\rangle. \tag{5.76}$$

This is the second result we wanted, and to which we shall have recourse in the next chapter.

Appendix: some useful integrals

We begin by stating a well-known formula

$$\int_{-\infty}^{\infty} e^{-\alpha x^2}\,dx = \left(\frac{\pi}{\alpha}\right)^{1/2} \quad (\alpha > 0). \tag{5A.1}$$

Proving it is clearly the same as proving that

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-\alpha(x^2+y^2)}\,dx\,dy = \frac{\pi}{\alpha}, \tag{5A.2}$$

and this is shown by going over to polar co-ordinates (r, θ):

$$\begin{aligned}\int_0^{2\pi}\int_0^{\infty} e^{-\alpha r^2} r\,dr\,d\theta &= 2\pi\int_0^{\infty} e^{-\alpha r^2}\,dr\\ &= \pi\int_0^{\infty} e^{-\alpha r^2}\,d(r^2)\\ &= \frac{\pi}{\alpha}.\end{aligned}$$

Thus, (5A.1) is proved.

Now we pass from the integration of Gaussians to that of quadratic forms

$$\int_{-\infty}^{\infty} e^{-ax^2+bx+c}\,dx \equiv \int_{-\infty}^{\infty} e^{q(x)}\,dx.$$

Let $\bar{x}$ be the value of x giving a minimum of q:

$$\bar{x} = \frac{b}{2a}, \quad q(\bar{x}) = \frac{b^2}{4a} + c.$$

This allows us to 'uncomplete' the square:

$$q(x) = q(\bar{x}) - a(x - \bar{x})^2.$$

Hence

$$\int_{-\infty}^{\infty} e^{q(x)}\,dx = e^{q(\bar{x})}\int_{-\infty}^{\infty} e^{-a(x-\bar{x})^2}\,dx$$

$$= e^{q(\bar{x})}\left(\frac{\pi}{a}\right)^{1/2}$$

from (5A.1). Finally, we have

$$\int_{-\infty}^{\infty} \exp(-ax^2 + bx + c)\,dx = \exp\left(\frac{b^2}{4a} + c\right)\left(\frac{\pi}{a}\right)^{1/2}. \qquad (5A.3)$$

Lastly, we show that

$$\int_{-\infty}^{\infty} \exp\{i\lambda[(x_1 - a)^2 + (x_2 - x_1)^2 + \ldots + (b - x_n)^2]\}\,dx_1 \ldots dx_n$$

$$= \left[\frac{i^n\pi^n}{(n+1)\lambda^n}\right]^{1/2} \exp\left[\frac{i\lambda}{n+1}(b-a)^2\right]. \qquad (5A.4)$$

It is proved by induction; we assume it is true for n, and show it is true for $n + 1$. We have

$$\int_{-\infty}^{\infty} \exp\{i\lambda[(x_1 - a)^2 + \ldots + (b - x_{n+1})^2]\}\,dx_1 \ldots dx_{n+1}$$

$$= \left[\frac{i^n\pi^n}{(n+1)\lambda^n}\right]^{1/2}\int_{-\infty}^{\infty} \exp\left[\frac{i\lambda}{n+1}(x_{n+1} - a)^2\right]\exp[i\lambda(b - x_{n+1})^2]\,dx_{n+1}$$

$$= \left[\frac{i^n\pi^n}{(n+1)\lambda^n}\right]^{1/2}\int_{-\infty}^{\infty} \exp\left\{i\lambda\left[\frac{1}{n+1}(x_{n+1} - a)^2 + (b - x_{n+1})^2\right]\right\}dx_{n+1}.$$

Putting $x_{n+1} - a = y$, the term in square brackets becomes

$$\frac{1}{n+1}y^2 + (b - a - y)^2 = \frac{n+2}{n+1}y^2 - 2y(b-a) + (b-a)^2$$

$$= \frac{n+2}{n+1}\left[y - \frac{n+1}{n+2}(b-a)\right]^2 + \frac{1}{n+2}(b-a)^2.$$

Now we put $\lambda - (n + 1/n + 2)(b - a) = z$ and find that the integral is

$$\left(\frac{i^n\pi^n}{(n+1)\lambda^n}\right)^{1/2}\int_{-\infty}^{\infty} \exp\left[i\lambda\frac{n+2}{n+1}z^2 + \frac{i\lambda}{n+2}(b-a)^2\right]dz$$

$$= \left[\frac{i^{n+1}\pi^{n+1}}{(n+2)\lambda^{n+1}}\right]^{1/2}\exp\left[\frac{i\lambda}{n+2}(b-a)^2\right]$$

which is (5A.4) with $n + 1$ instead of n. It only remains to show that the formula holds when $n = 1$. In this case the integral is

$$I = \int_{-\infty}^{\infty} \exp\{i\lambda[(x-a)^2 + (b-x)^2]\}\, dx$$
$$= \exp\left[i\frac{\lambda(a-b)^2}{2}\right]\left(\frac{i\pi}{2\lambda}\right)^{1/2}$$

where in the last step (5A.3) has been used, but with a in that equation imaginary. This value for I is the same as the value obtained from (5A.4) by putting $n = 1$. We have therefore proved (5A.4) for all n.

Summary

[1]Feynman's path integral formulation of quantum mechanics is explained, and [2]a perturbation series (the Born series) developed. The S matrix (for scattering of 'particles') is defined and it is shown how the resulting transition amplitudes may be obtained by reference to the 'Feynman rules'. These are written down in co-ordinate space and momentum space. [3]It is shown how the case of Coulomb scattering results in Rutherford's formula. [4]A brief account of functional differentiation is followed by [5]a demonstration that the scattering amplitude, written as a vacuum-to-vacuum transition amplitude in the presence of a source J, is a functional integral of J, and relates the vacuum expectation values of time-ordered products of operators to corresponding functional derivatives of this functional integral. The appendix proves the integrals needed in the course of the chapter.

Guide to further reading

The first papers on path-integral quantisation were Dirac (1933) and Feynman (1948); these are both reprinted in Schwinger (1958). An expanded account is to be found in Feynman & Hibbs (1965). There are by now a number of good reviews of path-integral quantisation as used in physics, among which are the following: Marinov (1980), DeWitt-Morette, Maheshwari & Nelson (1979), Schulman (1981), Lee (1981, ch. 19), J.R. Klauder in Papadopoulos & Devreese (1978), Blokhinstev & Barbashov (1972), and Abers & Lee (1973). Good introductions to the mathematical aspects of functional integration are Gel'fand & Yaglom (1960), Kac (1959), Keller & McLaughlin (1975). For more rigorous treatment, see Gudder (1979), Simon (1979), and M.C. Reed in Velo & Wightman (1973). Schwinger's philosophy of sources is explained in, for example, Schwinger (1969).