Further reading

The reader interested in the mathematical aspects of the theory can read the book [von Neumann (1932)]. A proof of Stone's theorem and von Neumann's theorems can be found in Vol. 1 of the book [Reed and Simon (1980a)], Chapter 8. A pedagogical introduction to self-adjoint extensions is in [Bonneau, Faraut, and Valent (2001)].

Guide to the Supplements

One of the main postulates of quantum mechanics is that each physical state corresponds to a ray in the Hilbert space (P1) (see Section 7.1). Does the inverse statement, "each vector in the Hilbert space describes a physical state", hold true as well? The question puts the superposition principle under scrutiny: given two physical states $|\alpha\rangle$, $|\beta\rangle$, is the state $|\alpha\rangle + |\beta\rangle$ also a physical state, for *whatever* choice of $|\alpha\rangle$ and $|\beta\rangle$? Supplement 20.14 is dedicated to the discussion of this subtle issue. The conclusion will be that the superposition principle actually admits exceptions. A well-known example is related to the exactly conserved electric charge. Only superpositions among the states with the same electric charge are allowed. An analogous restriction holds for the fermion number. Superposition of states with different fermion numbers is unphysical. These restrictions are known as *superselection rules*.

In a second Supplement some details of the von Neumann theorem are given. The theorem basically ensures the uniqueness of the Schrödinger representation for the Heisenberg commutation relations. Related questions on the relevance of canonical transformations in quantum mechanics and the problem of self-adjoint extensions of the operators are briefly addressed.

Problems

(7.1) Solve the Heisenberg equations of motion for a free particle and for a particle in an external uniform field.

(7.2) Solve the Heisenberg equations of motion for a harmonic oscillator in a uniform constant external field. Generalize the solution for a uniform time dependent force $F(t)$.

(7.3) Suppose that the system described by the wave function $\psi_S(x)$ at the instant $t = 0$ is an eigenstate of the operator f, with eigenvalue, f_0. Show that the wave function at time t is an eigenstate of the Heisenberg operator $\hat{f}_H(-t)$, with the same eigenvalue. (This technique is used in the book [Kogan and Galitsky (1963)] to compute the Green functions of several simple models).

Path integrals

8

An elegant alternative formalism of quantum mechanics was given by R. P. Feynman in 1948. The importance of this formalism, known as the path integral, functional integral, etc. approach, first of all lies in its vivid, intuitive description of quantum fluctuations. At the same time, it provides us with a formidable tool of calculus, of both perturbative effects (Feynman diagrams) and non-perturbative effects (e.g., tunnel effects, instantons).

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8.1 Green functions

An important concept in quantum mechanics is that of the (probability) amplitude for two successive events; in particular, the (probability) amplitude for finding a particle at the point x at time t, *knowing* that the particle was at $x = x_0$ at some earlier instant $t = t_0$. This amplitude is called the *Green function*, and as will be seen below, it is precisely this quantity the path integral is concerned with. Let us therefore review a few elementary aspects of Green functions, before discussing the path integral itself. In the cases in which the Hamiltonian is independent of time, the Green function is given by

$$G(x, x_0; t, t_0) = \langle x | e^{-iH(t-t_0)/\hbar} | x_0 \rangle \ . \tag{8.1}$$

In other words the Green function is the time evolution operator, written in the x representation.

From the very definition it follows immediately that the Green function possesses a fundamental property, i.e. the property of convolution,

$$G(x, x_0; t, t_0) = \int dx_1 \, G(x, x_1; t, t_1) \, G(x_1, x_0; t_1, t_0) \ , \tag{8.2}$$

where x_1 is the position occupied by the particle at *any fixed* intermediate time t_1 (Figure 8.1). As G represents the amplitude for the two successive events, the *probability* of $(x_0; t_0) \to (x; t)$ is the square of $G(x, x_0; t, t_0)$, and from eqn (8.2) we see that it contains various interference terms coming from the contributions of differrent "paths", $x_0 \to x_1 \to x$, with all possible intermediate positions, x_1.

The concept of the Green function is closely related to that of the wave function. G can be interpreted as the wave function with the special initial condition that the particle was a position eigenstate at

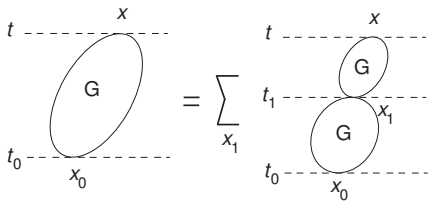

Fig. 8.1

the initial time: $\psi(x,t_0)=\delta(x-x_0)$. Indeed,

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}G(x,x_0;t,t_0) &= i\hbar\frac{\partial}{\partial t}\langle x|e^{-iH(t-t_0)/\hbar}|x_0\rangle = \langle x|He^{-iH(t-t_0)/\hbar}\,|x_0\rangle \\ &= H_{\rm Sch}\langle x|e^{-iH(t-t_0)/\hbar}|x_0\rangle = H_{\rm Sch}\,G(x,x_0;t,t_0)\ . \end{aligned}$$

The probability of finding the particle in the interval $(x,x+dx)$ at time t is then given by $|G(x,x_0;t,t_0)|^2dx$.

For simplicity we briefly review the properties of the Green function in one-dimensional systems. By definition the Green function G gives the solution of the general problem of time evolution in a given system, in the sense that the solution of Schrödinger's equation for *any* initial condition

$$\psi(x,t)|_{t=t_0}=\psi_0(x,t_0),$$

is given by

$$\psi(x,t)=\int dx'\,G(x,x';t,t_0)\,\psi_0(x',t_0)\ , \tag{8.3}$$

in terms of the Green function.[1]

[1] **Exercise.** Show that $\psi(x,t)$ in eqn (8.3) indeed satisfies both Schrödinger's equation and the initial condition.

The Green function (8.1) can be written, by inserting the completeness relation in terms of the energy eigenstates,

$$\mathbb{1}=\sum_n|\psi_n\rangle\langle\psi_n|$$

as

$$G(x,x_0;t,t_0)=\sum_n e^{-iE_n(t-t_0)/\hbar}\,\psi_n(x)\,\psi_n^*(x_0)\ . \tag{8.4}$$

[2] **Exercise.** Show that the integral in the last factor in eqn (8.5) can be brought to the form of the ordinary gaussian integration over the real axis, by using Cauchy's theorem.

[3] **Exercise.** Evaluate the wave function at $t>t_0$ of a particle, which at time t_0 is described by a wave packet,

$$\psi_0(x,t_0)=\frac{1}{\sqrt{2\pi a^2}}e^{-x^2/4a^2}\ .$$

[2][3]

In some simple cases the Green function can be evaluated explicitly. For a free particle, by subsituting

$$E_n\to\frac{p^2}{2m};\quad \psi_n(x)\to\frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar};\quad \sum_n\to\int_{-\infty}^{\infty}dp$$

into (8.4), one finds that

$$\begin{aligned} G(x,x_0;t,t_0) &= \int_{-\infty}^{\infty}\frac{dp}{2\pi\hbar}e^{-ip^2(t-t_0)/2m\hbar}e^{ip(x-x_0)/\hbar} \\ &= e^{im(x-x_0)^2/2\hbar(t-t_0)}\int_{-\infty}^{\infty}\frac{dp}{2\pi\hbar}\exp-\left[\frac{i(t-t_0)}{2m\hbar}\left(p-\frac{m(x-x_0)}{t-t_0}\right)^2\right] \\ &= \frac{1}{2\pi\hbar}\sqrt{\frac{2m\hbar}{i(t-t_0)}}\,e^{im(x-x_0)^2/2\hbar(t-t_0)}\,\left(\int_C d\xi\,e^{-\xi^2}\right)\ , \end{aligned} \tag{8.5}$$

where the contour of integration C in ξ is along the straight line $(1+i)\alpha$; $\alpha=-\infty\to\infty$. The integral is equal to $\sqrt{\pi}$, so the result is

$$G(x,x_0;t,t_0)=\sqrt{\frac{m}{2i\hbar\pi(t-t_0)}}\,e^{i\,m\,(x-x_0)^2/2\hbar(t-t_0)}\ . \tag{8.6}$$

The harmonic oscillator

The harmonic oscillator

$$H = \frac{P^2}{2m} + \frac{1}{2}\, m\,\omega^2\, Q^2$$

is another system in which the Green function is known explicitly. It can be explicitly evaluated by the path integral method; here we derive the same result by making use of a theorem proposed as a problem in Chapter 7. The Green function $G(q, q_0; t, 0) = \langle q|e^{-i\,H\,t/\hbar}|q_0\rangle$ is equal to the wave function $\psi(q,t)$ with a particular boundary condition

$$\psi(q,0) = \delta(q - q_0), \qquad \therefore \quad Q\,\psi(q,0) = q_0\,\psi(q,0)\ . \tag{8.7}$$

According to the theorem mentioned, $\psi(q,t)$ satisfies the equation

$$Q(-t)\,\psi(q,t) = \left(Q\,\cos\omega t - \frac{P}{m\,\omega}\,\sin\omega t\right)\,\psi(q,t) = q_0\,\psi(q,t)\ ,$$

where $Q(t)$ is the Heisenberg position operator at time t; $Q = Q(0)$, $P = P(0)$ are the ordinary Schrödinger operators, and the known solution of Heisenberg's equations for $Q(t)$ has been used. Thus

$$\frac{i\,\hbar}{m\,\omega}\sin\omega t\,\frac{\partial}{\partial q}\psi(q,t) = (-q\,\cos\omega t + q_0)\,\psi(q,t)\ :$$

and its solution is

$$\psi(q,t) = \exp\left[\,\frac{i\,m\,\omega\,(q\,\cos\omega t - q_0)^2}{\hbar\,\sin 2\omega t} + c(t)\,\right],$$

where $c(t)$ is an integration constant, independent of q. To determine it, we impose the condition

$$\left(i\hbar\frac{\partial}{\partial t} - H\right)\,\psi(q,t) = 0,$$

which yields a differential equation for $\dot{c}$:

$$\dot{c}(t) = -\frac{\omega}{2}\,\cot\omega t - \frac{i\,m\,\omega^2}{2\,\hbar}\frac{q_0^2}{\cos^2\omega t};$$

integrating it, one finds that

$$c(t) = -\frac{1}{2}\log(\sin\omega t) - \frac{i\,m\,\omega}{2\,\hbar}\,q_0^2\,\tan\omega t + \text{const.}\,,$$

where the constant depends neither on t nor on q. Collecting the factors and fixing the constant with boundary condition (8.7), we find that

$$G^{HO}(q, q_0; t, t_0) \tag{8.8}$$
$$= \sqrt{\frac{m\,\omega}{2\pi i\hbar\,\sin\omega(t-t_0)}}\,\exp\left[\,\frac{im\omega}{\hbar}\,\frac{(q^2+q_0^2)\,\cos\omega(t-t_0) - 2\,q_0\,q}{2\,\sin\omega(t-t_0)}\right]\ .$$

8.2 Path integrals

In the path integral formulation the Green function

$$\langle q_1 | e^{-iH(T_1-T_0)/\hbar} | q_0 \rangle$$

is given by the expression

$$\int_{q(T_0)=q_0}^{q(T_1)=q_1} [\mathcal{D}q]\, e^{\frac{i}{\hbar}S}, \qquad S = \int_{T_0}^{T_1} dt\, L(q,\dot{q}), \tag{8.9}$$

where $L(q,\dot{q})$ is the Lagrangian (S is the classical action).[4] The symbol $\int [\mathcal{D}q] \ldots$ will be defined in the following: its meaning is however quite clear: the Green function is given by the sum over all possible paths connecting the initial point $q(T_0) = q_0$ to the final point $q(T_1) = q_1$, each weighed with the factor $e^{iS/\hbar}$, where S is the classical action corresponding to each path (see Figure 8.9). Without entering into the details, one notes several salient features:

- The "virtual paths" introduced in the Lagrangian formalism of classical mechanics with the minimal action principle appear here as real paths: in quantum mechanics all trajectories—whether or not they satisfy the classical equation of motion—contribute, each with weight $e^{iS/\hbar}$. The fact that the electron "sees" both of the double slits (see Chapter 1) simultaneously, a rather counterintuitive fact, is here expressed in a very natural way.
- The sum over different paths is in the amplitude; contributions from different paths interfere nontrivially in the probability for a given event. This is of course a well-known, characteristic aspect of quantum mechanics.
- In the limit $\hbar \to 0$, only the stationary path for which $\delta S = 0$ contributes: the contributions of non-stationary paths cancel out due to the rapid phase oscillations. We thus recover the minimal principle of classical mechanics in the limit $\hbar \to 0$, as required.

[4] "This formula contains in one all of the three melodies of theoretical physics of the 20th century: quantization, qymmetry and phase factor", C. N. Yang, Int. Conf. of Theoretical Physics, TH2002, Paris (2002).

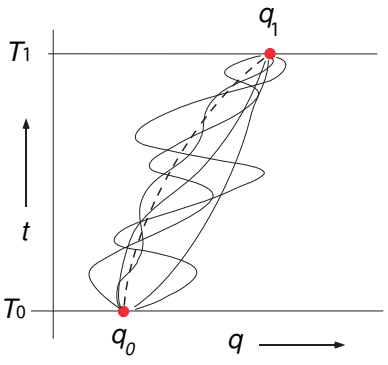

Fig. 8.2

8.2.1 Derivation

To derive eqn (8.9), we start by dividing the time interval $[T_1, T_0]$ into many tiny segments:

$$t_N = T_1 > t_{N-1} > t_{N-2} > \ldots t_2 > t_1 > t_0 = T_0,$$

$$t_i - t_{i-1} = \epsilon, \quad N\,\epsilon = T_1 - T_0\ .$$

The evolution operator can be factorized as

$$e^{-iH\,(T_1-T_0)/\hbar} = e^{-iH\,\epsilon/\hbar}\, e^{-iH\,\epsilon/\hbar} \ldots e^{-iH\,\epsilon/\hbar}\ .$$

Inserting the completeness relation

$$\sum_{q_i} |q_i\rangle\langle q_i| = \mathbf{1}$$

into each time slice, one gets

$$G(q,q_0;T_1,T_0)=\int\prod_i dq_i\,\prod_i G_{i+1,i}(q_{i+1},q_i;t_{i+1},t_i),$$

where

$$G_{i+1,i}=\langle q_{i+1}|e^{-iH\,\epsilon/\hbar}|q_i\rangle\simeq\langle q_{i+1}|\mathbf{1}-i\,H\,\epsilon/\hbar+\ldots|q_i\rangle\ .$$

For a Hamiltonian of the form, $H=\frac{p^2}{2\,m}+V(q)$, it follows that

$$\langle q_{i+1}|H|q_i\rangle=\langle q_{i+1}|\frac{p^2}{2\,m}+V(q)|q_i\rangle=\int dp\,\langle q_{i+1}|p\rangle\,\langle p|\frac{p^2}{2\,m}+V(q)|q_i\rangle$$
$$=\int\frac{dp}{2\pi\hbar}\,e^{ip(q_{i+1}-q_i)/\hbar}\left(\frac{p^2}{2\,m}+V(q_i)\right)=\int\frac{dp}{2\pi\hbar}\,e^{ip\Delta q/\hbar}\left(\frac{p^2}{2\,m}+V(q_i)\right)\ .$$

Thus

$$G_{i+1,i}\simeq\int\frac{dp}{2\pi\hbar}\,e^{ip\Delta q/\hbar}\left(1-i\frac{H(p,q_i)\epsilon}{\hbar}+\ldots\right)=\int\frac{dp}{2\pi\hbar}\,e^{ip\Delta q/\hbar-i\epsilon H/\hbar}\ .$$

Collecting the factors one finds that[5]

$$G(q,q_0;T_1,T_0)=\lim_{N\to\infty}\int\prod\frac{dq_i\,dp_i}{2\pi\hbar}e^{i\sum_i\left[\frac{p_i(q_{i+1}-q_i)}{\hbar}-H(p_i,q_i)\right]}\ .$$

[5] Feynman's inspiration came from some observations made by Dirac. In fact all the basic ideas about the path integral can be already found in a somewhat mysterious §32 of Dirac's book [Dirac (1958)].

Finally, performing the integration over p_i,

$$\begin{aligned}G_{i+1,i}&=\int\frac{dp}{2\pi\hbar}\,e^{ip\Delta q/\hbar-i\epsilon p^2/2m\hbar-i\epsilon V(q_i)/\hbar}\\&=\text{const.}\,e^{i\epsilon m(\Delta q/\epsilon)^2/2-i\epsilon V(q_i)/\hbar}=e^{i\,\epsilon\,L(q_i,\dot q_i)/\hbar},\end{aligned}$$

where we have written

$$L(q_i,\dot q_i)=\frac{m}{2}\left(\frac{\Delta q}{\epsilon}\right)^2-V(q_i)\simeq\frac{m\,(\dot q)^2}{2}-V(q_i)\ .$$

Thus

$$G(q,q_0;T_1,T_0)=\lim_{N\to\infty;\,\epsilon\to0}\int\prod dq_i\,e^{i\sum_i\,\epsilon\,L(q_i,\dot q_i)/\hbar}\equiv\int[\mathcal{D}q]\,e^{iS/\hbar}\ .$$

Remarks. The reader with a tendency for mathematical rigor might be appalled to see the omnipresent symbol $\simeq$ and the limit with infinite-dimensional integrals taken with nonchalance. Actually, the derivation can be made rigorous. First of all, we consider the Euclidean time, i.e., a continuation $t=-it_E$, which makes all the integrals of Gaussian type,

$$i\,S\to-S_E,\qquad S_E=\int dt_E\,\left[\left(\frac{dq(t_E)}{dt_E}\right)^2+V(q(t_E))\right]\ .$$

As for the infinite product, the convergence of the limit (Trotter's formula)

$$\lim_{N\to\infty}\left(e^{-(T+V)/N}\right)^N=\lim_{N\to\infty}\left(e^{-T/N}\,e^{-V/N}\right)^N$$

can be proved for any *self-adjoint* operators (see Section 7.3.1) T,V.

The convolution property of the path integral

$$\int_{q(T_0)=q_0}^{q(T_1)=q_1} [\mathcal{D}q]\, e^{\frac{i}{\hbar}S} = \int dq \left[\int_{q(t)=q}^{q(T_1)=q_1} [\mathcal{D}q]\, e^{\frac{i}{\hbar}S}\right] \left[\int_{q(T_0)=q_0}^{q(t)=q} [\mathcal{D}q]\, e^{\frac{i}{\hbar}S}\right]$$

(valid for any fixed t, $T_1 > t > T_0$) follows immediately from the very definition of the path integral. In agreement with the general principles of quantum mechanics, the amplitude for the particle at q_0 initially ($t = T_0$) to travel to q_1 at time $t = T_1$, is a coherent sum of the amplitudes for the particle traveling first from q_0 to q, then from q to q_1, summed over the intermediate position q.

The amplitude studied above can also be written as a matrix element between two Heisenberg states,

$$G(q_1, q_0; T_1, T_0) = {}_H\langle q_1, T_1 | q_0, T_0\rangle_H,$$

where $|q_1, t\rangle_H = e^{iHt/\hbar}|q_1\rangle$ is an eigenstate of the Heisenberg operator[6]

$$Q_H(t) = e^{iHt}\, Q\, e^{-iHt}, \qquad Q_H(t)\,|q_1, t\rangle_H = q_1\,|q_1, t\rangle_H\ .$$

[6] As this point might be confusing, let us remind the reader that the state $|q_1, t\rangle_H$ is *not* the same as the Schrödinger state at time t, which is $e^{-iHt/\hbar}|q_1\rangle$; the latter is certainly not an eigenstate of any postition operator. On the contrary, $|q_1, t\rangle_H$ *is* an eigenstate of $Q_H(t)$ with eigenvalue q_1.

The states without suffix H stands for the position eigenstates of the standard Schrödinger operator Q. Let us now consider a matrix element,

$$\begin{aligned} {}_H\langle q_1, T_1 | Q_H(t) | q_0, T_0\rangle_H &= \langle q_1 | e^{-iH(T_1-t)/\hbar}\, Q\, e^{-iH(t-T_0)/\hbar} | q_0\rangle \\ &= \int dq\, \langle q_1 | e^{-iH(T_1-t)/\hbar} | q\rangle\, q\, \langle q | e^{-iH(t-T_0)/\hbar} | q_0\rangle\ ; \end{aligned}$$

calculating it between the time intervals $[T_1, t]$ and $[t, T_0]$ as above, one finds that

$${}_H\langle q_1, T_1 | Q_H(t) | q_0, T_0\rangle_H = \int [\mathcal{D}q]\, q(t)\, e^{\frac{i}{\hbar}\int_{T_0}^{T_1} L}\ ;$$

analogously, one finds for $t_1 > t_2$

$${}_H\langle q_1, T_1 |\, Q_H(t_1)\, Q_H(t_2)\, | q_0, T_0\rangle_H = \int [\mathcal{D}q]\, q(t_1)\, q(t_2)\, e^{\frac{i}{\hbar}\int_{T_0}^{T_1} L}\ ;$$

and so on. In general, we find a remarkable result,

$$\begin{aligned} &\int [\mathcal{D}q]\, q(t_1)\, q(t_2) \dots q(t_n)\, e^{\frac{i}{\hbar}\int_{T_0}^{T_1} L} \\ &\qquad = {}_H\langle q_1, T_1 | T\{Q_H(t_1) Q_H(t_2) \dots Q_H(t_n)\}\, | q_0, T_0\rangle_H, \end{aligned}$$

where the chronological product $T\{\dots\}$ is defined as

$$T\{Q_H(t_1)Q_H(t_2)Q_H(t_3)\} = \begin{cases} Q_H(t_1)Q_H(t_2)Q_H(t_3) & \text{if} \quad t_1 > t_2 > t_3; \\ Q_H(t_2)Q_H(t_3)Q_H(t_1) & \text{if} \quad t_2 > t_3 > t_1; \end{cases}, \tag{8.10}$$

etc.

We further modify the Lagrangian by introducing a "source term" $J(t)$, as

$$L \to L + J(t)\, q(t)\ .$$

If one assumes that the source is non-vanishing only during the time interval between t and t',

$$T_1 > t' > t > T_0,$$

then the Green function (path integral) in the presence of such a source term

$$W^{(J)} = \int [\mathcal{D}q]\, e^{\frac{i}{\hbar}\int (L + J\, q)}$$

is equal to

$${}_H\langle q_1, T_1 | q_0, T_0\rangle_H^{\{J\}} = \int dq' dq\, {}_H\langle q_1, T_1 | q', t'\rangle_H\, {}_H\langle q', t' | q, t\rangle_H^{\{J\}}\, {}_H\langle q, t | q_0, T_0\rangle_H\ .$$

We now let

$$T_1 \to -i\,\infty, \qquad T_0 \to +i\,\infty.$$

By inserting a completeness relation constructed with the energy eigenstates, we have

$$\begin{aligned} {}_H\langle q, t | q_0, T_0\rangle_H &= \langle q | e^{-iH(t-T_0)/\hbar} | q_0\rangle = \textstyle\sum_n \phi_n(q)\, \phi^{n\,*}(q_0)\, e^{-iE_n(t-T_0)/\hbar} \\ &\xrightarrow{T_0 \to +i\,\infty} \phi_0(q)\, \phi_0^*(q_0)\, e^{-iE_0(t-T_0)/\hbar}\ , \end{aligned} \tag{8.11}$$

i.e., in this limit the sum is dominated by a single term. In other words the path integral becomes proportional to the "vacuum to vacuum" amplitude (i.e., ground state to ground state). This important result is known as *Feynman's theorem.*

In analogy to the ordinary derivative, a "functional derivative" can be defined as

$$\frac{\delta}{\delta J(t)}\, J(t') = \delta(t - t').$$

Then ($T_1 \to -i\,\infty$, $T_0 \to +i\,\infty$)

$$\left.\frac{\delta^n\, W^{(J)}}{\delta J(t_1)\delta J(t_2)\ldots\delta J(t_n)}\right|_{J=0} = \langle 0 | T\{Q_H(t_1) Q_H(t_2)\ldots Q_H(t_n)\} | 0\rangle\ . \tag{8.12}$$

In other words, $W^{(J)}$ acts as the generating functional for the n-point *correlation functions.*

The generalization of the path integral to systems with s variables is immediate:

$$\begin{aligned} G(\{q_1\}, \{q_0\}; T_1, T_0) &= \langle \{q_1\} | e^{-iH(T_1 - T_0)/\hbar} | \{q_0\}\rangle \\ &= \int \prod_n \mathcal{D}q^{(n)}\, e^{i\,\frac{i}{\hbar}\int_{T_0}^{T_1} L(q^{(n)}(t), \dot{q}^{(n)}(t))}\ . \end{aligned}$$

Systems with infinite degrees of freedom (quantum fields) can be found as a limit of the multiple degrees of freedom. In quantum field theories the analogues of quantity (8.12) are the so-called causal correlation functions (the propagator and n-point functions). (See Section 17.2.)

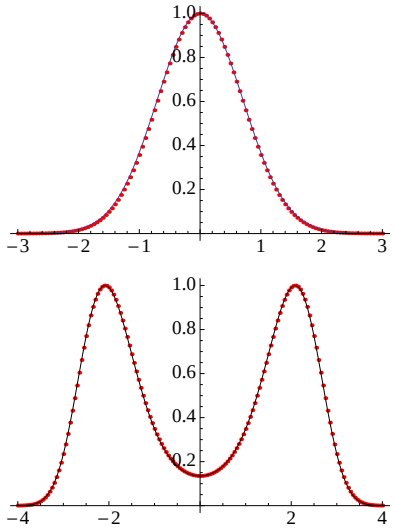

Fig. 8.3 The ground state $|\psi|^2$ computed with the Feynman path integral for the harmonic oscillator and a double well potential; see NB-8.1, NB-8.2.

Important identities can be found by considering the functional change of variables,

$$q(t) \to q(t) + \delta q(t) \ .$$

To start with, consider a general path integral with an "argument" $G[q]$,

$$\langle G[q] \rangle = \int [\mathcal{D}q]\, G[q(t)]\, e^{\frac{i}{\hbar} S},$$

where $G[q]$ is a generic function (or a functional) of $q(t)$. Applying a change of variable, one has

$$\left\langle \frac{\delta G}{\delta q(t)} - \frac{i}{\hbar} G[q(t)]\, \frac{\delta S}{\delta q(t)} \right\rangle = 0 \ .$$

By using such identities with various choices for $G[q]$ it is possible to reproduce known theorems such as Ehrenfest's theorem, the virial theorem, and so on. It is quite curious that the relation corresponding to the fundamental commutator in the usual operator formalism of quantum mechanics $[\hat{q}, \hat{p}] = i\,\hbar$ emerges this way (with $F(q) = q_i$).

8.2.2 Mode expansion

Two particular advantages of the path integral method are the following. First, the ease with which perturbative contributions (Chapter 9) can be organized in a diagrammatic fashion (Feynman graphs), which makes the concrete task of calculations much simpler, especially in complex systems with many degrees of freedom. Second, certain non-perturbative effects (tunnel effects) are elegantly captured by solutions of the classical equation of motion analytically continued to the Euclidean time. These solutions play the role of a sort of functional saddle point.

By going to the Euclidean time,

$$t \to t = -i\tau,$$

the factor e^{iS} becomes

$$e^{i \int dt \left[\frac{m}{2} \left(\frac{dq}{dt} \right)^2 - V(q) \right]} \to e^{- \int d\tau \left[\frac{m}{2} \left(\frac{dq}{d\tau} \right)^2 + V(q) \right]} = e^{-S_E},$$

where the Euclidean action is defined as

$$S_E = \int d\tau \ \left[\frac{m}{2} \left(\frac{dq}{d\tau} \right)^2 + V(q) \right] = \int d\tau\, L_E(q, \dot{q}) \ :$$

it describes the motion of the particle in the potential $-V(q)$. The generating functional in the presence of the source term is

$$W_E(J) = \int \mathcal{D}q\, e^{- \int d\tau\, [L_E(q,\dot{q}) - J \cdot q]},$$

and

$$\frac{1}{W(J)} \frac{\delta^n W}{\delta J(t_1) \ldots \delta J(t_n)} \bigg|_{J=0} = i^n \ \frac{1}{W_E(J)} \frac{\delta^n W_E}{\delta J(\tau_1) \ldots \delta J(\tau_n)} \bigg|_{J=0, \tau_i = i t_i} \ .$$

This last relation tells us how to retrieve the results for the n-point function in standard real time (Minkowski time), after the calculations have been done in the Euclidean-time formalism.

For the harmonic oscillator, $V(q) = \frac{\omega^2}{2}\, q^2$, and in the Euclidean time Lagrangian is (by setting $m = 1$)

$$L_E = \frac{\dot{q}^2}{2} + \frac{\omega^2}{2}\, q^2 \ .$$

Once the path integral

$$\langle q_1 |\, e^{-H\,\tau}\, | q_0 \rangle = \mathcal{N} \int \mathcal{D}q\, e^{-S_E} \ , \tag{8.13}$$

$$S_E = \int_{-\tau_0/2}^{\tau_0/2} \left(\frac{\dot{q}^2}{2} + \frac{\omega^2}{2}\, q^2 \right) \ ,$$

is calculated, the ground-state energy can be computed by studying its behavior at $\tau_0 \to \infty$,

$$\langle q_1 |\, e^{-H\,\tau}\, | q_0 \rangle \simeq e^{-E_0\,\tau}\, \psi_0(q_1)\, \psi_0(q_0)^* \ . \tag{8.14}$$

In more general cases, with the potential containing the cubic or higher powers of q, we write

$$S_E = \int d\tau\, [q(\tau) \hat{A}(\tau) q(\tau) + V_{int}(q(\tau))],$$

where $\hat{A}(\tau) = -\frac{1}{2}\frac{d^2}{d\,\tau^2} + \frac{1}{2}\omega^2$ is the quadratic part of the (Euclidean) Lagrangian; the remaining part $V_{int} = \lambda\, q(\tau)^3 + \eta\, q(\tau)^4 + \ldots$ represents the interactions. By introducing a complete set of eigenfunctions of the operator $\hat{A}$:

$$\hat{A}(\tau)\, f_k(\tau) = \epsilon_k\, f_k(\tau), \qquad \int d\tau\, f_k^*(\tau) f_\ell(\tau) = \delta_{k\,\ell}, \tag{8.15}$$

and by defining

$$[\mathcal{D}q] \equiv \prod_k dc_k, \qquad q(t) = \sum_k c_k\, f_k(\tau), \tag{8.16}$$

the functional integration reduces to the ordinary integrals over the coefficients of the mode expansion, $\prod_k\, dc_k$. The quadratic part gives

$$\int [\mathcal{D}q]\, e^{-q\cdot\hat{A}\cdot q} = \prod_k \epsilon_k^{-1/2} = (\det\, \hat{A})^{-1/2}; \tag{8.17}$$

the interaction part can be treated perturbatively, by introducing the source term, and writing things concisely:[7]

$$\begin{aligned} \int [\mathcal{D}q]\, e^{-q\cdot\hat{A}\cdot q - J\cdot q - V(q)} &= e^{-V\left(-\frac{\delta}{\delta J}\right)} \int [\mathcal{D}q]\, e^{-q\cdot\hat{A}\cdot q - J\cdot q} \\ &= e^{-V\left(-\frac{\delta}{\delta J}\right)}\, e^{J\cdot\hat{A}^{-1}\cdot J/4}\, (\det\, \hat{A})^{-1/2} \ . \end{aligned} \tag{8.18}$$

[7] Equation (8.18) is the key formula.

where

$$J \cdot \hat{A}^{-1} \cdot J \equiv \int d\tau_1 \, d\tau_2 \int \int J(\tau_1) D(\tau_1 - \tau_2) J(\tau_2), \tag{8.19}$$

$D(\tau_1 - \tau_2) \equiv \hat{A}^{-1}_{\tau_1,\tau_2}$, etc.

Equation (8.18) is the key formula both for the standard perturbation theory, i.e., computation of the fluctuations about the trivial minimum (in which case $\omega(t) = \omega = \text{const.}$), as well as for the evaluation of non-perturbative effects, i.e., determination of the effects due to some nontrivial classical minima $q(t) = q^{(cl)}(t)$ and to the fluctuations around it.

8.2.3 Feynman graphs

In order to get an expansion in the interaction potentials, let us first determine the value of the functional integral (8.13) for the harmonic oscillator, with $q_0 = q_1 = 0$ (with $S_{cl} = 0$), and without the interaction and source term ($V_{int} = J = 0$). It is formally equal to

$$(\det \hat{A})^{-1/2}, \qquad A = -\frac{d^2}{d\tau^2} + \omega^2,$$

which we shall now compute explicitly. In this case, the "classical solution" in the inverted oscillator potential is just the trivial solution, $q(\tau) = 0, \forall\tau$. (Figure 8.4). As the fluctuations must vanish at $\tau = \pm\frac{T}{2}$, the problem of finding the eigenvalues of the operator A is identical to the simple quantum mechanical problem of a particle in an infinitely deep well at $x = \pm\frac{T}{2}$:

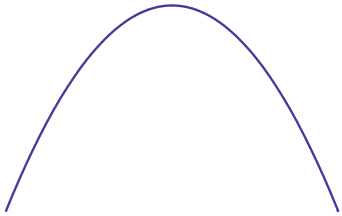

Fig. 8.4

$$\left(-\frac{d^2}{d\tau^2} + \omega^2\right) f_n = \epsilon_n \, f_n, \tag{8.20}$$

$$f_n\left(\frac{T}{2}\right) = f_n\left(-\frac{T}{2}\right) = 0,$$

which has solutions (Section 3.3.1)

$$\epsilon_n - \omega^2 = \frac{\pi^2 \, n^2}{T^2} \equiv \lambda_n^2; \quad f_n(\tau) = A_n \, \sin \lambda_n \left(\tau + \frac{T}{2}\right) .$$

By expanding

$$\delta q(\tau) = \sum_n c_n \, f_n(\tau),$$

and using the orthonormality of the eigenfunctions f_k,

$$S_E = \int d\tau \, \delta q(\tau) \, A \, \delta q(\tau) = \sum_n c_n^2 \, \epsilon_n,$$

we find that

$$\mathcal{N} \int \mathcal{D}q(\tau) e^{-S_E} = \mathcal{N} \, e^{-S_{cl}} \int \prod_n dc_n \, e^{-c_n^2 \, \epsilon_n}$$

$$= \left[\mathcal{N} \int \mathcal{D}q(\tau) e^{-S_E}\right]_{\omega=0} \prod_n \left(1 + \frac{\omega^2 \, T^2}{\pi^2 \, n^2}\right)^{-1/2} .$$

The part we factorized corresponds to the propagation of the free particle, so (with Euclidean time and with $m = \hbar = 1$)

$$\mathcal{N} \int \mathcal{D}q(\tau) e^{-S_E}|_{\omega=0} = \langle 0|e^{-p^2 T/2}|0\rangle = \frac{1}{\sqrt{2\pi T}},$$

(see eqn (8.6)). The "correction" factor is determined by using the formula

$$\prod_{n=1}^{\infty} \left(1 + \frac{z^2}{n^2}\right) = \frac{\sinh \pi z}{\pi z}$$

to be

$$\prod_{n=1}^{\infty} \left(1 + \frac{\omega^2 T^2}{\pi^2 n^2}\right)^{-1/2} = \left(\frac{\sinh \omega T}{\omega T}\right)^{-1/2} .$$

Thus the sum over fluctuations (paths) gives

$$\langle 0|\, e^{-H\tau}\, |0\rangle = \mathcal{N} \int \mathcal{D}q\, e^{-S_E} = \sqrt{\frac{\omega}{2\pi}}\, \sinh^{-1/2} \omega T \, . \tag{8.21}$$

This, of course, agrees with eqn (8.8), after setting $q_1 = q_0 = 0$ and going to the Euclidean time. Equation (8.21) yields in the limit $T \to \infty$,

$$\langle 0|\, e^{-H\tau}\, |0\rangle \to \sqrt{\frac{\omega}{\pi}}\, e^{-\omega T/2},$$

and gives, in view of eqn (8.14), $E_0 = \frac{\omega}{2}$, $\psi(0) = (\frac{\omega}{\pi})^{1/4}$, in agreement with what was obtained by solving Schrödinger's equation (Section 3.4).

Next we note that the *propagator* $\hat{A}^{-1}$ in eqn (8.18) is explicitly given by

$$\hat{A}^{-1} \equiv D(\tau_1 - \tau_2) = \frac{1}{2\,\omega}\, e^{-\omega|\tau_1 - \tau_2|} \, . \tag{8.22}$$

To obtain it, first make a Fourier transform to the energy space

$$q(\tau) = \int_{-\infty}^{\infty} \frac{dE}{2\pi}\, e^{-iE\tau}\, \tilde{q}(E) \, ,$$

in which the operator $\hat{A}$ is equal to $E^2 + \omega^2$. The inverse is thus $1/(E^2 + \omega^2)$ and $\hat{A}^{-1}$ is given by the inverse Fourier transform,

$$\hat{A}^{-1} \equiv D(\tau_1 - \tau_2) = \int_{-\infty}^{\infty} \frac{dE}{2\pi}\, \frac{1}{E^2 + \omega^2}\, e^{-iE(\tau_1 - \tau_2)} \, . \tag{8.23}$$

We leave it as an exercise to work out the integration by using the residues theorem, to get eqn (8.22). The propagator is just the two-point correlation function in the free theory ($V_{int} = 0$), as it corresponds to the second derivative with respect to the source function.

To get a taste of how things work, let us consider the case of the the cubic potential, $V = \lambda\, q^3(\tau)$, that is, the system

$$H = \frac{p^2}{2} + \frac{\omega^2}{2} q^2 + \lambda\, q^3$$

(we set $m = \hbar = 1$) and we are going to calculate the corrections to the ground-state energy $\frac{\omega}{2}$ due to the cubic interactions. The strategy is to compute the path integral (8.18) by setting $J = 0$, *after* an appropriate number of derivatives $\delta/\delta J$ are taken to extract the desired powers of λ, and then to use Feynman's theorem, (8.11). The potential enters eqn (8.18) through

$$e^{-\lambda \int d\tau \frac{\delta^3}{\delta J(\tau)^3}} = 1 - \lambda \int d\tau \, \frac{\delta^3}{\delta J(\tau)^3} + \frac{\lambda^2}{2!} \int d\tau \, \frac{\delta^3}{\delta J(\tau)^3} \int d\tau' \, \frac{\delta^3}{\delta J(\tau')^3} + \dots \, .$$

To the order λ^2 for instance, we have

$$\frac{\lambda^2}{2!} \int_\tau \frac{\delta^3}{\delta J^3} \int_{\tau'} \frac{\delta^3}{\delta J^3} \, \frac{1}{3!} \left(\int_1 \int_2 \frac{JDJ}{2} \right) \left(\int_3 \int_4 \frac{JDJ}{2} \right) \left(\int_5 \int_6 \frac{JDJ}{2} \right) .$$

With the use of the functional derivatives, various contributions arise. For instance if three derivatives in $\delta^3/\delta J^3(\tau)$ act on J's inside three different parentheses, the result would be proportional to

$$\int \int (D_{\tau,\tau'})^3 = \int d\tau \int d\tau' \, \frac{e^{-3\omega|\tau-\tau'|}}{(2\omega)^3} = \frac{T}{12\omega^4} \, , \tag{8.24}$$

where T is the total time interval. But the same contribution arises many times as the derivatives $\delta^3/\delta J^3(\tau)$ and $\delta^3/\delta J^3(\tau')$ are distributed in the three groups: taking into account the factorials in the expansion and the combinatoric factor, the above contribution gets multiplied by

$$\frac{\lambda^2}{2!} \, \frac{1}{3!} \, 3! \, 3! = 3 \, \lambda^2 \, .$$

Another type of contribution occurs when two of the derivatives in $\delta^3/\delta J^3(\tau)$ act on two J's inside a parenthesis. Necessarily the same occurs for the derivatives in $\delta^3/\delta J^3(\tau')$. In this case the result is

$$\int \int D_{\tau,\tau} D_{\tau,\tau'} D_{\tau',\tau'} = \int d\tau \int d\tau' \, \frac{e^{-\omega|\tau-\tau'|}}{(2\omega)^3} = \frac{T}{4\omega^4} \, . \tag{8.25}$$

The combinatorics for this case is a little more tricky: it is

$$\frac{\lambda^2}{2!} \, \frac{1}{3!} \, \frac{3!}{2} \, 3! \, \frac{3!}{2} = \frac{9 \, \lambda^2}{2},$$

which multiplies the above contribution. The total contribution to this order is equal to

$$\frac{11 \, T}{8 \, \omega^4} \, .$$

This kind of calculation can be pushed to higher orders, but obviously the counting will very quickly become cumbersome. The elegant observation due to Feynman which makes life considerably easier is that these contributions can be reorganized diagrammatically. Indeed, one has a simple set of rules (*Feynman's rules*):

(i) Each vertex (Figure 8.5) gives a factor $-\lambda$.

(ii) Each propagator gives $D(\tau_1 - \tau_2)$ (Figure 8.6) .

(iii) For a given number of vertices (to a given order in λ), draw all graphs combining vertices and propagators.

(iv) Integrate over all τ's (interaction time).

(v) Insert a factor $1/n!$ if there are n identical vertices.

(vi) Count how many times a given graph arises.

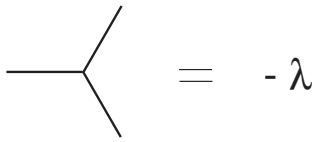

Fig. 8.5

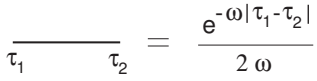

Fig. 8.6

Thus to the second-order contribution in λ considered above in the system with a cubic potential, there are two graphs A and B of Figure 8.7 contributing to the "vacuum-to-vacuum" amplitude. Their combinatorial factors (i.e., in how many ways the given graph can be formed) are

$$3 \cdot 3 = 9, \qquad 3 \cdot 2 = 6,$$

for the graphs A and B, respectively, while the value of the graphs is easily seen to be equal to eqns (8.24) and (8.25).

To sew things up and to apply Feynman's theorem, there is one more step needed. As we are really looking for the correction proportional to λ^2 in the ground-state energy, which appears in the *exponent* of the functional integral we are computing,

$$\langle q_1 |\, e^{-H\,T}\, | q_0 \rangle \simeq e^{-E_0\,T}\, \psi_0(q_1)\, \psi_0(q_0)^* \,,$$

we must exponentiate the contribution we have just computed:

$$1 + (A + B) + \frac{1}{2!}(A + B) \cdot (A + B) + \ldots = e^{A+B} \,.$$

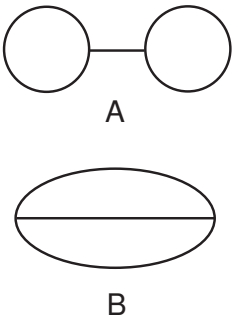

Fig. 8.7

More precisely we are to calculate the vacuum-to-vacuum amplitude to all orders in λ, however keeping only those graphs in which the *connected part* (let us call Σ) consists of the second-order contributions only. Thus the path integral has been computed to be

$$W|_{J=0} = \sqrt{\frac{\omega}{2\pi}}\, \sinh^{-1/2} \omega\, T\, e^{11\lambda^2 T/8\omega^2} \simeq e^{-(\omega/2 - 11\lambda^2/8\omega^2)T} \,,$$

so that

$$E_0 = \frac{\omega}{2} - \frac{11\,\lambda^2}{8\,\omega^2} + \ldots$$

where $\ldots$ indicates the corrections to higher orders in λ. This result coincides with the one found by using standard perturbation theory, developed in the next chapter (Section 9.1).

In the case of the quartic potential,

$$H = \frac{p^2}{2} + \frac{\omega^2}{2} q^2 + g\, q^4,$$

the only difference to the previous case is the vertex, see Figure 8.8. In this case, there is a vacuum-to-vacuum graph already at the first order, Figure 8.9, given by

$$-g\, \frac{4 \cdot 3}{2}\, \frac{1}{2} \int \frac{e^{-2\omega|\tau - \tau|}}{(2\,\omega)^2} = -\,\frac{3}{4}\, \frac{T}{\omega^2} \,.$$

To the second order, we find the two graphs shown in Figure 8.10, which sum up to yield

$$\frac{21}{8}\,\frac{T}{\omega^5}\,.$$

The correction to the ground-state energy is thus

$$E_0 = \frac{\omega}{2} + \frac{3}{4}\,\frac{g}{\omega^2} - \frac{21}{8}\,\frac{g^2}{\omega^5} + \dots\,,$$

which again, of course, agrees with the result of standard perturbation theory.

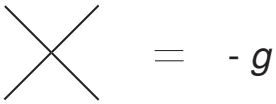

Fig. 8.8

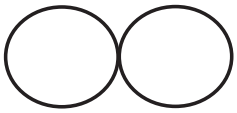

Fig. 8.9

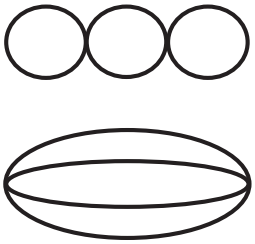

Fig. 8.10

Remarks

- Feynman's rules and graphs (diagrams) can be easily generalized to cases with more than one degree of freedom, and in fact to the case of infinite degrees of freedom (quantum field theory).
- A great advantage of the diagrammatic method is that the organization of the various contributions, in particular, the combinatorial factors, are identical in quantum mechanics considered here and in quantum field theory in any dimensions; the only difference is in the propagator (8.23), which is replaced by

  $$D(x_1^\mu - x_2^\mu) = \int \frac{d^D p}{(2\pi)^D}\,\frac{e^{ip\cdot(x_1-x_2)}}{p^2+m^2},$$

  where the mass of a propagating particle replaces ω of a quantum mechanical oscillator. Also the internal "loop" momenta (Fourier conjugate of the relative positions of the two vertices connected by the propagator) become D-dimensional.
- The power of the path integral formulation is truly appreciated when one faces much more complex problems such as relativistic quantum field theories or statistical mechanics (theories of infinite degrees of freedom). To try to solve a simple quantum mechanical problem with this method is a little like trying to crush a nut with a hydraulic press, not always the smartest thing to do.
- In the problems of elementary particle physics—relativistic quantum field theories—the fact that the formalism is intrinsically relativistic (the Lagrangian density which plays the central role in this formalism is a Lorenz-invariant quantity, while the Hamiltonian density is not), is a great advantage.
- From the formal point of view, the path integral with configurations $\{q\}$ periodic (and summed over) in Euclidean time (call $T = \beta$),

  $$\sum_q \langle q|e^{-\beta H}|q\rangle = \mathrm{Tr}\, e^{-\beta H}$$

  can be interpreted as the *partition function* of statistical mechanics, with $\beta \equiv 1/kT$, with T standing now for the temperature. This simple observation is at the basis of an enormously rich

(and successful) fields of research, encompassing condensed matter physics (phase transitions and critical phenomena) on the one hand and quantum field theories and elementary particle physics, on the other [Zinn-Justin (1989)]. Two fields have been enriched by mutual exportation of the techniques and theoretical concepts (even some physicists themselves!), such as the renormalization group, universality, scaling, phase structures of the systems, duality, and so on and so forth.

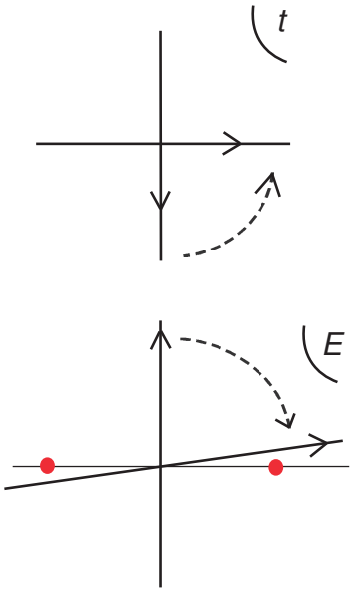

Fig. 8.11

8.2.4 Back to ordinary (Minkowski) time

The continuation back to the ordinary, real time description must be done with some care. We shall choose to rotate back the time variable as

$$t = -i\tau \longrightarrow t \quad \text{real},$$

90 degrees anti-clockwise, while at the same time

$$E = iE \longrightarrow E \quad \text{real},$$

by rotating 90 degrees in the clockwise direction. See Figure 8.11. This choice is dictated by the particular type of correlation functions we are interested in. Indeed, the propagator (8.23) is continued back to

$$D_M(t_1 - t_2) = -i \int_{-\infty}^{\infty} \frac{dE}{2\pi} \frac{1}{E^2 - \omega^2 + i\epsilon} e^{-iE(\tau_1 - \tau_2)} , \qquad (8.26)$$

where $+i\epsilon$ in the denominator indicates that the singularity at $\pm\omega$ must be avoided by shifting them slightly off the real axis, $\pm(\omega - i\epsilon)$. By picking up the appropriate residues for $t_1 - t_2 > 0$ or $t_1 - t_2 < 0$, one finds the propagator

$$D_M(t_1 - t_2) = \begin{cases} -e^{-i\omega(t_1 - t_2)}/2\omega, & t_1 > t_2; \\ -e^{i\omega(t_1 - t_2)}/2\omega, & t_1 < t_2 \, . \end{cases}$$

As the two-point correlation function in general has the form, e.g., for $t_1 > t_2$ (see eqn (8.10))

$$\begin{aligned} &D_M(t_1 - t_2) = \langle 0|T(Q(t_1)Q(t_2))|0\rangle \\ &= \sum_n \langle 0|Q(t_1)|n\rangle \, \langle n|Q(t_2)|0\rangle = \sum_n e^{-iE_n(t_1 - t_2)/\hbar} |\langle 0|Q|n\rangle|^2 \, , \end{aligned}$$

and analogously

$$D_M(t_1 - t_2) = \sum_n e^{+iE_n(t_1 - t_2)/\hbar} |\langle 0|Q|n\rangle|^2 \, , \qquad t_1 < t_2 \, ,$$

we see that $D_M(t)$ represents the *causal* propagator: only the positive (negative) energy states propagate in the future (past) direction.

A similar reasoning explains the form of the causal (Feynman) propagator of a scalar particle in Minkowski spacetime,

$$D_M(x_1^\mu - x_2^\mu) = i \int \frac{d^D p}{(2\pi)^D} \frac{e^{ip\cdot x}}{p^2 - m^2 + i\epsilon},$$

with the so-called $i\epsilon$ prescription.

8.2.5 Tunnel effects and instantons

As an example of the application of the path integral to non-perturbative effects in quantum mechanics (e.g., tunnel effects) consider a double-well potential,

$$H = \frac{p^2}{2\,m} + V(q), \qquad V(q) = \lambda\,(q^2 - \eta^2)^2\,, \tag{8.27}$$

shown in Figure 8.12. We know from the standard considerations based on Schrödinger's equation that the ground state of the system is a symmetric combination of the approximate ground state of the two wells, the first excited state antisymmetric combination thereof, and the splitting of the two levels is characterized by the tunneling amplitude between the two wells,

$$\Delta E_{\pm} \sim e^{-\frac{1}{\hbar}\int |p|\,dq}\,.$$

(For a more detailed discussion based on the semi-classical approximation see Section 11.1). In this section we are going to analyze the problem by making use of the "sum-over-paths" approach.

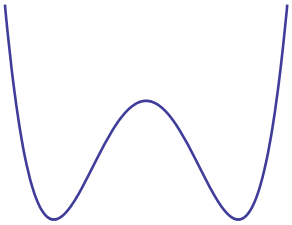

Fig. 8.12

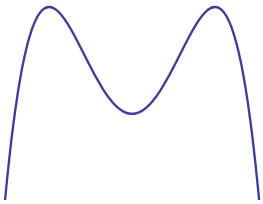

Fig. 8.13

We are mainly interested in studying the amplitudes

$$\langle \eta | e^{-HT} | -\eta \rangle = \int_{q(-T/2)=-\eta}^{q(T/2)=\eta} \mathcal{D}q\, e^{-S_E}; \tag{8.28}$$

$$\langle -\eta | e^{-HT} | -\eta \rangle = \int_{q(-T/2)=-\eta}^{q(T/2)=-\eta} \mathcal{D}q\, e^{-S_E}; \tag{8.29}$$

and similar ones with $\eta \leftrightarrow -\eta$, where S_E is the Euclidean action

$$S_E = \int d\tau\, \left(\frac{m}{2}\dot{q}^2 + V(q)\right)\,.$$

Note that near the bottom of each well the potential looks like a harmonic oscillator with

$$V''(q)|_{\eta} = 8\,\lambda\,\eta^2 \equiv m\,\omega^2, \qquad \omega = \sqrt{\frac{8\,\lambda\,\eta^2}{m}};$$

while the barrier height is

$$V(0) = \lambda\,\eta^4 = \frac{m^2\,\omega^4}{64\,\lambda} \gg \omega, \qquad \text{if} \quad \frac{m^2\,\omega^3}{\lambda} \gg 1\,.$$

Let us first consider the amplitude (8.29) for the particle traveling from $-\eta$ to η during the time T. The (functional) stationary point of S_E is given by the solution of the Euclidean equation of motion

$$\frac{\delta S_E}{\delta q} = -m\,\ddot{q} + \frac{dV}{dq} = 0\,.$$

Note that this describes a particle moving in the potential $-V(q)$ (Figure 8.13). The desired solution, satisfying the boundary condition $q(-T/2) = -\eta,\ q(T/2) = \eta$, is clearly a solution in which the particle, staying for a long time near $q(-T/2) = -\eta$, moves quickly through the central

ditch and approaches asymptotically towards $q(T/2) = \eta$. Such a solution in the Euclidean equation of motion is known as an *instanton*. (Figure 8.14).

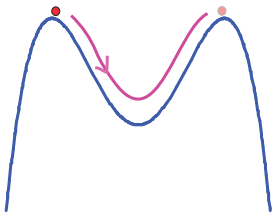

Fig. 8.14

In the case of the concrete model (8.27), the instanton solution is given by (for large T)

$$q^{(class)}(\tau) = q^{(inst)}(\tau) = \eta \tanh \frac{\omega}{2}(\tau - \tau_0)\,, \tag{8.30}$$

where τ_0, the center of the instanton, is arbitrary. It is clear from classical mechanics that an analogous solution always exists for a particle moving in a potential with the same general characteristics as in Figure 8.13, even though the detailed dependence on τ will depend on the potential. The classical instanton action can be expressed as follows. By integrating the equation of motion, one gets

$$\frac{m}{2}\left(\frac{dq}{d\tau}\right)^2 - V(q) = E = 0,$$

where we used the boundary condition to fix the value of the energy. This gives

$$\frac{dq}{d\tau} = \sqrt{\frac{2\,V(q)}{m}},$$

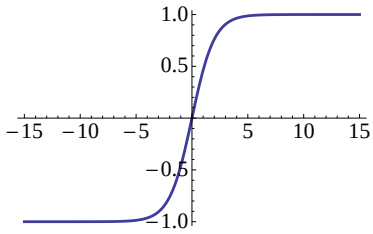

Fig. 8.15

and thus (by using the virial theorem)

$$\begin{aligned} S_E^{(inst)} &= \int d\tau \left[\frac{m}{2}\dot{q}^2 + V(q)\right] = \int d\tau\, m\,\dot{q}^2 \\ &= \int_{-\eta}^{\eta} dq\,\sqrt{2\,m\,V(q)} = \int_{-\eta}^{\eta} dq\,|p| \end{aligned} \tag{8.31}$$

which is the well-known reduced action for the tunneling amplitude. In the specific case of the quartic potential (8.27) we find $S_E^{(inst)} = \omega^3/12\lambda$.

We now expand $q(\tau)$ around the instanton solution

$$q(\tau) = q^{(class)}(\tau) + \delta q(\tau),$$

$$S_E = S_E^{(inst)} + \frac{1}{2}\int d\tau\,\delta q(\tau)\,\left[-m\frac{d^2}{d\tau^2} + V''(q^{(inst)}(\tau))\right]\,\delta q(\tau) + \dots\,;$$

by integrating over the fluctuations δq we formally get

$$\int \mathcal{D}q\, e^{-S_E} = \mathcal{N}\, e^{-S_E^{(inst)}}\,\det\left[-m\frac{d^2}{d\tau^2} + V''(q^{(inst)})\right]^{-1/2}\,.$$

But there are problems. First, as the classical solution (8.30) contains a free parameter x_0 and as the action S_E does not depend on it, among the fluctuations around that solution there must be those corresponding to *simple translations* in the time direction, which do not require extra action. There will therefore be a zero eigenvalue among the mode expansion associated with the quadratic operator

$$\left[-m\frac{d^2}{d\tau^2} + V''(q^{(inst)}(\tau))\right]\,\xi_n(\tau) = \epsilon_n\,\xi_n,$$

(cf. eqn (8.20)) with $\epsilon_0 = 0$, and this makes the factor $\det[\cdots]^{-1/2}$ meaningless. Also, in view of the fact that there are other instanton solutions in which the center is shifted, it is clear that contributions from these solutions (many saddle points) must be somehow summed up to get a sensible answer.

These two points are of course intimately related, and indeed the solution to *both* problems is given by the following (standard) trick. The idea is to explicitly extract the *zero mode*, corresponding to the translation in time,

$$dq^{(class)}(\tau) = \frac{dq^{(class)}(\tau)}{d\tau_0}\, d\tau_0 \equiv dc_0\, \xi_0(\tau),$$

[8]The normalization of the zero mode is known from an integral appearing in eqn (8.31).

where ξ_0 is the normalized zero mode function[8]

$$\xi_0(\tau) = \left(\frac{S_E^{(inst)}}{m}\right)^{-1/2} \frac{dq^{(class)}(\tau)}{d\tau}\,,$$

and therefore

$$dc_0 = (2\pi\hbar)^{1/2} \left(\frac{S_E^{(inst)}}{m}\right)^{1/2} d\tau_0\ .$$

[9]This kind of theoretical tool is used in studying *solitons*, *kinks*, *vortices*, etc. which are various finite-energy solutions of non-linear field equations, appearing in diverse fields of physics, from optics, solid state physics, fluid dynamics, superconductivity, and particle physics to cosmology.

Namely we traded the part of the (functional) integration over a particular fluctuation mode with an ordinary integration over the center of the instanton! This type of manipulation is known as the method of collective coordinates (of which τ_0 is an example). The functional integral is defined as[9]

$$\mathcal{D}q \equiv \frac{dc_0}{(2\pi\hbar)^{1/2}} \prod_{n\neq 0} \frac{dc_n}{(2\pi\hbar)^{1/2}} = \left(\frac{S_E^{(inst)}}{m}\right)^{1/2} d\tau_0 \prod_{n\neq 0} \frac{dc_n}{(2\pi\hbar)^{1/2}}\ .$$

The integration around an instanton solution then gives a contribution

$$\int \mathcal{D}q\, e^{-S_E} = (2\pi\hbar)^{1/2} \left(\frac{S_E^{(inst)}}{m}\right)^{1/2} T\ \det{}' \left[-m\frac{d^2}{d\tau^2} + V''(q^{(inst)})\right]^{-1/2},$$

where the prime on the determinant indicates that the product is over the nonzero eigenvalues only. By normalizing it to the determinant in the case of the oscillator ($V = 0$), (8.21), we write

$$\mathcal{N}\, \det{}' \left[-m\frac{d^2}{d\tau^2} + V''(q^{(inst)})\right]^{-1/2} = \sqrt{\frac{m\omega}{\pi\hbar}}\, e^{-\omega T/2}\, K\,,$$

where K is the ratio of the quadratic fluctuations around the instanton and those around the trivial solution $q^{(class)} = 0$. We shall not be concerned here with the computation of K, although in the case of the concrete model (8.27) the calculation can be carried through and gives $K = \omega\sqrt{6\, S_E^{(inst)}}/\pi\hbar$.

We are almost done. At $T \to \infty$, there must be many solutions which correspond to the particle going between the two peaks of the inverted potential many times. See Figure 8.16. As the action is concentrated near the center of the instanton (with a finite time spread of the order of $\Delta\tau \sim 1/\omega$)—and this is the reason for its name—the contribution corresponding to n instantons will be roughly proportional to $(Ke^{-S^{inst}/\hbar}T)^n$. Clearly n must be even for amplitude (8.29) whereas only odd-n solutions contribute to amplitude (8.28). Summing over the centers of the instantons we finally get

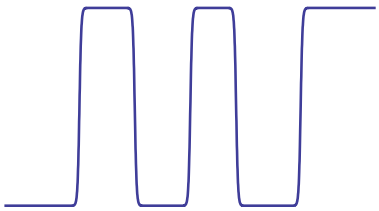

Fig. 8.16

$$\langle -\eta|e^{-HT}|-\eta\rangle = \langle \eta|e^{-HT}|\eta\rangle \simeq \left(\frac{m\omega}{\hbar}\right)^{1/2} e^{-\omega T/2} \cosh\left(Ke^{-S^{(inst)}/\hbar}T\right);$$

$$\langle \eta|e^{-HT}|-\eta\rangle = \langle -\eta|e^{-HT}|\eta\rangle \simeq \left(\frac{m\omega}{\hbar}\right)^{1/2} e^{-\omega T/2} \sinh\left(Ke^{-S^{(inst)}/\hbar}T\right).$$

Clearly the states $|\eta\rangle$ and $|-\eta\rangle$ are not eigenstates of the evolution operator, i.e., of the Hamiltonian. The correct eigenstates are the combinations $|\psi_\pm\rangle = (|\eta\rangle \pm |-\eta\rangle)/\sqrt{2}$, in the basis of which e^{-HT} is diagonal. The energy eigenvalues are ($\cosh x \pm \sinh x = e^{\pm x}$)

$$E_\pm = \frac{\hbar\omega}{2} \mp K\hbar\, e^{-S^{(inst)}/\hbar}.$$

Chapter summary

- The quantum mechanical Green function is given by the sum over paths, each path weighted by $e^{iS/\hbar}$.

Further reading

Special advice for the interested reader: read the original article by Feynman, *Space-time approach to non-relativistic quantum mechanics*, [Feynman (1948)]. For more details on the path integral formulation of quantum mechanics, the reader will find the book *Quantum Mechanics and path integrals* [Feynman and Hibbs (1965)] very stimulating. The first chapters of the book *Quantum Field Theory and Critical Phenomena* [Zinn-Justin (1989)] is a good introduction; this is also an example of a book dedicated both to quantum field theory and to critical phenomena. The review article [Abers and Lee (1973)] gives a very neat introduction to the path integral, as well as to the modern gauge theories. There are many other good books specialized in path integrals such as [Schulman (1981)] and [Kleinert (2006)].

The path integral method helped as the basis for an enormous advance in the numerical investigations of quantum field theory and statistical mechanics. Many approaches are based on the *Monte Carlo* method. In the numerical problems we give a brief account of these techniques in the case of simple quantum mechanical problems.

Numerical analyses

(8.1) Write a Monte Carlo simulation for one-dimensional quantum systems. Apply the method to the computation of the propagator for harmonic and anharmonic oscillators.

(8.2) Compute the path integral, by defining a transfer matrix between the adjacent time slices.