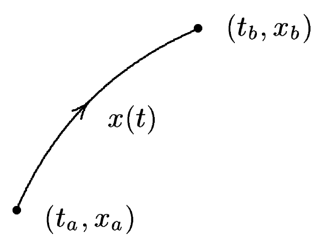
Chapter 2

Feynman path-integral formulation of quantum mechanics

2.1 Classical action

Suppose a particle starts at initial time t_a and point x_a, and goes to a final point x_b at time t_b:



Write the path of the particle between these two points as a function of t: $x(t)$ with $x(t_a) = x_a$ and $x(t_b) = x_b$. The classical path $\bar{x}(t)$ is singled out of all the possible paths as the one having the least action S, given by

$$S = \int_{t_a}^{t_b} \mathrm{d}t \, L(x, \dot{x}, t) \,, \tag{2.1}$$

where the Lagrangian is

$$L = \tfrac{1}{2} m \dot{x}^2 - V(x, t) \,. \tag{2.2}$$

This minimum would remain unchanged to first order if the path is varied away from $\bar{x}(t)$ by the amount $\delta x(t)$, such that the end-points are kept fixed:

$$\delta x(t_a) = \delta x(t_b) = 0\,. \tag{2.3}$$

In other words, the variation

$$\delta S \equiv S[\bar{x} + \delta x] - S[\bar{x}]\,, \tag{2.4}$$

vanishes to first order in δx. But

$$\begin{aligned} S[x+\delta x] &= \int_{t_a}^{t_b} \mathrm{d}t\, L(x+\delta x, \dot{x}+\delta\dot{x}, t) \\ &= \int_{t_a}^{t_b} \mathrm{d}t\, \left(L(x,\dot{x},t) + \delta\dot{x}\frac{\partial L}{\partial \dot{x}} + \delta x \frac{\partial L}{\partial x} \right) \\ &= S[x] + \int_{t_a}^{t_b} \mathrm{d}t\, \left(\delta\dot{x}\frac{\partial L}{\partial \dot{x}} + \delta x \frac{\partial L}{\partial x} \right). \end{aligned} \tag{2.5}$$

Hence

$$\delta S = \delta x \frac{\partial L}{\partial \dot{x}}\bigg|_{t_a}^{t_b} - \int_{t_a}^{t_b} \mathrm{d}t\, \delta x \left(\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} \right), \tag{2.6}$$

where the boundary term vanishes by (2.3). Since δx is arbitrary, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} = 0\,. \tag{2.7}$$

This is the Euler–Lagrange equation and it gives the usual classical equation of motion.

2.2 Quantum mechanical propagator

Instead of only considering the classical trajectory, we now consider every possible path between a and b. Each path contributes a different phase to the total amplitude to go from a to b. The phase of the contribution from a given path is equal to the action S for that path in units of the quantum of action $\hbar$. This amplitude can be written as

$$\begin{aligned} K(b,a) &= \sum_{\substack{\text{all paths} \\ \text{from a to b}}} \phi[x(t)]\,, \\ \phi[x(t)] &= \text{const}\ \mathrm{e}^{\frac{i}{\hbar}S[x(t)]}. \end{aligned} \tag{2.8}$$

The probability to go from point x_a at time t_a to point x_b at time t_b is then

$$P(b,a) = |K(b,a)|^2. \tag{2.9}$$

We shall write the sum over all paths as the (path) integral:

$$K(b,a) = \int_a^b \mathcal{D}x(t)\, \mathrm{e}^{\frac{i}{\hbar}S[b,a]}, \tag{2.10}$$

although the measure $\mathcal{D}x(t)$ is not defined at this stage.

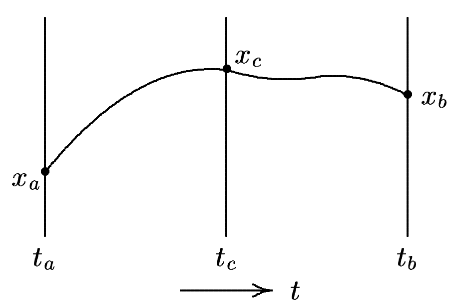
Suppose that $t_a < t_c < t_b$. Then the action along any path between a and b can be written as

$$S[b,a] = S[b,c] + S[c,a]\,. \tag{2.11}$$

This follows from the definition of the action as an integral in time, and also from the fact that L does not depend on derivatives higher than velocity (otherwise, we would have to specify values of velocity and perhaps higher derivatives at point c). Hence

$$K(b,a) = \int_a^b \mathcal{D}x(t)\, \mathrm{e}^{\frac{i}{\hbar}\{S[b,c]+S[c,a]\}}. \tag{2.12}$$

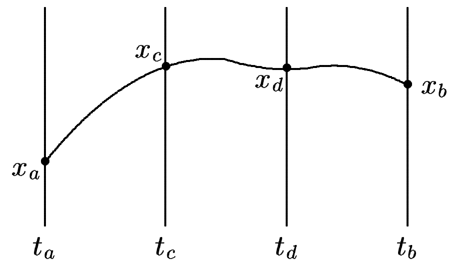
For any path between a and b, we split it into two parts:



The first part will have end points x_a and $x_c \equiv x(t_c)$, while the second part will have end points x_c and x_b. So we integrate first over all paths from a to c, then over all paths from c to b, and then finally integrate over all possible values of x_c:

$$\begin{aligned} K(b,a) &= \int_{x_c} \mathrm{d}x_c \int_c^b \mathcal{D}x(t)\, \mathrm{e}^{\frac{i}{\hbar}S[b,c]} K(c,a) \\ &= \int_{x_c} \mathrm{d}x_c\, K(b,c)K(c,a)\,. \end{aligned} \tag{2.13}$$

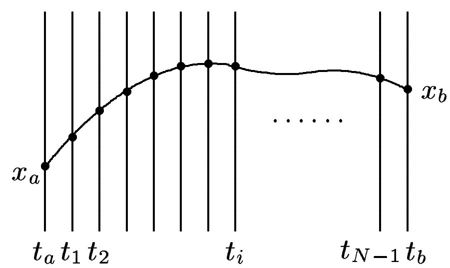
Similarly, if we make two divisions in all the paths, say at times t_c and t_d:



then we can write

$$K(b,a) = \int_{x_c}\int_{x_d} \mathrm{d}x_c \mathrm{d}x_d \, K(b,d)K(d,c)K(c,a)\,. \tag{2.14}$$

And for N intervals in the time scale:



the propagator is

$$K(b,a) = \int_{x_1}\int_{x_2}\cdots\int_{x_{N-1}} \mathrm{d}x_1\mathrm{d}x_2\cdots\mathrm{d}x_{N-1}\, K(b,N-1)K(N-1,N-2) \cdots K(i+1,i)\cdots K(1,a)\,. \tag{2.15}$$

Now suppose $N\to\infty$, i.e., consider infinitesimal time intervals. Then the propagator for a particle to go between two points separated by an infinitesimal time interval ϵ is

$$\begin{aligned} K(i+1,i) &= \text{const } \mathrm{e}^{\frac{i}{\hbar}S[i+1,i]} = \frac{1}{A}\exp\left[\frac{i}{\hbar}\int \mathrm{d}t\, L\right] \\ &= \frac{1}{A}\exp\left[\frac{i\epsilon}{\hbar}L\left(\frac{x_{i+1}+x_i}{2}, \frac{x_{i+1}-x_i}{\epsilon}, \frac{t_{i+1}+t_i}{2}\right)\right]. \end{aligned} \tag{2.16}$$

2.3 Schrödinger equation

Denote the probability of finding a particle at the point x and the time t by $|\psi(x,t)|^2$. We call this type of amplitude a wave function, and it differs from the other type of amplitude

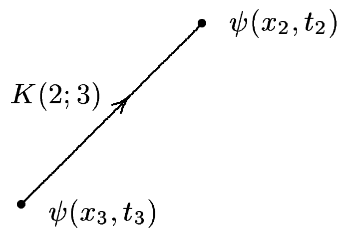
$K(x_2, t_2; x_1, t_1)$ in that the former does not worry about where the particle originated from. The difference between the two is just a matter of notation:

$$K(x_2, t_2; x_1, t_1) = \psi(x_2, t_2)\,. \tag{2.17}$$

The notation on the left-hand side gives us more information. Recalling the property (2.13), we can write

$$\psi(x_2, t_2) = \int_{-\infty}^{\infty} \mathrm{d}x_3\, K(x_2, t_2; x_3, t_3)\psi(x_3, t_3)\,. \tag{2.18}$$

Physically, this means that the total amplitude to arrive at (x_2, t_2) [i.e., $\psi(x_2, t_2)$] is the sum over all possible values of x_3, of the total amplitude to arrive at x_3 [i.e., $\psi(x_3, t_3)$], multiplied by the amplitude to go from 3 to 2 [i.e., $K(x_2, t_2; x_3, t_3)$]:



Consider now an infinitesimal time interval of length ϵ. Using the approximation of K obtained in (2.16), we have

$$\psi(x, t+\epsilon) = \frac{1}{A}\int_{-\infty}^{\infty} \mathrm{d}y\, \exp\left[\frac{i\epsilon}{\hbar} L\left(\frac{x+y}{2}, \frac{x-y}{\epsilon}, t\right)\right]\psi(y, t)\,. \tag{2.19}$$

For a particle moving in a potential $V(x, t)$ in one dimension,

$$\psi(x, t+\epsilon) = \frac{1}{A}\int_{-\infty}^{\infty} \mathrm{d}y\, \exp\left[\frac{i}{\hbar}\frac{m(x-y)^2}{2\epsilon}\right]\exp\left[-\frac{i\epsilon}{\hbar} V\left(\frac{x+y}{2}, t\right)\right]\psi(y, t)\,. \tag{2.20}$$

The quantity $\frac{(x-y)^2}{\epsilon}$ appears in the exponent of the first factor. If y is appreciably different from x, this quantity is very large and the exponential oscillates very rapidly as y varies. So the integral over y gives a very small value. Appreciable contributions to the integral will only occur when y is near x. Write $y = x + \eta$, so that

$$\psi(x, t+\epsilon) = \frac{1}{A}\int_{-\infty}^{\infty} \mathrm{d}\eta\, \exp\left(\frac{im\eta^2}{2\hbar\epsilon}\right)\exp\left[-\frac{i\epsilon}{\hbar} V\left(x+\frac{\eta}{2}, t\right)\right]\psi(x+\eta, t)\,. \tag{2.21}$$

The phase of the first exponential changes by order of one radian when η is of order $\sqrt{\epsilon\hbar/m}$, so that most of that integral is contributed by values of η in this order.

Now expand (2.21) to first order in ϵ and second order in η:

$$\psi(x,t)+\epsilon\frac{\partial\psi}{\partial t}=\frac{1}{A}\int_{-\infty}^{\infty}\mathrm{d}\eta\,\exp\left(\frac{im\eta^2}{2\hbar\epsilon}\right)\left[1-\frac{i\epsilon}{\hbar}V(x,t)\right]\left[\psi(x,t)+\eta\frac{\partial\psi}{\partial x}+\frac{\eta^2}{2}\frac{\partial^2\psi}{\partial x^2}\right]. \tag{2.22}$$

Considering the leading term on the right-hand side, we have $\psi(x,t)$ multiplied by

$$\frac{1}{A}\int_{-\infty}^{\infty}\mathrm{d}\eta\,\exp\left(\frac{im\eta^2}{2\hbar\epsilon}\right)=\frac{1}{A}\left(\frac{2\pi i\hbar\epsilon}{m}\right)^{\frac{1}{2}}. \tag{2.23}$$

On the left-hand side, we just have $\psi(x,t)$, so taking the limit $\epsilon\to 0$, we get

$$A=\left(\frac{2\pi i\hbar\epsilon}{m}\right)^{\frac{1}{2}}. \tag{2.24}$$

Now, recall the two integrals:

$$\begin{aligned}\frac{1}{A}\int_{-\infty}^{\infty}\mathrm{d}\eta\,\eta\exp\left(\frac{im\eta^2}{2\hbar\epsilon}\right)&=0\,,\\ \frac{1}{A}\int_{-\infty}^{\infty}\mathrm{d}\eta\,\eta^2\exp\left(\frac{im\eta^2}{2\hbar\epsilon}\right)&=\frac{i\hbar\epsilon}{m}.\end{aligned} \tag{2.25}$$

We thus have

$$\psi(x,t)+\epsilon\frac{\partial\psi}{\partial t}=\psi(x,t)-\frac{i\epsilon}{\hbar}V(x,t)\psi-\frac{\hbar\epsilon}{2im}\frac{\partial^2\psi}{\partial x^2}\,, \tag{2.26}$$

or

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+V(x,t)\psi\,. \tag{2.27}$$

This is the Schrödinger equation for a particle restricted to one dimension. It is in the differential equation form.

The equations which result from various problems corresponding to different forms of the Lagrangian can all be written as

$$i\hbar\frac{\partial\psi}{\partial t}=H\psi\,, \tag{2.28}$$

where H is the Hamiltonian operator. In the above example, this operator is

$$H=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x,t)\,. \tag{2.29}$$

Since $K(2,1)$, thought of as a function of the variables 2, is a special wave function (namely, that for a particle which starts at 1), we see that K must also satisfy a Schrödinger equation. Thus, for the above case,

$$i\hbar\frac{\partial}{\partial t_2}K(2,1) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial {x_2}^2}K(2,1) + V(2)K(2,1)\,, \tag{2.30}$$

for $t_2 > t_1$. In general, we have

$$i\hbar\frac{\partial}{\partial t_2}K(2,1) = H_2 K(2,1)\,, \tag{2.31}$$

where the operator H_2 acts on variables 2 only. The function $K(2,1)$ defined by the path integral is defined for $t_2 > t_1$. It is convenient to define $K(2,1)$ to be zero for $t_2 < t_1$. The above equation is trivially satisfied for this case. However, this equation is not satisfied when $t_2 = t_1$, because $K(2,1)$ is discontinuous at this point.

Now recall that

$$\int_{-\infty}^{\infty} \mathrm{d}x_2\, K(x_3,t_3;x_2,t_2)K(x_2,t_2;x_1,t_1) = K(x_3,t_3;x_1,t_1)\,, \tag{2.32}$$

for $t_2 \to t_1 + 0$. Then in this limit,

$$K(x_2,t_2;x_1,t_1) = \delta(x_2 - x_1)\,, \tag{2.33}$$

since

$$\int_{-\infty}^{\infty} \mathrm{d}x_2\, K(x_3,t_3;x_2,t_1)\delta(x_2 - x_1) = K(x_3,t_3;x_1,t_1)\,. \tag{2.34}$$

Hence the derivative of $K(x_2,t_2;x_1,t_1)$ with respect to t_2 gives a delta function in the time, multiplied by the height of the jump $\delta(x_2 - x_1)$. $K(2,1)$ therefore satisfies

$$i\hbar\frac{\partial}{\partial t_2}K(2,1) - H_2 K(2,1) = i\hbar\delta(x_2 - x_1)\delta(t_2 - t_1)\,. \tag{2.35}$$

This equation could serve to define $K(2,1)$ if one were to start out from the Schrödinger equation as the fundamental definition in quantum mechanics. It is clear that the quantity $K(2,1)$ is a kind of Green's function for the Schrödinger equation.

2.4 Free-particle propagator

We now describe a free particle in one dimension using the path-integral approach. The Lagrangian in this case is

$$L = \tfrac{1}{2} m \dot{x}^2. \tag{2.36}$$

Then the propagator is

$$\begin{aligned} K(b,a) = \lim_{\epsilon\to 0} \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{-\frac{N}{2}} \int_{x_1}\int_{x_2}\cdots\int_{x_{N-1}} \mathrm{d}x_1\mathrm{d}x_2\cdots\mathrm{d}x_{N-1} \exp\left[\frac{i\epsilon}{\hbar}\frac{m}{2}\left(\frac{x_N - x_{N-1}}{\epsilon}\right)^2\right] \\ \exp\left[\frac{i\epsilon}{\hbar}\frac{m}{2}\left(\frac{x_{N-1} - x_{N-2}}{\epsilon}\right)^2\right]\cdots\exp\left[\frac{i\epsilon}{\hbar}\frac{m}{2}\left(\frac{x_1 - x_0}{\epsilon}\right)^2\right] \\ = \lim_{\epsilon\to 0} \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{-\frac{N}{2}} \int_{x_1}\int_{x_2}\cdots\int_{x_{N-1}} \mathrm{d}x_1\mathrm{d}x_2\cdots\mathrm{d}x_{N-1} \exp\left[\frac{im}{2\hbar\epsilon}\sum_{i=1}^{N}(x_i - x_{i-1})^2\right]. \end{aligned} \tag{2.37}$$

This can be calculated by successive application of gaussian integrals.[1] First notice that

$$\begin{aligned} &\left(\frac{2\pi i\hbar\epsilon}{m}\right)^{-\frac{2}{2}} \int_{-\infty}^{\infty} \mathrm{d}x_1 \exp\left\{-\frac{m}{2i\hbar\epsilon}[(x_2-x_1)^2 + (x_1-x_0)^2]\right\} \\ &= \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{-\frac{2}{2}} \left(\int_{-\infty}^{\infty} \mathrm{d}x_1 \exp\left\{-\frac{m}{2i\hbar\epsilon}[2{x_1}^2 - 2(x_2+x_0)x_1]\right\}\right) \exp\left\{-\frac{m}{2i\hbar\epsilon}[{x_2}^2 + {x_0}^2]\right\} \\ &= \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{-\frac{2}{2}} \sqrt{\frac{\pi i\hbar\epsilon}{m}} \exp\left\{\frac{m}{4i\hbar\epsilon}[x_0 + x_2]^2\right\} \exp\left\{-\frac{m}{2i\hbar\epsilon}[{x_0}^2 + {x_2}^2]\right\} \\ &= \left(\frac{2\pi i\hbar\cdot 2\epsilon}{m}\right)^{-\frac{1}{2}} \exp\left\{-\frac{m}{2i\hbar\cdot 2\epsilon}(x_2 - x_0)^2\right\}. \end{aligned} \tag{2.38}$$

Next we multiply this result by

$$\left(\frac{2\pi i\hbar\epsilon}{m}\right)^{-\frac{1}{2}} \exp\left\{-\frac{m}{2i\hbar\epsilon}(x_3 - x_2)^2\right\}, \tag{2.39}$$

and integrate over x_2. We get

$$\left(\frac{2\pi i\hbar\cdot 3\epsilon}{m}\right)^{-\frac{1}{2}} \exp\left\{-\frac{m}{2i\hbar\cdot 3\epsilon}(x_3 - x_0)^2\right\}, \tag{2.40}$$

and so on. After $n-1$ steps, we have

$$\left(\frac{2\pi i\hbar\cdot n\epsilon}{m}\right)^{-\frac{1}{2}} \exp\left\{-\frac{m}{2i\hbar\cdot n\epsilon}(x_n - x_0)^2\right\}. \tag{2.41}$$

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[1] $\int_{-\infty}^{\infty} \mathrm{d}x \, \exp(-p^2x^2 \pm qx) = \frac{\sqrt{\pi}}{p}\exp\left(\frac{q^2}{4p^2}\right)$.

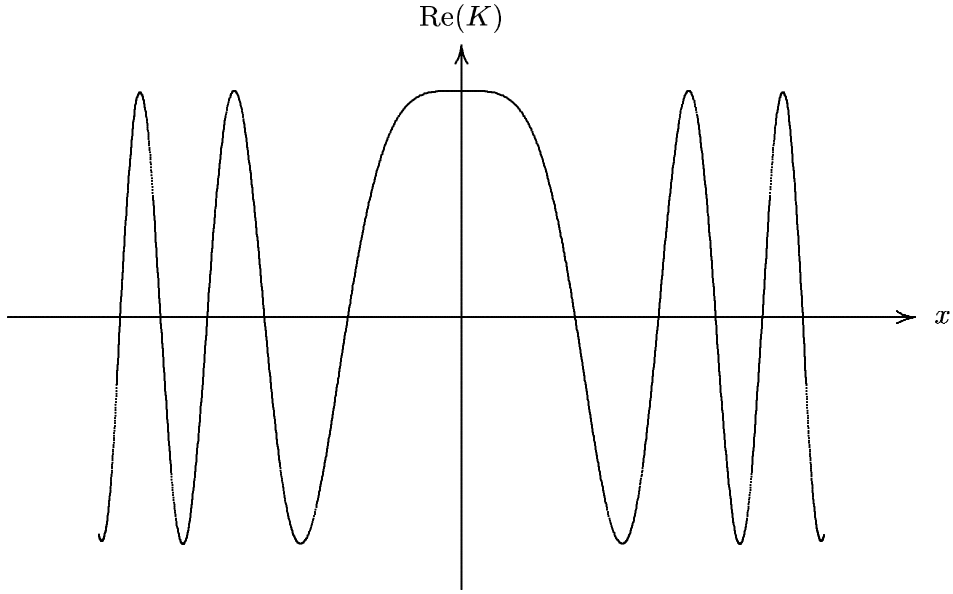


Fig. 1

Since $n\epsilon = t_n - t_0$,

$$K(b,a) = \left(\frac{2\pi i\hbar(t_b - t_a)}{m}\right)^{-\frac{1}{2}} \exp\left\{\frac{im(x_b - x_a)^2}{2\hbar(t_b - t_a)}\right\}. \tag{2.42}$$

This is the free-particle propagator. It can be checked to satisfy the differential Schrödinger equation

$$i\hbar\frac{\partial K(b,a)}{\partial t_b} = -\frac{\hbar^2}{2m}\frac{\partial^2 K(b,a)}{\partial {x_b}^2}, \tag{2.43}$$

whenever t_b is greater than t_a.

For convenience, let the point a represent the origin in both space and time. The amplitude to go to some other point $b = (x,t)$ is

$$K(x,t;0,0) = \left(\frac{2\pi i\hbar t}{m}\right)^{-\frac{1}{2}} \exp\left(\frac{imx^2}{2\hbar t}\right). \tag{2.44}$$

The real part of this amplitude is plotted in Fig. 1. As we get farther from the origin, the oscillations become more and more rapid. If x is so large that many oscillations have occurred, the distance between successive nodes is nearly constant, at least for the following few oscillations. That is, the amplitude behaves much like a sine wave of slowly varying

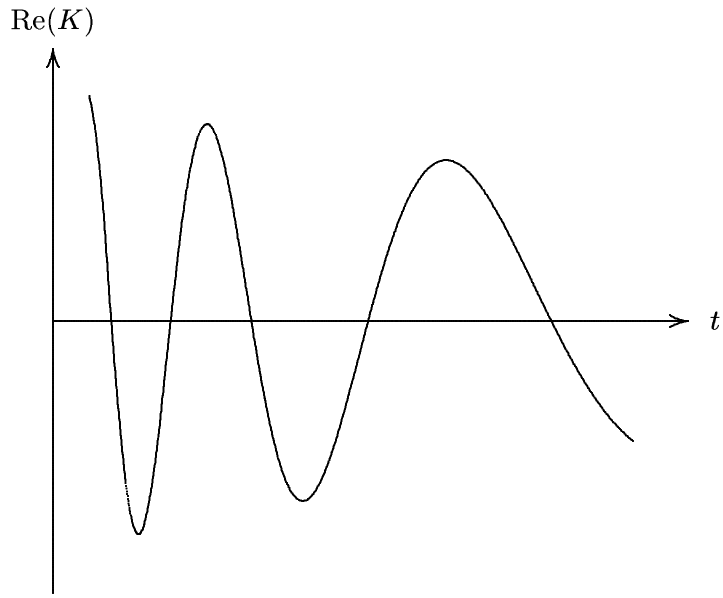


Fig. 2

wavelength. We can evaluate this wavelength λ. Changing x by λ must increase the phase of the amplitude by 2π, i.e.,

$$2\pi = \frac{m(x+\lambda)^2}{2\hbar t} - \frac{mx^2}{2\hbar t} = \frac{mx\lambda}{\hbar t} + \frac{m\lambda^2}{2\hbar t}\,. \tag{2.45}$$

Assuming $x \gg \lambda$, we can neglect the second term on the right-hand side, and so

$$\lambda = \frac{2\pi\hbar}{m(x/t)}\,. \tag{2.46}$$

From a classical point of view, a particle which moves from the origin to x in time interval t has a velocity x/t and momentum $p = m(x/t)$. From the quantum mechanical point of view, when the motion can be adequately described by assigning a classical momentum p to the particle, we have from (2.46) $\lambda = h/p$, which is nothing but the de Broglie wavelength.

Instead of varying distance, we now fix x and vary time. The variation of the real part of the propagator is plotted in Fig. 2. Both frequency and amplitude change with t. Suppose t is very large and ignore the change in amplitude with variations of t. The period of oscillation T is defined as the time required to increase the phase by 2π. Thus

$$2\pi = \frac{mx^2}{2\hbar t} - \frac{mx^2}{2\hbar(t+T)} = \frac{mx^2}{2\hbar t^2}\left(\frac{T}{1+T/t}\right)\,. \tag{2.47}$$

By introducing the angular frequency $\omega = 2\pi/T$ and assuming that $t \gg T$, we have

$$\omega \simeq \frac{m}{2\hbar}\left(\frac{x}{t}\right)^2 . \tag{2.48}$$

Since $\frac{m}{2}\left(\frac{x}{t}\right)^2$ is the classical energy E of a free particle, this equation says that

$$E = \hbar\omega . \tag{2.49}$$

2.5 Harmonic oscillator

The alert reader would have noticed that the free-particle propagator is of the form

$$K(b,a) \sim \exp\left(\frac{i}{\hbar} S_{\text{cl}}[b,a]\right) , \tag{2.50}$$

where S_{cl} is the classical action. In fact, this property holds exactly for any Lagrangian quadratic in x and $\dot{x}$. Let us demonstrate this for the case of a harmonic oscillator with the Lagrangian

$$L = \tfrac{m}{2}(\dot{x}^2 - \omega^2 x^2) , \tag{2.51}$$

for constants m and ω. The classical action is readily checked to be

$$S_{\text{cl}} = \frac{m\omega}{2\sin\omega(t_b - t_a)}\left[({x_a}^2 + {x_b}^2)\cos\omega(t_b - t_a) - 2x_a x_b\right] .$$

As before, we shall denote the classical path between the specified end-points a and b by $\bar{x}(t)$. We can then write some other alternative path as $x(t)$, with

$$x(t) = \bar{x}(t) + \eta(t) . \tag{2.52}$$

Hence

$$\begin{aligned} S[x(t)] &= S[\bar{x}(t) + \eta(t)] \\ &= \int_{t_a}^{t_b} \text{d}t \, \left\{\tfrac{m}{2}[\dot{\bar{x}}^2 + 2\dot{\bar{x}}\dot{\eta} + \dot{\eta}^2] - \tfrac{m}{2}\omega^2[\bar{x}^2 + 2\bar{x}\eta + \eta^2]\right\} \\ &= S[\bar{x}(t)] + \int_{t_a}^{t_b} \text{d}t \, \{m\dot{\bar{x}}\dot{\eta} - m\omega^2\bar{x}\eta\} + \int_{t_a}^{t_b} \text{d}t \, \left\{\tfrac{m}{2}\dot{\eta}^2 - \tfrac{m}{2}\omega^2\eta^2\right\} . \end{aligned} \tag{2.53}$$

The first integral on the right-hand side consists of terms linear in η, which vanish by the Euler–Lagrange equations (some integrations by parts would be involved). Hence

$$S[x(t)] = S_{\rm cl}[b,a] + \int_{t_a}^{t_b} {\rm d}t \left\{ \tfrac{m}{2}\dot\eta^2 - \tfrac{m}{2}\omega^2\eta^2 \right\}. \tag{2.54}$$

Now because the path-integral does not depend on the classical path, i.e., $\mathcal{D}x(t) = \mathcal{D}\eta(t)$, we have

$$K(b,a) = F(t_a,t_b)\exp\left(\frac{i}{\hbar}S_{\rm cl}[b,a]\right), \tag{2.55}$$

where

$$F(t_a,t_b) = \int_0^0 \mathcal{D}\eta(t)\, \exp\left(\frac{i}{\hbar}\int_{t_a}^{t_b} {\rm d}t \left\{ \tfrac{m}{2}\dot\eta^2 - \tfrac{m}{2}\omega^2\eta^2 \right\}\right). \tag{2.56}$$

The path-integral $F(t_a,t_b)$ is over all paths $\eta(t)$ which start from and return to the point $\eta = 0$, and so can only be a function of the times at the end-points. In fact, it is a function of the difference $t_b - t_a$.

Let us evaluate $F(t_a,t_b)$. For simplicity, we set $t_a = 0$ and $t_b = T$. Every path $\eta(t)$ going from 0 at $t = 0$ to 0 at $t = T$ can then be written as a Fourier sine series with a fundamental period of T. Thus,

$$\eta(t) = \sum_n a_n \sin\left(\frac{n\pi t}{T}\right). \tag{2.57}$$

We may consider the paths as functions of the coefficients a_n instead of functions of η at any particular value of t. The Jacobian J is a constant which is independent of $\hbar$, m and ω.

The integral for the action can be written in terms of the Fourier series (2.57). The kinetic energy term becomes

$$\begin{aligned}\int_0^T {\rm d}t\,\dot\eta^2 &= \sum_m\sum_n \frac{m\pi}{T}\frac{n\pi}{T}a_m a_n \int_0^T {\rm d}t\,\cos\left(\frac{m\pi t}{T}\right)\cos\left(\frac{n\pi t}{T}\right)\\ &= T\cdot\tfrac{1}{2}\sum_n\left(\frac{n\pi}{T}\right)^2 {a_n}^2,\end{aligned} \tag{2.58}$$

and the potential energy term becomes

$$\int_0^T {\rm d}t\,\eta^2 = T\cdot\tfrac{1}{2}\sum_n {a_n}^2. \tag{2.59}$$

With the time interval T divided into N discrete steps each of length ϵ, the path integral becomes

$$F(T) = J \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \frac{da_1}{A} \frac{da_2}{A} \cdots \frac{da_N}{A} \exp\left\{ \sum_{n=1}^{N} \frac{im}{2\hbar} \frac{T}{2} \left[\left(\frac{n\pi}{T} \right)^2 - \omega^2 \right] {a_n}^2 \right\}, \tag{2.60}$$

with A is defined in (2.16) and explicitly given in (2.24). Since the exponent can be separated into factors, the integral over each coefficient a_n can be done separately. For example,

$$\int_{-\infty}^{\infty} \frac{da_n}{A} \exp\left\{ \frac{im}{2\hbar} \frac{T}{2} \left[\left(\frac{n\pi}{T} \right)^2 - \omega^2 \right] {a_n}^2 \right\} = \left(\frac{n^2\pi^2}{T^2} - \omega^2 \right)^{-\frac{1}{2}}. \tag{2.61}$$

The path-integral then becomes

$$\begin{aligned} F(T) &= J \prod_{n=1}^{N} \left(\frac{n^2\pi^2}{T^2} \right)^{-\frac{1}{2}} \prod_{n=1}^{N} \left(1 - \frac{\omega^2 T^2}{n^2\pi^2} \right)^{-\frac{1}{2}} \\ &= C \left(\frac{\sin \omega T}{\omega T} \right)^{-\frac{1}{2}}, \end{aligned} \tag{2.62}$$

in the limit $N \to \infty$. Here, C is a constant independent of ω. But for $\omega = 0$, our integral reduces to the case of a free particle, for which we have already derived in (2.44). Hence, for the harmonic oscillator, we have

$$F(T) = \left(\frac{m\omega}{2\pi i\hbar \sin \omega T} \right)^{\frac{1}{2}}.$$

The full propagator is, finally,

$$K(b,a) = \left(\frac{m\omega}{2\pi i\hbar \sin \omega T} \right)^{\frac{1}{2}} \exp\left(\frac{im\omega}{2\hbar \sin \omega T} \left[({x_a}^2 + {x_b}^2) \cos \omega T - 2x_a x_b \right] \right). \tag{2.63}$$

2.6 Stationary states

The special case when the Hamiltonian H is independent of time is of great importance in quantum mechanics. The harmonic oscillator is an example of this. In this section, we shall relate the Schrödinger description of stationary states to the path-integral formalism. In doing so, we shall rederive the well-known energy levels of the harmonic oscillator in this new formalism.

Recall that the wave function of a stationary state can be written in the form

$$\psi(x,t) = \mathrm{e}^{-\frac{i}{\hbar}Et}\phi(x)\,, \tag{2.64}$$

where $\phi(x)$ satisfies the eigenvalue equation

$$H\phi(x) = E\phi(x)\,. \tag{2.65}$$

It is possible to choose an orthonormal basis of solutions $\phi_n(x)$ such that

$$\int_{-\infty}^{\infty} \mathrm{d}x\, \phi_m^*(x)\phi_n(x) = \delta_{mn}\,. \tag{2.66}$$

Any solution to (2.65) can then be expanded as

$$f(x) = \sum_{n=1}^{\infty} a_n\phi_n(x)\,, \tag{2.67}$$

with

$$a_n = \int_{-\infty}^{\infty} \mathrm{d}x\, \phi_n^*(x)f(x)\,. \tag{2.68}$$

We then have the relation

$$\begin{aligned} f(x) &= \sum_{n=1}^{\infty} \phi_n(x) \int_{-\infty}^{\infty} \mathrm{d}y\, \phi_n^*(y)f(y) \\ &= \int_{-\infty}^{\infty} \mathrm{d}y \left(\sum_{n=1}^{\infty} \phi_n(x)\phi_n^*(y)\right) f(y)\,. \end{aligned} \tag{2.69}$$

In the case when $f(x) = \psi(x,t_1)$, for some time t_1, we have

$$\psi(x,t_2) = \sum_{n=1}^{\infty} a_n \mathrm{e}^{-\frac{i}{\hbar}E_n(t_2-t_1)}\phi_n(x)\,, \tag{2.70}$$

and hence, using (2.68),

$$\psi(x,t_2) = \int_{-\infty}^{\infty} \mathrm{d}y \left(\sum_{n=1}^{\infty} \phi_n(x)\phi_n^*(y)\mathrm{e}^{-\frac{i}{\hbar}E_n(t_2-t_1)}\right) \psi(y,t_1)\,. \tag{2.71}$$

Recalling the property (2.18) of wave functions, it is now possible to express the propagator in terms of $\phi_n(x)$:

$$K(x_2,t_2;x_1,t_1) = \sum_{n=1}^{\infty} \mathrm{e}^{-\frac{i}{\hbar}E_n(t_2-t_1)}\phi_n(x_2)\phi_n^*(x_1)\,, \tag{2.72}$$

when $t_2 > t_1$, and zero otherwise.

The equation (2.72) can now be used to deduce the energy levels and energy eigenfunctions of the harmonic oscillator, for it implies that

$$\left(\frac{m\omega}{2\pi i\hbar \sin\omega T}\right)^{\frac{1}{2}} \exp\left(\frac{im\omega}{2\hbar\sin\omega T}\left[({x_1}^2+{x_2}^2)\cos\omega T - 2x_1x_2\right]\right) = \sum_{n=1}^{\infty} \mathrm{e}^{-\frac{i}{\hbar}E_nT}\phi_n(x_2)\phi_n^*(x_1)\,. \tag{2.73}$$

Using the relations

$$\begin{aligned} i\sin\omega T &= \tfrac{1}{2}\mathrm{e}^{i\omega T}(1-\mathrm{e}^{-2i\omega T})\,, \\ \cos\omega T &= \tfrac{1}{2}\mathrm{e}^{i\omega T}(1+\mathrm{e}^{-2i\omega T})\,, \end{aligned} \tag{2.74}$$

we can write the left-hand side of (2.73) as

$$\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}} \mathrm{e}^{-i\omega T/2}(1-\mathrm{e}^{-2i\omega T})^{-\frac{1}{2}} \times \exp\left\{-\frac{m\omega}{2\hbar}\left[({x_1}^2+{x_2}^2)\left(\frac{1+\mathrm{e}^{-2i\omega T}}{1-\mathrm{e}^{-2i\omega T}}\right) - \frac{4x_1x_2\mathrm{e}^{-i\omega T}}{1-e^{-2i\omega T}}\right]\right\}. \tag{2.75}$$

If we expand this in powers of $\mathrm{e}^{-i\omega T}$, we obtain a series having the form of the right-hand side of (2.73). Because of the initial factor of $\mathrm{e}^{-i\omega T/2}$, the energy levels would be shifted correspondingly:

$$E_n = \hbar\omega(n+\tfrac{1}{2})\,. \tag{2.76}$$

The is the well-known result for the harmonic oscillator.

To obtain the corresponding energy eigenfunctions, we have to carry out the expansion explicitly. Expanding the left-hand side of (2.73) to second order, we have

$$\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}} \mathrm{e}^{-i\omega T/2}(1+\tfrac{1}{2}\mathrm{e}^{-2i\omega T}+\cdots)\exp\left[-\frac{m\omega}{2\hbar}({x_1}^2+{x_2}^2) - \frac{m\omega}{\hbar}({x_1}^2+{x_2}^2)(\mathrm{e}^{-2i\omega T}+\cdots) + \frac{2m\omega}{\hbar}x_1x_2\mathrm{e}^{-i\omega T}+\cdots\right], \tag{2.77}$$

or

$$\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}} \mathrm{e}^{-(m\omega/2\hbar)({x_1}^2+{x_2}^2)}\mathrm{e}^{-i\omega T/2}(1+\tfrac{1}{2}\mathrm{e}^{-2i\omega T})\left[1+\frac{2m\omega}{\hbar}x_1x_2\mathrm{e}^{-i\omega T} + \frac{4m^2\omega^2}{2\hbar^2}{x_1}^2{x_2}^2\mathrm{e}^{-2i\omega T} - \frac{m\omega}{\hbar}({x_1}^2+{x_2}^2)\mathrm{e}^{-2i\omega T}+\cdots\right]. \tag{2.78}$$

From this, we see that the lowest-order term is

$$\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}} \mathrm{e}^{-(m\omega/2\hbar)(x_1{}^2+x_2{}^2)}\mathrm{e}^{-i\omega T/2} = \mathrm{e}^{-\frac{i}{\hbar}E_0 T}\phi_0(x_2)\phi_0^*(x_1)\,. \tag{2.79}$$

This means that $E_0 = \frac{1}{2}\hbar\omega$, and

$$\phi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \mathrm{e}^{-m\omega x^2/2\hbar}, \tag{2.80}$$

where we have chosen $\phi_0(x)$ to be real. The next-order term is

$$\mathrm{e}^{-i\omega T/2}\mathrm{e}^{-i\omega T}\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}} \mathrm{e}^{-(m\omega/2\hbar)(x_1{}^2+x_2{}^2)}\frac{2m\omega}{\hbar}x_1x_2 = \mathrm{e}^{-\frac{i}{\hbar}E_1 T}\phi_1(x_2)\phi_1^*(x_1)\,, \tag{2.81}$$

which implies that $E_1 = \frac{3}{2}\hbar\omega$, and

$$\phi_1(x) = \left(\frac{2m\omega}{\hbar}\right)^{\frac{1}{2}} x\phi_0(x)\,. \tag{2.82}$$

Higher-order terms can be analysed in the same way. These results are in agreement with those obtained from the Schrödinger description of the harmonic oscillator.

2.7 Perturbation theory

Recall that the propagator for a particle moving from point a to b in a potential $V(x,t)$, is given by

$$K(b,a) = \int_a^b \mathcal{D}x(t)\,\exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b}\mathrm{d}t\,\left[\tfrac{1}{2}m\dot{x}^2 - V(x,t)\right]\right\}. \tag{2.83}$$

We have already seen that in some cases, K can be determined exactly, as for the harmonic oscillator. This can in general be done for potentials which are quadratic in x. However, many of the interesting potentials which arise in quantum mechanics problems are not of this type and thus cannot be handled so easily. In this section, we study a technique known as perturbation theory, which is useful when the effect of the potential is small.

Suppose the potential is small, or more precisely, suppose the time integral of $V(x,t)$ is small compared with $\hbar$. Then the exponential of the potential term in (2.83) can be written as

$$\exp\left[-\frac{i}{\hbar}\int_{t_a}^{t_b}\mathrm{d}t\,V(x,t)\right] = 1 - \frac{i}{\hbar}\int_{t_a}^{t_b}\mathrm{d}t\,V(x,t) + \frac{1}{2!}\left(\frac{i}{\hbar}\right)^2\left[\int_{t_a}^{t_b}\mathrm{d}t\,V(x,t)\right]^2 + \cdots\,. \tag{2.84}$$

This is the perturbative expansion. Substituting into (2.83), we get the expansion

$$K(b,a) = K_0(b,a) + K_1(b,a) + K_2(b,a) + \cdots \,, \tag{2.85}$$

where K_0 is the free-particle propagator (2.42), and

$$\begin{aligned} K_1(b,a) &= -\frac{i}{\hbar}\int_a^b \mathcal{D}x(t)\,\exp\left(\frac{i}{\hbar}\int_{t_a}^{t_b}\mathrm{d}t\,\tfrac{1}{2}m\dot{x}^2\right)\int_{t_a}^{t_b}\mathrm{d}t_c\,V[x(t_c),t_c]\,, \\ K_2(b,a) &= -\frac{1}{2\hbar^2}\int_a^b \mathcal{D}x(t)\,\exp\left(\frac{i}{\hbar}\int_{t_a}^{t_b}\mathrm{d}t\,\tfrac{1}{2}m\dot{x}^2\right)\int_{t_a}^{t_b}\mathrm{d}t_c\,V[x(t_c),t_c] \\ &\qquad\qquad \times\int_{t_a}^{t_b}\mathrm{d}t_d\,V[x(t_d),t_d]\,, \end{aligned} \tag{2.86}$$

and so on.

Let us first consider the propagator K_1. After interchanging the order of integration over the time variable t_c and the path $x(t)$, we have

$$K_1(b,a) = -\frac{i}{\hbar}\int_{t_a}^{t_b}\mathrm{d}t_c\,F(t_c)\,, \tag{2.87}$$

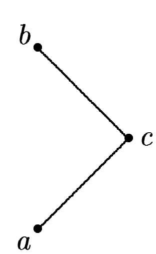
with

$$F(t_c) = \int_a^b \mathcal{D}x(t)\,\exp\left(\frac{i}{\hbar}\int_{t_a}^{t_b}\mathrm{d}t\,\tfrac{1}{2}m\dot{x}^2\right)V[x_c,t_c]\,. \tag{2.88}$$

We have set $x_c = x(t_c)$ here. The path integral $F(t_c)$ can be written, like in (2.13), as a path integral over all paths from a to c, and from c to b, integrated over x_c:

$$\begin{aligned} F(t_c) &= \int_{-\infty}^{\infty}\mathrm{d}x_c\int_c^b\mathcal{D}x(t)\int_a^c\mathcal{D}x(t) \\ &\qquad \exp\left(\frac{i}{\hbar}\int_{t_c}^{t_b}\mathrm{d}t\,\tfrac{1}{2}m\dot{x}^2\right)V[x_c,t_c]\exp\left(\frac{i}{\hbar}\int_{t_a}^{t_c}\mathrm{d}t\,\tfrac{1}{2}m\dot{x}^2\right) \\ &= \int_{-\infty}^{\infty}\mathrm{d}x_c\,K_0(b,c)V(c)K_0(c,a)\,. \end{aligned} \tag{2.89}$$

The meaning of this should be clear. A particle starts from a and moves as a free particle to c. At this point, it is acted upon or scattered by the potential $V(c)$. Thereafter, it moves again as a free particle to b:



The amplitude for such a scattering at time t_c is given by $F(t_c)$. If this amplitude is integrated over all possible times $t_a < t_c < t_b$, we recover the first term in the perturbative expansion (2.85).

Similarly, it can be shown that

$$K_2(b,a) = \left(-\frac{i}{\hbar}\right)^2 \int \mathrm{d}\tau_c \int \mathrm{d}\tau_d \, K_0(b,d)V(d)K_0(d,c)V(c)K_0(c,a)\,, \tag{2.90}$$

where $\int \mathrm{d}\tau = \int \mathrm{d}t \int \mathrm{d}x$. Reading from right to left, this formula means: The particle moves as a free particle from a to c. At c, the particles gets scattered by the potential $V(c)$ at that point. It then moves as a free particle from c to d, where it is scattered by the potential $V(d)$. After that, it moves from d to b, again as a free particle. We sum over all the alternatives, i.e., all the places and times that the scattering may take place.

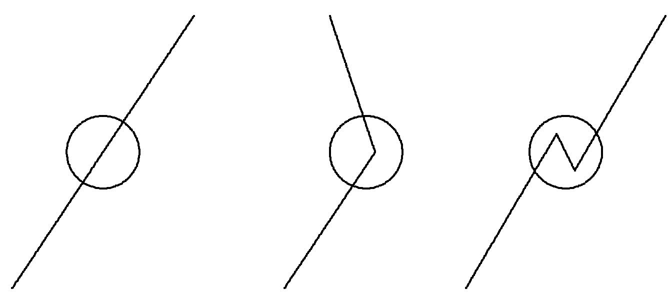
With this interpretation, we can describe K in the following way. It is a sum over different ways in which the particle may move from point a to b. The alternatives are:

1 The particle may not be scattered at all $[K_0(b,a)]$;

2 The particle may be scattered once $[K_1(b,a)]$;

3 The particle may be scattered twice $[K_2(b,a)]$;

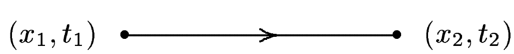
and so on:



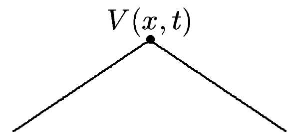
$$K(b,a) \quad = \quad K_0(b,a) \quad + \quad K_1(b,a) \quad + \quad K_2(b,a) \quad + \quad \cdots$$

Each one of these alternatives is itself a sum over alternatives by integrating over t and x.

Conversely, given a particular scattering process, one can derive its amplitude. This is done using the so-called Feynman rules. In this case, we associate to each line



the free propagator $K_0(x_2,t_2;x_1,t_1)$, and to each vertex,



the factor $-\frac{i}{\hbar}V(x,t)$, followed by integration over x and t. In the non-relativistic quantum mechanics that we are presently considering, these rules are hardly necessary to do calculations. But in quantum field theory to be considered below, they are a great aid to calculations.

2.8 Momentum representation

The above Feynman rules were derived in the coordinate representation. It is sometimes more convenient to work in the momentum representation, where the Feynman rules often simplify. So we now briefly examine this case. The momentum propagator is related to the one in coordinate space by the formula

$$k(p_2,E_2;p_1,E_1) = \int\!\!\int\!\!\int\!\!\int \mathrm{d}x_1\mathrm{d}t_1\mathrm{d}x_2\mathrm{d}t_2\,\mathrm{e}^{-\frac{i}{\hbar}p_2x_2}\mathrm{e}^{\frac{i}{\hbar}E_2t_2}K(x_2,t_2;x_1,t_1)\mathrm{e}^{\frac{i}{\hbar}p_1x_1}\mathrm{e}^{-\frac{i}{\hbar}E_1t_1}. \tag{2.91}$$

Let us work out the corresponding propagator for a free particle. Using (2.42), we first perform the spatial integrals:

$$\int\!\!\int \mathrm{d}x_1\mathrm{d}x_2\,\mathrm{e}^{-\frac{i}{\hbar}(p_2x_2-p_1x_1)}K_0(x_2,t_2;x_1,t_1) = \begin{cases} (2\pi\hbar)\delta(p_1-p_2)\exp\left[-\frac{i{p_1}^2}{2\hbar m}(t_2-t_1)\right], & t_2>t_1; \\ 0\,, & t_2<t_1. \end{cases} \tag{2.92}$$

So we are left with the integrals over t_1 and t_2. Make the substitution $t_2 = t_1+\tau$, so that the integral becomes

$$\int_{-\infty}^{\infty}\mathrm{d}t_1\,\mathrm{e}^{\frac{i}{\hbar}(E_2-E_1)t_1}\int_0^{\infty}\mathrm{d}\tau\,\mathrm{e}^{\frac{i}{\hbar}(E_2-\frac{p^2}{2m})\tau}. \tag{2.93}$$

The first of these two integrals is $2\pi\hbar\delta(E_2-E_1)$. The second integral is of the form

$$\int_0^{\infty}\mathrm{d}\tau\,\mathrm{e}^{i\omega\tau}. \tag{2.94}$$

If ω is real, it does not converge. So we replace ω by a complex number $\omega + i\epsilon$, for an infinitesimal real number ϵ. This integral then has value $\frac{i}{\omega+i\epsilon}$. Although the limit $\epsilon \to 0$ is implied, we do not take the limit yet, as this would mean that the path integral would have a pole at $\omega = 0$.

Returning to the evaluation of the propagator, we replace ω with $E_2 - \frac{p^2}{2m}$ to find

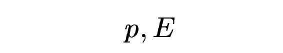
$$k_0(p_2, E_2; p_1, E_1) = (2\pi\hbar)^2 \delta(p_2 - p_1)\delta(E_2 - E_1)\frac{i\hbar}{E_1 - \frac{{p_1}^2}{2m} + i\epsilon}. \tag{2.95}$$

The existence of delta functions in this expression means that neither the energy nor the momentum changes during the motion of a free particle. But these two quantities affect the motion of the particle, as shown by the last term of this equation. So the amplitude for a free particle to move from one point to another, with energy E and momentum p, is proportional to $\frac{i\hbar}{E_1 - \frac{{p_1}^2}{2m} + i\epsilon}$.

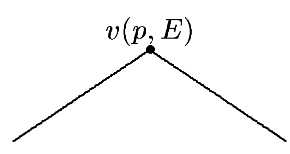
Similarly, we may introduce the Fourier transform of the potential $V(x,t)$ by

$$V(x,t) = \int \mathrm{d}p\mathrm{d}E\, \mathrm{e}^{\frac{i}{\hbar}(px - Et)} v(p,E)\,. \tag{2.96}$$

We are now in the position to write down the Feynman rules in momentum space, from which scattering amplitudes in terms of p and E may be derived. To each propagator



we include a factor of $\frac{1}{(2\pi\hbar)^2}\frac{i\hbar}{E - \frac{p^2}{2m} + i\epsilon}$; and to each vertex



we associate the factor $-\frac{i}{\hbar}(2\pi\hbar)^2 v(p,E)$, with the appropriate delta functions for energy and momentum conservation.

2.9 References and further reading

This chapter is almost exclusively based on Feynman and Hibbs, *Quantum Mechanics and Path Integrals*, which is the most authoratative text on the subject. (But beware of a large number of misprints in it!) Other books are Swanson, *Path Integrals and Quantum Processes* and Khandekar et. al., *Path-Integral Methods and Their Applications.* Shorter treatments include Ryder, *Quantum Field Theory*, and Brown, *Quantum Field Theory*. For applications of path integrals to other areas of physics, see Schulman, *Techniques and Applications of Path Integration* or Wiegel, *Introduction to Path-Integral Methods in Physics and Polymer Science*.