20
Path integrals

20.1 Path integrals and Richard Feynman

Since Richard Feynman invented them some 80 years ago, path integrals have been used with increasing frequency in particle physics and condensed-matter physics, in optics and biophysics, and even in finance. They express the amplitude for a process as a sum of all the ways the process can occur each weighted by an exponential of its classical action $\exp(iS/\hbar)$. (Richard Feynman, 1918–1988)

20.2 Gaussian integrals and Trotter's formula

Path integrals are based upon the gaussian integral (6.184) which holds for real $a \neq 0$ and real b

$$\int_{-\infty}^{\infty} e^{iax^2+2ibx}\, dx = \sqrt{\frac{i\pi}{a}}\; e^{-ib^2/a} \tag{20.1}$$

and upon the gaussian integral (6.138)

$$\int_{-\infty}^{\infty} e^{-ax^2+2ibx}\, dx = \sqrt{\frac{\pi}{a}}\; e^{-b^2/a} \tag{20.2}$$

which holds both for $\mathrm{Re}\, a > 0$ and also for $\mathrm{Re}\, a = 0$ with b real and $\mathrm{Im}\, a \neq 0$.

The extension of the integral formula (20.1) to any $n \times n$ real symmetric nonsingular matrix s_{jk} and any real vector c_j is (exercises 20.1 & 20.2)

$$\int_{-\infty}^{\infty} e^{is_{jk}x_jx_k+2ic_jx_j}\, dx_1 \ldots dx_n = \sqrt{\frac{(i\pi)^n}{\det s}}\; e^{-ic_j(s^{-1})_{jk}c_k} \tag{20.3}$$

in which $\det a$ is the determinant of the matrix a, a^{-1} is its inverse, and sums over the repeated indices j and k from 1 to n are understood. One may similarly extend the gaussian integral (20.2) to any positive symmetric $n \times n$ matrix s_{jk} and any vector c_j (exercises 20.3 & 20.4)

$$\int_{-\infty}^{\infty} e^{-s_{jk}x_j x_k + 2ic_j x_j} \, dx_1 \dots dx_n = \sqrt{\frac{\pi^n}{\det s}} \, e^{-c_j (s^{-1})_{jk} c_k}. \tag{20.4}$$

Path integrals also are based upon Trotter's product formula (Trotter, 1959; Kato, 1978)

$$e^{a+b} = \lim_{n\to\infty} \left(e^{a/n} \, e^{b/n} \right)^n \tag{20.5}$$

both sides of which are symmetrically ordered and obviously equal when $ab = ba$.

Separating a given hamiltonian $H = K + V$ into a kinetic part K and a potential part V, we can use Trotter's formula to write the time-evolution operator $e^{-itH/\hbar}$ as

$$e^{-it(K+V)/\hbar} = \lim_{n\to\infty} \left(e^{-itK/(n\hbar)} \, e^{-itV/(n\hbar)} \right)^n \tag{20.6}$$

and the Boltzmann operator $e^{-\beta H}$ as

$$e^{-\beta(K+V)} = \lim_{n\to\infty} \left(e^{-\beta K/n} \, e^{-\beta V/n} \right)^n. \tag{20.7}$$

20.3 Path integrals in quantum mechanics

Path integrals can represent matrix elements of the time-evolution operator $\exp(-i(t_b - t_a)H/\hbar)$ in which H is the hamiltonian. For a particle of mass m moving nonrelativistically in one dimension in a potential $V(q)$, the hamiltonian is

$$H = \frac{p^2}{2m} + V(q). \tag{20.8}$$

The position and momentum operators q and p obey the commutation relation $[q, p] = i\hbar$. Their eigenstates $|q'\rangle$ and $|p'\rangle$ have eigenvalues q' and p' for all real numbers q' and p'

$$q\,|q'\rangle = q'\,|q'\rangle \quad \text{and} \quad p\,|p'\rangle = p'\,|p'\rangle. \tag{20.9}$$

These eigenstates are complete. Their outer products $|q'\rangle\langle q'|$ and $|p'\rangle\langle p'|$ provide expansions for the identity operator I and have inner products (4.73) that are phases

$$I = \int_{-\infty}^{\infty} |q'\rangle\langle q'|\, dq' = \int_{-\infty}^{\infty} |p'\rangle\langle p'|\, dp' \quad \text{and} \quad \langle q'|p'\rangle = \frac{e^{iq'p'/\hbar}}{\sqrt{2\pi\hbar}}. \tag{20.10}$$

Setting $\epsilon = (t_b - t_a)/n$ and writing the hamiltonian (20.8) over $\hbar$ as $H/\hbar = p^2/(2m\hbar) + V/\hbar = k + v$, we can write Trotter's formula (20.6) for the time-evolution operator as the limit as $n \to \infty$ of n factors of $e^{-i\epsilon k}e^{-i\epsilon v}$

$$e^{-i(t_b-t_a)(k+v)} = e^{-i\epsilon k}\, e^{-i\epsilon v}\ e^{-i\epsilon k}\, e^{-i\epsilon v} \cdots e^{-i\epsilon k}\, e^{-i\epsilon v}\ e^{-i\epsilon k}\, e^{-i\epsilon v}. \tag{20.11}$$

The advantage of using Trotter's formula is that we now can evaluate the matrix element $\langle q_1|e^{-i\epsilon k}\, e^{-i\epsilon v}|q_a\rangle$ between eigenstates $|q_a\rangle$ and $|q_1\rangle$ of the position operator q by inserting the momentum-state expansion (20.10) of the identity operator I between the two exponentials

$$\langle q_1|e^{-i\epsilon k}\, e^{-i\epsilon v}|q_a\rangle = \langle q_1|\, e^{-i\epsilon p^2/(2m\hbar)} \int_{-\infty}^{\infty} |p'\rangle\langle p'|\, dp'\ e^{-i\epsilon\, V(q)/\hbar}|q_a\rangle \tag{20.12}$$

and using the eigenvalue formulas (20.9)

$$\langle q_1|e^{-i\epsilon k}\, e^{-i\epsilon v}|q_a\rangle = \int_{-\infty}^{\infty} e^{-i\epsilon p'^2/(2m\hbar)}\, \langle q_1|p'\rangle\, e^{-i\epsilon V(q_a)/\hbar}\, \langle p'|q_a\rangle\, dp'. \tag{20.13}$$

Now using the formula (20.10) for the inner product $\langle q_1|p'\rangle$ and the complex conjugate of that formula for $\langle p'|q_a\rangle$, we get

$$\langle q_1|e^{-i\epsilon k}\, e^{-i\epsilon v}|q_a\rangle = e^{-i\epsilon\, V(q_a)/\hbar} \int_{-\infty}^{\infty} e^{-i\epsilon p'^2/(2m\hbar)}\, e^{i(q_1-q_a)p'/\hbar}\, \frac{dp'}{2\pi\hbar}. \tag{20.14}$$

In this integral, the momenta that are important are very high, being of order $\sqrt{m\hbar/\epsilon}$ which diverges as $\epsilon \to 0$; nonetheless, the integral converges.

If we adopt the suggestive notation $q_1 - q_a = \epsilon\, \dot q_a$ and use the gaussian integral (20.1) with $a = -\epsilon/(2m\hbar)$, $x = p$, and $b = \epsilon\dot q/(2\hbar)$

$$\int_{-\infty}^{\infty} \exp\left(-\, i\, \epsilon\, \frac{p^2}{2m\hbar} + i\, \epsilon\, \frac{\dot q\, p}{\hbar} \right) \frac{dp}{2\pi\hbar} \;=\; \sqrt{\frac{m}{2\pi i\epsilon\hbar}}\ \exp\left(i\, \frac{\epsilon}{\hbar}\, \frac{m\dot q^2}{2} \right), \tag{20.15}$$

then we find

$$\begin{aligned}
\langle q_1|e^{-i\epsilon k}\, e^{-i\epsilon v}|q_a\rangle &= \frac{1}{2\pi\hbar}\, e^{-\epsilon\, V(q_a)} \int_{-\infty}^{\infty} \exp\left(-\, i\frac{\epsilon p'^2}{2m\hbar} + i\frac{\epsilon\, \dot q_a\, p'}{\hbar} \right) dp' \\
&= \left(\frac{m}{2\pi i\hbar\epsilon} \right)^{1/2} \exp\left[i\, \frac{\epsilon}{\hbar} \left(\frac{m\dot q_a^2}{2} - V(q_a) \right) \right].
\end{aligned} \tag{20.16}$$

The dependence of the amplitude $\langle q_1|e^{-i\epsilon k}\, e^{-i\epsilon v}|q_a\rangle$ upon q_1 is hidden in the formula $\dot q_a = (q_1 - q_a)/\epsilon$.

The next step is to use the position-state expansion (20.10) of the identity operator to link two of these matrix elements together

$$\begin{aligned}\langle q_2|\left(e^{-i\epsilon k}\, e^{-i\epsilon v}\right)^2|q_a\rangle &= \int_{-\infty}^{\infty} \langle q_2|\, e^{-i\epsilon k}\, e^{-i\epsilon v}\, |q_1\rangle\langle q_1|\, e^{-i\epsilon k}\, e^{-i\epsilon v}\, |q_a\rangle\, dq_1 \\ &= \frac{m}{2\pi i\hbar\epsilon}\int_{-\infty}^{\infty} \exp\left[i\frac{\epsilon}{\hbar}\left(\frac{m\dot{q}_1^2}{2} - V(q_1) + \frac{m\dot{q}_a^2}{2} - V(q_a)\right)\right] dq_1\end{aligned}$$

where now $\dot{q}_1 = (q_2 - q_1)/\epsilon$.

By stitching together $n = (t_b - t_a)/\epsilon$ time intervals each of length ϵ and letting $n \to \infty$, we get

$$\begin{aligned}\langle q_b|e^{-ni\epsilon H/\hbar}|q_a\rangle &= \int \langle q_b|e^{-i\epsilon k}\, e^{-i\epsilon v}|q_{n-1}\rangle \cdots \langle q_1|e^{-i\epsilon k}\, e^{-i\epsilon v}|q_a\rangle\, dq_{n-1}\cdots dq_1 \\ &= \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{n/2}\int \exp\left[i\frac{\epsilon}{\hbar}\sum_{j=0}^{n-1}\frac{m\dot{q}_j^2}{2} - V(q_j)\right] dq_{n-1}\cdots dq_1 \\ &= \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{n/2}\int \exp\left(i\frac{\epsilon}{\hbar}\sum_{j=0}^{n-1} L_j\right) dq_{n-1}\cdots dq_1 \qquad (20.17)\end{aligned}$$

in which $L_j = m\dot{q}_j^2/2 - V(q_j)$ is the lagrangian of the jth interval, and the q_j integrals run from $-\infty$ to ∞. In the limit $\epsilon \to 0$ with $n\epsilon = (t_b - t_a)/\epsilon$, this multiple integral is an integral over all paths $q(t)$ that go from q_a, t_a to q_b, t_b

$$\langle q_b|e^{-i\,(t_b-t_a)\,H/\hbar}|q_a\rangle = \int e^{iS[q]/\hbar}\, Dq \qquad (20.18)$$

in which each path is weighted by the phase of its classical action

$$S[q] = \int_{t_a}^{t_b} L(\dot{q}, q)\, dt = \int_{t_a}^{t_b}\left(\frac{m\dot{q}(t)^2}{2} - V(q(t))\right) dt \qquad (20.19)$$

in units of $\hbar$ and $Dq = (mn/(2\pi i\hbar(t_b - t_a)))^{n/2}\, dq_{n-1}\ldots dq_1$.

If we multiply the path-integral (20.18) for $\langle q_b|e^{-i\,(t_b-t_a)\,H/\hbar}|q_a\rangle$ from the left by $|q_b\rangle$ and from the right by $\langle q_a|$ and integrate over q_a and q_b as in the resolution (20.10) of the identity operator, then we can write the time-evolution operator as an integral over all paths from t_a to t_b

$$e^{-i\,(t_b-t_a)\,H/\hbar} = \int |q_b\rangle\, e^{iS[q]/\hbar}\, \langle q_a|\, Dq\, dq_a\, dq_b \qquad (20.20)$$

with $Dq = (mn/(2\pi i\hbar(t_b - t_a)))^{n/2}\, dq_{n-1}\ldots dq_1$ and $S[q]$ the action (20.19).

The path integral for a particle moving in three-dimensional space is

$$\langle \boldsymbol{q}_b | e^{-i(t_b - t_a)H/\hbar} | \boldsymbol{q}_a \rangle = \int \exp\left[\frac{i}{\hbar} \int_{t_a}^{t_b} \tfrac{1}{2}\, m\, \dot{\boldsymbol{q}}^2(t) - V(\boldsymbol{q}(t))\, dt \right] D\boldsymbol{q} \tag{20.21}$$

where $D\boldsymbol{q} = (mn/(2\pi i\hbar(t_b - t_a)))^{3n/2}\, d\boldsymbol{q}_{n-1} \cdots d\boldsymbol{q}_1$.

Let us first consider macroscopic processes whose actions are large compared to $\hbar$. Apart from the factor $D\boldsymbol{q}$, the amplitude (20.21) is a sum of phases $e^{iS[\boldsymbol{q}]/\hbar}$ one for each path from $\boldsymbol{q}_a, t_a$ to $\boldsymbol{q}_b, t_b$. When is this amplitude big? When is it small? Suppose there is a path $\boldsymbol{q}_c(t)$ from $\boldsymbol{q}_a, t_a$ to $\boldsymbol{q}_b, t_b$ that obeys the classical equation of motion (19.14–19.15)

$$\frac{\delta S[\boldsymbol{q}_c]}{\delta \boldsymbol{q}_{jc}} = m\ddot{\boldsymbol{q}}_{jc} + V'(\boldsymbol{q}_c) = 0. \tag{20.22}$$

Its action may be minimal. It certainly is stationary: a path $\boldsymbol{q}_c(t) + \delta\boldsymbol{q}(t)$ that differs from $\boldsymbol{q}_c(t)$ by a small detour $\delta\boldsymbol{q}(t)$ has an action $S[\boldsymbol{q}_c + \delta\boldsymbol{q}]$ that differs from $S[\boldsymbol{q}_c]$ only by terms of second order and higher in $\delta\boldsymbol{q}$. Thus a classical path has infinitely many neighboring paths whose actions differ only by integrals of $(\delta\boldsymbol{q})^n$, $n \ge 2$, and so have the same action to within a small fraction of $\hbar$. These paths add with nearly the same phase to the path integral (20.21) and so make a huge contribution to the amplitude $\langle \boldsymbol{q}_b | e^{-i(t_b - t_a)H/\hbar} | \boldsymbol{q}_a \rangle$. But if no classical path goes from $\boldsymbol{q}_a, t_a$ to $\boldsymbol{q}_b, t_b$, then the nonclassical, nonstationary paths that go from $\boldsymbol{q}_a, t_a$ to $\boldsymbol{q}_b, t_b$ have actions that differ from each other by large multiples of $\hbar$. These amplitudes cancel each other, and their sum, which is the amplitude for going from $\boldsymbol{q}_a, t_a$ to $\boldsymbol{q}_b, t_b$, is small. **Thus the path-integral formula for an amplitude in quantum mechanics explains why macroscopic processes have stationary action** (section 7.13).

What about microscopic processes whose actions are tiny compared to $\hbar$? The path integral (20.21) gives large amplitudes for all microscopic processes. On very small scales, anything can happen that doesn't break a conservation law.

The path integral for two or more particles $\{\boldsymbol{q}\} = \{\boldsymbol{q}_1, \dots, \boldsymbol{q}_k\}$ interacting with a potential $V(\{\boldsymbol{q}\})$ is

$$\langle \{\boldsymbol{q}\}_b | e^{-i(t_b - t_a)H/\hbar} | \{\boldsymbol{q}\}_a \rangle = \int e^{iS[\{q\}]/\hbar}\, D\{\boldsymbol{q}\} \tag{20.23}$$

where

$$S[\{\boldsymbol{q}\}] = \int_{t_a}^{t_b} \left[\frac{m_1 \dot{\boldsymbol{q}}_1^2(t)}{2} + \cdots + \frac{m_k \dot{\boldsymbol{q}}_k^2(t)}{2} - V(\{\boldsymbol{q}(t)\}) \right] dt \tag{20.24}$$

and $D\{\boldsymbol{q}\} = D\boldsymbol{q}_1 \cdots D\boldsymbol{q}_k$.

Example 20.1 (A free particle) For a free particle, the potential is zero, $H = p^2/(2m)$, and the path integral (20.18, 20.19) is the $\epsilon \to 0, n \to \infty$ limit of

$$\langle q_b|e^{-i\,t\,H/\hbar}|q_a\rangle = \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{n/2} \times \int \exp\left[i\frac{m\epsilon}{2\hbar}\left(\frac{(q_b - q_{n-1})^2}{\epsilon^2} + \cdots + \frac{(q_1 - q_a)^2}{\epsilon^2}\right)\right] dq_{n-1}\cdots dq_1. \tag{20.25}$$

The q_1 integral is by the gaussian formula (20.1)

$$\frac{m}{2\pi i\hbar\epsilon}\int e^{im[(q_2-q_1)^2+(q_1-q_a)^2]/(2\hbar\epsilon)}dq_1 = \sqrt{\frac{m}{2\pi i\hbar 2\epsilon}}\, e^{im(q_2-q_a)^2/(2\hbar 2\epsilon)}. \tag{20.26}$$

The q_2 integral is (exercise 20.5)

$$\frac{m}{2\sqrt{2}\,\pi i\hbar\epsilon}\int e^{im[(q_3-q_2)^2+(q_2-q_a)^2/2]/(2\hbar\epsilon)}dq_2 = \sqrt{\frac{m}{2\pi i\hbar 3\epsilon}}\, e^{im(q_3-q_a)^2/(2\hbar 3\epsilon)}. \tag{20.27}$$

Doing all $n-1$ integrals (20.25) in this way and setting $n\epsilon = t_b - t_a$, we get

$$\begin{aligned}\langle q_b|\, e^{-i\,(t_b-t_a)\,H/\hbar}\,|q_a\rangle &= \sqrt{\frac{m}{2\pi i\hbar n\epsilon}}\,\exp\left[\frac{im(q_b-q_a)^2}{2\hbar n\epsilon}\right]\\ &= \sqrt{\frac{m}{2\pi i\hbar(t_b-t_a)}}\,\exp\left[\frac{im(q_b-q_a)^2}{2\hbar(t_b-t_a)}\right].\end{aligned} \tag{20.28}$$

It is easier to compute this amplitude (20.28) by using the outer products (20.10) (exercise 20.6).

In three dimensions, the amplitude to go from $\boldsymbol{q}_a, t_a$ to $\boldsymbol{q}_b, t_b$ is

$$\langle \boldsymbol{q}_t|e^{-i(t_b-t_a)H/\hbar}|\boldsymbol{q}_0\rangle = \left(\frac{m}{2\pi i\hbar(t_b-t_a)}\right)^{3/2}\exp\left[\frac{im(\boldsymbol{q}_b-\boldsymbol{q}_a)^2}{2\hbar(t_b-t_a)}\right]. \tag{20.29}$$

□

Example 20.2 (The ubiquitous phase factor $e^{ipx/\hbar}$) The phase factor $e^{ipx/\hbar}$ is actually the exponential of the classical action of a particle of mass m going from the origin to the point $x = (ct, \boldsymbol{x})$ both non-relativistically

$$ipx/\hbar = i(\boldsymbol{p}\cdot\boldsymbol{x} - Et)/\hbar = i(m\boldsymbol{v}\cdot\boldsymbol{v}t - \tfrac{1}{2}m\boldsymbol{v}^2t)/\hbar = i\tfrac{1}{2}m\boldsymbol{v}^2t/\hbar \tag{20.30}$$

and relativistically

$$ipx/\hbar = \frac{m\boldsymbol{v}\cdot\boldsymbol{v}\,t}{\hbar\sqrt{1-\boldsymbol{v}^2/c^2}} - \frac{mc^2\,t}{\hbar\sqrt{1-\boldsymbol{v}^2/c^2}} = -mc^2\sqrt{1-\boldsymbol{v}^2/c^2}\,t/\hbar. \tag{20.31}$$

□

20.4 Path integrals for quadratic actions

If a path $q(t) = q_c(t) + x(t)$ differs from a classical path $q_c(t)$ by a detour $x(t)$ that vanishes at the endpoints $x(t_a) = 0 = x(t_b)$ so that both paths go from q_a, t_a to q_b, t_b, then the difference $S[q_c + x] - S[q_c]$ in their actions that is of first order in $x(t)$ vanishes (section 7.13). Thus the actions of the two paths differ by a time integral of quadratic and higher powers of the detour $x(t)$

$$\begin{aligned} S[q_c + x] &= \int_{t_a}^{t_b} \tfrac{1}{2} m \dot{q}(t)^2 - V(q(t))\, dt \\ &= \int_{t_a}^{t_b} \tfrac{1}{2} m \left(\dot{q}_c(t) + \dot{x}(t)\right)^2 - V(q_c(t) + x(t))\, dt \\ &= \int_{t_a}^{t_b} \left[\frac{m}{2} \dot{q}_c^2 + m \dot{q}_c \dot{x} + \frac{m}{2} \dot{x}^2 - V(q_c) - V'(q_c) x - \frac{V''(q_c)}{2} x^2 \right. \\ &\qquad \left. - \frac{V'''(q_c)}{6}\, x^3 - \frac{V''''(q_c)}{24}\, x^4 - \dots \right] dt. \end{aligned} \tag{20.32}$$

We integrate the linear terms by parts

$$\int_{t_a}^{t_b} \left[m \dot{q}_c \dot{x} - V'(q_c) x \right] dt = - \int_{t_a}^{t_b} \left[m \ddot{q}_c + V'(q_c) \right] x \, dt = 0 \tag{20.33}$$

and see that they vanish because on the classical path $m\ddot{q}_c = -V'(q_c)$ and $x(t_a) = x(t_b) = 0$ at its end points. Thus the action of the deviant path is

$$\begin{aligned} S[q_c + x] &= \int_{t_a}^{t_b} \left[\frac{m}{2} \dot{q}_c^2 - V(q_c) \right] dt + \int_{t_a}^{t_b} \left[\frac{m}{2} \dot{x}^2 - \frac{V''(q_c)}{2} x^2 \right. \\ &\qquad \left. - \frac{V'''(q_c)}{6}\, x^3 - \frac{V''''(q_c)}{24}\, x^4 - \dots \right] dt \\ &= S[q_c] + \Delta S[q_c, x] \end{aligned}$$

in which $S[q_c]$ is the action of the classical path, and the detour $x(t)$ is a loop that goes from $x(t_a) = 0$ to $x(t_b) = 0$.

If the potential $V(q)$ is quadratic in the position q, then the third V''' and higher derivatives of the potential vanish, and the second derivative is a constant $V''(q_c(t)) = V''$. In this quadratic case, the correction $\Delta S[q_c, x]$ depends only on the time interval $t_b - t_a$ and on $\hbar$, m, and V''

$$\Delta S[q_c, x] = \Delta S[x] = \int_{t_a}^{t_b} \left[\tfrac{1}{2} m\, \dot{x}^2(t) - \tfrac{1}{2} V''\, x^2(t) \right] dt. \tag{20.34}$$

It is independent of the classical path.

Thus for quadratic actions, the path integral (20.18) is simply the exponential $\exp(iS[q_c]/\hbar)$ of the classical action apart from a factor $f(t_b - t_a, \hbar, m, V'')$ that depends only on the time interval $t_b - t_a$ and on the parameters $\hbar$, m, and V''

$$\begin{aligned} \langle q_b | e^{-i(t_b - t_a)H/\hbar} | q_a \rangle &= \int e^{iS[q]/\hbar} Dq = \int e^{i(S[q_c] + \Delta S[x])/\hbar} Dq \\ &= e^{iS[q_c]/\hbar} \int e^{i\Delta S[x])/\hbar}\, Dx \\ &= f(t_b - t_a, \hbar, m, V'')\, e^{iS[q_c]/\hbar}. \end{aligned} \tag{20.35}$$

The function $f = f(t_b - t_a, \hbar, m, V'')$ is the limit as $n \to \infty$ of the $(n-1)$-dimensional integral

$$f = \left[\frac{mn}{2\pi i\hbar(t_b - t_a)} \right]^{n/2} \int e^{i\Delta S[x])/\hbar} dx_{n-1} \dots dx_1 \tag{20.36}$$

where

$$\Delta S[x] = \frac{t_b - t_a}{n} \sum_{j=1}^{n} \frac{1}{2} m \frac{(x_j - x_{j-1})^2}{[(t_b - t_a)/n]^2} - \frac{1}{2} V''\, x_j^2 \tag{20.37}$$

and $x_n = 0 = x_0$.

More generally, the path integral for any quadratic action of the form

$$S[q] = \int_{t_a}^{t_b} u\, \dot{q}^2(t) + v\, q(t)\dot{q}(t) + w\, q^2(t) + s(t)\, \dot{q}(t) + j(t)\, q(t)\, dt \tag{20.38}$$

is (exercise 20.7)

$$\langle q_b | e^{-i(t_b - t_a)H/\hbar} | q_a \rangle = f(t_a, t_b, \hbar, u, v, w)\, e^{iS[q_c]/\hbar}. \tag{20.39}$$

The dependence of the amplitude upon $s(t)$ and $j(t)$ is contained in the classical action $S[q_c]$ of the classical path q_c.

These formulas (20.35–20.39) may be generalized to any number of particles with coordinates $\{\boldsymbol{q}\} = \{\boldsymbol{q}^1, \dots, \boldsymbol{q}^k\}$ moving nonrelativistically in a space of multiple dimensions as long as the action is quadratic in the $\{\boldsymbol{q}\}$'s and their velocities $\{\dot{\boldsymbol{q}}\}$. The amplitude is then an exponential of the action $S[\{\boldsymbol{q}\}_c]$ of the classical path multiplied by a function $f(t_a, t_b, \hbar, \dots)$ that is independent of the classical path q_c

$$\langle \{\boldsymbol{q}\}_b | e^{-i(t_b - t_a)H/\hbar} | \{\boldsymbol{q}\}_a \rangle = f(t_a, t_b, \hbar, \dots)\, e^{iS[\{\boldsymbol{q}\}_c]/\hbar}. \tag{20.40}$$

Example 20.3 (Free particle) The classical path of a free particle going from $\boldsymbol{q}_a$ at time t_a to $\boldsymbol{q}_b$ at time t_b is

$$\boldsymbol{q}_c(t) = \boldsymbol{q}_a + \frac{t - t_a}{t_b - t_a} (\boldsymbol{q}_b - \boldsymbol{q}_a). \tag{20.41}$$

Its action is

$$S[\boldsymbol{q}_c] = \int_{t_a}^{t_b} \frac{1}{2}\, m\, \dot{\boldsymbol{q}}_c^2\, dt = \frac{m(\boldsymbol{q}_b - \boldsymbol{q}_a)^2}{2(t_b - t_a)} \tag{20.42}$$

and for this case our quadratic-potential formula (20.40) is

$$\langle \boldsymbol{q}_b | e^{-i(t_b - t_a)H/\hbar} | \boldsymbol{q}_a \rangle = f(t_b - t_a, \hbar, m)\, \exp\left[i \frac{m(\boldsymbol{q}_b - \boldsymbol{q}_a)^2}{2\hbar(t_b - t_a)} \right] \tag{20.43}$$

which agrees with our explicit calculation (20.29) when $f(t_b - t_a, \hbar, m) = [m/(2\pi i\hbar(t_b - t_a))]^{3/2}$. □

Example 20.4 (Bohm-Aharonov effect) From the formula (12.70) for the action of a relativistic particle of mass m and charge e, it follows (exercise 20.18) that the action of a nonrelativistic particle in an electromagnetic field with no scalar potential is

$$S = \int_{t_a}^{t_b} \left[\tfrac{1}{2} m \dot{\boldsymbol{q}}^2 + e\boldsymbol{A} \cdot \dot{\boldsymbol{q}} \right]\, dt = \int_{\boldsymbol{q}_a}^{\boldsymbol{q}_b} \left[\tfrac{1}{2} m \dot{\boldsymbol{q}} + e\, \boldsymbol{A} \right] \cdot \boldsymbol{dq}\, . \tag{20.44}$$

Since this action is quadratic in $\dot{\boldsymbol{q}}$, the amplitude for a particle to go from $\boldsymbol{q}_a$ at t_a to $\boldsymbol{q}_b$ at t_b is an exponential of the classical action

$$\langle \boldsymbol{q}_b | e^{-i(t_b - t_a)H/\hbar} | \boldsymbol{q}_a \rangle = f(t_b - t_a, \hbar, m, e)\, e^{iS[\boldsymbol{q}_c]/\hbar} \tag{20.45}$$

multiplied by a function $f(t_b - t_a, \hbar, m, e)$ that is independent of the path $\boldsymbol{q}_c$. A beam of such particles goes horizontally past but not through a vertical pipe in which a vertical magnetic field is confined. The particles can go both ways around the pipe of cross-sectional area S but do not enter it. The difference in the phases of the amplitudes for the two paths is a loop integral from the source to the detector around the pipe and back to the source

$$\oint \left[\frac{m\dot{\boldsymbol{q}}}{2} + e\, \boldsymbol{A} \right] \cdot \frac{\boldsymbol{dq}}{\hbar} = \oint \frac{m\dot{\boldsymbol{q}} \cdot \boldsymbol{dq}}{2\hbar} + \frac{e}{\hbar} \int_S \boldsymbol{B} \cdot \boldsymbol{dS} = \oint \frac{m\dot{\boldsymbol{q}} \cdot \boldsymbol{dq}}{2\hbar} + \frac{e\Phi}{\hbar} \tag{20.46}$$

in which Φ is the magnetic flux through the cylinder. □

Example 20.5 (Harmonic oscillator) The action

$$S = \int_{t_a}^{t_b} \frac{1}{2} m\dot{q}^2(t) - \frac{1}{2} m\omega^2 q^2(t)\, dt \tag{20.47}$$

of a harmonic oscillator is quadratic in q and $\dot{q}$. So apart from a factor f, its path integral (20.35–20.37) is an exponential

$$\langle q_b | e^{-i(t_b - t_a)H/\hbar} | q_a \rangle = f\, e^{iS[q_c]/\hbar} \tag{20.48}$$

of the action $S[q_c]$ (exercise 20.8)

$$S[q_c] = \frac{m\omega\left[\left(q_a^2+q_b^2\right)\cos(\omega(t_b-t_a)) - 2q_aq_b\right]}{2\sin(\omega(t_b-t_a))} \tag{20.49}$$

of the classical path

$$q_c(t) = q_a\cos\omega(t-t_a) + \frac{q_b - q_a\cos\omega(t_b-t_a)}{\sin\omega(t_b-t_a)}\,\sin\omega(t-t_a) \tag{20.50}$$

that runs from q_a, t_a to q_b, t_b and obeys the classical equation of motion $m\ddot{q}_c(t) = -\omega^2 q_c(t)$.

The factor f is a function $f(t_b-t_a, \hbar, m, m\omega^2)$ of the time interval and the parameters of the oscillator. Its actual value is

$$f = \sqrt{\frac{m\omega}{2\pi i\hbar\sin\omega T}}. \tag{20.51}$$

The amplitude (20.48) is then an exponential of the action $S[q_c]$ (20.49) of the classical path (20.50) multiplied by this factor f

$$\begin{aligned}\langle q_b|e^{-i(t_b-t_a)H/\hbar}|q_a\rangle = {}& \sqrt{\frac{m\omega}{2\pi i\hbar\sin\omega(t_b-t_a)}} \\ &\times\exp\left\{\frac{i}{\hbar}\frac{m\omega\left[\left(q_a^2+q_b^2\right)\cos(\omega(t_b-t_a)) - 2q_aq_b\right]}{2\sin(\omega(t_b-t_a))}\right\}.\end{aligned} \tag{20.52}$$

□

Example 20.6 (Computation of f) The factor f is the $n\to\infty$ limit of the $(n-1)$-dimensional integral (20.36)

$$f = \left[\frac{mn}{2\pi i\hbar(t_b-t_a)}\right]^{n/2}\int e^{i\Delta S[x])/\hbar}\,dx_{n-1}\dots dx_1 \tag{20.53}$$

over all loops that run from 0 to 0 in time t_b-t_a in which the quadratic correction to the classical action is (20.37)

$$\Delta S[x] = \frac{t_b-t_a}{n}\sum_{j=1}^{n}\frac{1}{2}m\frac{(x_j-x_{j-1})^2}{[(t_b-t_a)/n]^2} - \frac{1}{2}m\omega^2\,x_j^2, \tag{20.54}$$

and $x_n = 0 = x_0$.

Setting $t_b - t_a = T$, we use the many-variable imaginary gaussian integral (20.3) to write f as

$$f = \left[\frac{mn}{2\pi i\hbar T}\right]^{n/2}\int e^{ia_{jk}x_jx_k}dx_{n-1}\dots dx_1 = \left[\frac{mn}{2\pi i\hbar T}\right]^{n/2}\sqrt{\frac{(i\pi)^{n-1}}{\det a}} \tag{20.55}$$

in which the quadratic form $a_{jk}x_jx_k$ is

$$\frac{nm}{\hbar T}\sum_{j=1}^{n}\left[-x_jx_{j-1}+\frac{1}{2}(x_j^2+x_{j-1}^2)-\frac{(\omega T)^2}{2n^2}x_j^2\right] \tag{20.56}$$

which has no linear term because $x_0 = x_n = 0$.

The $(n-1)$-dimensional square matrix a is a tridiagonal Toeplitz matrix

$$a = \frac{nm}{2\hbar T}\begin{pmatrix} y & -1 & 0 & 0 & \cdots \\ -1 & y & -1 & 0 & \cdots \\ 0 & -1 & y & -1 & \cdots \\ 0 & 0 & -1 & y & \cdots \\ \vdots & \vdots & \vdots & \ddots & \ddots \end{pmatrix}. \tag{20.57}$$

Apart from the factor $nm/(2\hbar T)$, the matrix $a = (nm/(2\hbar T))\, C_{n-1}(y)$ is a tridiagonal matrix $C_{n-1}(y)$ whose off-diagonal elements are -1 and whose diagonal elements are $y = 2-(\omega T)^2/n^2$. Their determinants $|C_n(y)| = \det C_n(y)$ obey (exercise 20.9) the recursion relation

$$|C_{n+1}(y)| = y\,|C_n(y)| - |C_{n-1}(y)| \tag{20.58}$$

and have the initial values $|C_1(y)| = y$ and $|C_2(y)| = y^2-1$. The trigonometric functions $S_n(y) = \sin[(n+1)\theta]/\sin\theta$ with $y = 2\cos\theta$ obey the same recursion relation and have the same initial values (exercise 20.10), so

$$|C_n(y)| = \frac{\sin(n+1)\theta}{\sin\theta}. \tag{20.59}$$

Since for large n

$$\theta = \arccos(y/2) = \arccos\left(1-\frac{\omega^2t^2}{2n^2}\right) \approx \frac{\omega T}{n}, \tag{20.60}$$

the determinant of the matrix a is

$$\begin{aligned}\det a &= \left(\frac{nm}{2\hbar T}\right)^{n-1}|C_{n-1}(y)| = \left(\frac{nm}{2\hbar T}\right)^{n-1}\frac{\sin n\theta}{\sin\theta}\\ &\approx \left(\frac{nm}{2\hbar T}\right)^{n-1}\frac{\sin(\omega T)}{\sin(\omega T/n)} \approx \left(\frac{nm}{2\hbar T}\right)^{n-1}\frac{n\sin\omega T}{\omega T}.\end{aligned} \tag{20.61}$$

Thus the factor f is

$$\begin{aligned}f &= \left[\frac{mn}{2\pi i\hbar T}\right]^{n/2}\sqrt{\frac{(i\pi)^{n-1}}{\det a}} = \left[\frac{mn}{2\pi i\hbar T}\right]^{n/2}\sqrt{\left(\frac{2\pi i\hbar T}{nm}\right)^{n-1}\frac{\omega T}{n\sin\omega T}}\\ &= \sqrt{\frac{m\omega}{2\pi i\hbar\sin\omega T}}.\end{aligned} \tag{20.62}$$

$\square$

As these examples (20.1 & 20.5) suggest, path integrals are well defined.

20.5 Path integrals in statistical mechanics

At the imaginary time $t = -i\hbar\beta = -i\hbar/(kT)$, the time-evolution operator $e^{-itH/\hbar}$ becomes the **Boltzmann operator** $e^{-\beta H}$ whose trace is the **partition function** $Z(\beta)$ at inverse energy $\beta = 1/(kT)$

$$Z(\beta) = \mathrm{Tr}\big(e^{-\beta H}\big) = \sum_n \langle n|e^{-\beta H}|n\rangle \tag{20.63}$$

in which the states $|n\rangle$ form a complete orthonormal set, $k = 8.617 \times 10^{-5}$ eV/K is Boltzmann's constant, and T is the absolute temperature. Partition functions are used in statistical mechanics and quantum field theory.

Since the Boltzmann operator $e^{-\beta H}$ is the time-evolution operator $e^{-itH/\hbar}$ at the imaginary time $t = -i\hbar\beta$, we can write it as a path integral by imitating the derivation of the preceding section (20.3). We will use the same hamiltonian $H = p^2/(2m) + V(q)$ and the operators q and p which have complete sets of eigenstates (20.9) that satisfy (20.10).

Changing our definitions of ϵ, k, and v to $\epsilon = \beta/n$, $k = \beta p^2/(2m)$, and $v = \beta V(q)$, we can write Trotter's formula (20.7) for the Boltzmann operator as the $n \to \infty$ limit of n factors of $e^{-\epsilon k}\, e^{-\epsilon v}$

$$e^{-\beta H} = e^{-\epsilon k}\, e^{-\epsilon v}\; e^{-\epsilon k}\, e^{-\epsilon v} \cdots e^{-\epsilon k}\, e^{-\epsilon v}\; e^{-\epsilon k}\, e^{-\epsilon v}. \tag{20.64}$$

To evaluate the matrix element $\langle q_1|e^{-\epsilon k}\, e^{-\epsilon v}|q_a\rangle$, we insert the identity operator $\langle q_1|e^{-\epsilon k}\, I\, e^{-\epsilon v}|q_a\rangle$ as an integral (20.10) over outer products $|p'\rangle\langle p'|$ of momentum eigenstates and use the inner products $\langle q_1|p'\rangle = e^{iq_1p'/\hbar}/\sqrt{2\pi\hbar}$ and $\langle p'|q_a\rangle = e^{-iq_ap'/\hbar}/\sqrt{2\pi\hbar}$

$$\begin{aligned}\langle q_1|e^{-\epsilon k}\, e^{-\epsilon v}|q_a\rangle &= \int_{-\infty}^{\infty} \langle q_1|e^{-\epsilon p^2/(2m)}|p'\rangle\langle p'|e^{-\epsilon V(q)}|q_a\rangle\, dp' \\ &= e^{-\epsilon V(q_a)} \int_{-\infty}^{\infty} e^{-\epsilon p'^2/(2m)}\; e^{ip'(q_1-q_a)/\hbar}\, \frac{dp'}{2\pi\hbar}.\end{aligned} \tag{20.65}$$

If we adopt the suggestive notation $q_1 - q_a = \epsilon\hbar\,\dot{q}_a$ and use the gaussian integral (20.2) with $a = \epsilon/(2m)$, $x = p$, and $b = \epsilon\dot{q}/2$

$$\int_{-\infty}^{\infty} \exp\left(-\epsilon\,\frac{p^2}{2m} + i\epsilon\,\dot{q}\,p\right)\frac{dp}{2\pi\hbar} = \sqrt{\frac{m}{2\pi\epsilon\hbar^2}}\; \exp\left(-\epsilon\,\frac{m\dot{q}^2}{2}\right), \tag{20.66}$$

then we find

$$\langle q_1|e^{-\epsilon k}\, e^{-\epsilon v}|q_a\rangle = e^{-\epsilon\, V(q_a)} \int_{-\infty}^{\infty} \exp\left(-\epsilon\, \frac{p'^2}{2m} + i\, \epsilon\, p'\, \dot{q}_a\right) \frac{dp'}{2\pi\hbar}$$
$$= \left(\frac{m}{2\pi\hbar^2\epsilon}\right)^{1/2} \exp\left[-\epsilon\left(\frac{m\,\dot{q}_a^2}{2} + V(q_a)\right)\right] \quad (20.67)$$

in which q_1 is hidden in the formula $q_1 - q_a = \hbar\,\epsilon\,\dot{q}_a$.

The next step is to link two of these matrix elements together

$$\langle q_2|\left(e^{-\epsilon k}\, e^{-\epsilon v}\right)^2|q_a\rangle = \int_{-\infty}^{\infty} \langle q_2|e^{-\epsilon k}\, e^{-\epsilon v}|q_1\rangle\langle q_1|e^{-\epsilon k}\, e^{-\epsilon v}|q_a\rangle dq_1$$
$$= \frac{m}{2\pi\hbar^2\epsilon}\int_{-\infty}^{\infty} \exp\left\{-\epsilon\left[\frac{m\dot{q}_1^2}{2} + V(q_1) + \frac{m\dot{q}_0^2}{2} + V(q_a)\right]\right\} dq_1.$$

Passing from 2 to n and suppressing some integral signs, we get

$$\langle q_b|e^{-n\epsilon H}|q_a\rangle = \iiint_{-\infty}^{\infty} \langle q_b|e^{-\epsilon k}\, e^{-\epsilon v}|q_{n-1}\rangle \cdots \langle q_1|e^{-\epsilon k}\, e^{-\epsilon v}|q_a\rangle\, dq_{n-1}\ldots dq_1$$
$$= \left(\frac{m}{2\pi\hbar^2\epsilon}\right)^{n/2} \iiint_{-\infty}^{\infty} \exp\left[-\epsilon\sum_{j=0}^{n-1}\left(\frac{m\,\dot{q}_j^2}{2} + V(q_j)\right)\right] dq_{n-1}\ldots dq_1.$$

Setting $du = \hbar\epsilon = \hbar\beta/n$ and taking the limit $n \to \infty$, we find that the matrix element $\langle q_b|e^{-\beta H}|q_a\rangle$ is the path integral

$$\langle q_b|e^{-\beta H}|q_a\rangle = \int e^{-S_e[q]/\hbar}\, Dq \quad (20.68)$$

in which each path is weighted by its euclidian action

$$S_e[q] = \int_0^{\hbar\beta} \frac{m\dot{q}^2(u)}{2} + V(q(u))\ du, \quad (20.69)$$

$\dot{q}$ is the derivative of the coordinate $q(u)$ with respect to euclidian time $u = \hbar\beta$, and $Dq \equiv (n\, m/2\pi\, \hbar^2\beta)^{n/2}\, dq_{n-1}\ldots dq_1$.

A derivation identical to the one that led from (20.64) to (20.69) leads to

$$\langle q_b|e^{-(\beta_b-\beta_a)H}|q_a\rangle = \int e^{-S_e[q]/\hbar}\, Dq \quad (20.70)$$

in which each path is weighted by its euclidian action

$$S_e[q] = \int_{\hbar\beta_a}^{\hbar\beta_b} \frac{m\dot{q}^2(u)}{2} + V(q(u))\, du, \quad (20.71)$$

and $\dot{q}$ and Dq are the same as in (20.69).

If we multiply the path integral (20.70) from the left by $|q_b\rangle$ and from the right by $\langle q_a|$ and integrate over q_a and q_b as in the resolution (20.10) of the identity operator, then we can write the Boltzmann operator as an integral over all paths from t_a to t_b

$$e^{-(\beta_b-\beta_a)\,H} = \int |q_b\rangle\, e^{-S_e[q]/\hbar}\,\langle q_a|\, Dq\, dq_a\, dq_b \tag{20.72}$$

with $Dq = (mn/(2\pi i\hbar(t_b-t_a)))^{n/2}\, dq_{n-1}\ldots dq_1$ and $S_e[q]$ the action (20.71).

To get the partition function $Z(\beta)$, we set $q_b = q_a \equiv q_n$ and integrate over all n q's letting $n \to \infty$

$$\begin{aligned} Z(\beta) = \operatorname{Tr} e^{-\beta H} &= \int \langle q_n|e^{-\beta H}|q_n\rangle\, dq_n \\ &= \int \exp\left[-\frac{1}{\hbar}\int_0^{\hbar\beta} \frac{m\dot{q}^2(u)}{2} + V(q(u))\; du\right] Dq \end{aligned} \tag{20.73}$$

where $Dq \equiv (n\,m/2\pi\,\hbar^2\,\beta)^{n/2}\,dq_n\ldots dq_1$. We sum over all loops $q(u)$ that go from $q(0) = q_n$ at Boltzmann time 0 to $q(\hbar\beta) = q_n$ at Boltzmann time $\hbar\beta$.

In the low-temperature limit, $T \to 0$ and $\beta \to \infty$, the Boltzmann operator $\exp(-\beta H)$ projects out the ground state $|E_0\rangle$ of the system

$$\lim_{\beta\to\infty} e^{-\beta H} = \lim_{\beta\to\infty} \sum_n e^{-\beta E_n}|E_n\rangle\langle E_n| = e^{-\beta E_0}|E_0\rangle\langle E_0|. \tag{20.74}$$

The maximum-entropy **density operator** (section 1.40, example 1.64) is the Boltzmann operator $e^{-\beta H}$ divided by its trace $Z(\beta)$

$$\rho = \frac{e^{-\beta H}}{\operatorname{Tr}(e^{-\beta H})} = \frac{e^{-\beta H}}{Z(\beta)}. \tag{20.75}$$

Its matrix elements are matrix elements of the Boltzmann operator (20.69) divided by the partition function (20.73)

$$\langle q_b|\rho|q_a\rangle = \frac{\langle q_b|e^{-\beta H}|q_a\rangle}{Z(\beta)}. \tag{20.76}$$

For many particles $\{\boldsymbol{q}\}$ in three dimensions with $\dot{\boldsymbol{q}}_j(u) = d\boldsymbol{q}_j(u)/du$, the $\{\boldsymbol{q}_a\}, \{\boldsymbol{q}_b\}$ matrix element of the Boltzmann operator is the analog of equation (20.69) (exercise 20.36)

$$\langle\{\boldsymbol{q}_b\}|e^{-\beta H}|\{\boldsymbol{q}_a\}\rangle = \int \exp\left[-\frac{1}{\hbar}\int_0^{\hbar\beta} \frac{m\dot{\boldsymbol{q}}_j^2(u)}{2} + V(\{\boldsymbol{q}\}(u))\; du\right] D\{\boldsymbol{q}\} \tag{20.77}$$

where $D\{q\} \equiv (n\,m/2\pi\,\hbar^2\beta)^{3n/2}\,d\{\boldsymbol{q}\}_{n-1}\ldots d\{\boldsymbol{q}_1\}$, and the partition function is the integral over all loops that go from $\{q\}_0$ to anywhere and back to $\{q\}_0$ in time $\hbar\beta$

$$Z(\beta) = \int \exp\left[-\frac{1}{\hbar}\int_0^{\hbar\beta} \frac{m\dot{\boldsymbol{q}}_j^2(u)}{2} + V(\{\boldsymbol{q}\}(u))\, du\right] D\{\boldsymbol{q}\} \tag{20.78}$$

where now $D\{\boldsymbol{q}\} \equiv (n\, m/2\pi\, \hbar^2\, \beta)^{3n/2}\, d\{\boldsymbol{q}\}_n \ldots d\{\boldsymbol{q}\}_1$.

Because the Boltzmann operator $e^{-\beta H}$ is the time-evolution operator $e^{-itH/\hbar}$ at time $\hbar\beta$ and imaginary time $t = -iu = -i\hbar\beta = -i\hbar/(kT)$, the path integrals of statistical mechanics are called **euclidian path integrals**.

Example 20.7 (Density operator for a free particle) For a free particle, the matrix element of the Boltzmann operator $e^{-\beta H}$ is the $n = \beta/\epsilon \to \infty$ limit of the integral of n factors of the integral (20.67) with $V = 0$

$$\begin{aligned}\langle q_b|e^{-\beta H}|q_a\rangle = &\left(\frac{m}{2\pi\hbar^2\epsilon}\right)^{n/2}\\ &\times\int \exp\left[-\frac{m(q_b-q_{n-1})^2}{2\hbar^2\epsilon}\cdots - \frac{(q_1-q_a)^2}{2\hbar^2\epsilon}\right] dq_{n-1}\cdots dq_1.\end{aligned}$$

The formula (20.2) gives for the q_1 integral

$$\left(\frac{m}{2\pi\hbar^2\epsilon}\right)^{1/2}\int e^{-[m(q_2-q_1)^2+m(q_1-q_a)^2]/(2\hbar^2\epsilon)}dq_1 = \frac{e^{-m(q_2-q_a)^2/(2\hbar^2 2\epsilon)}}{\sqrt{2}}.$$

The q_2 integral is (exercise 20.11)

$$\left(\frac{m}{4\pi\hbar^2\epsilon}\right)^{1/2}\int e^{-m(q_3-q_2)^2/(2\hbar^2\epsilon)-m(q_2-q_a)^2/(4\hbar^2\epsilon)}dq_2 = \frac{e^{-m(q_3-q_a)^2/(2\hbar^2 3\epsilon)}}{\sqrt{3}}. \tag{20.79}$$

All $n-1$ integrations give

$$\langle q_b|e^{-\beta H}|q_a\rangle = \sqrt{\frac{m}{2\pi\hbar^2\epsilon}}\,\frac{e^{-m(q_b-q_a)^2/(2\hbar^2 n\epsilon)}}{\sqrt{n}} = \sqrt{\frac{m}{2\pi\hbar^2\beta}}\,e^{-m(q_b-q_a)^2/(2\hbar^2\beta)}.$$

The partition function is the integral of this matrix element over $q_a = q_b$

$$Z(\beta) = \left(\frac{m}{2\pi\hbar^2\beta}\right)^{1/2}\int dq_a = \left(\frac{m}{2\pi\hbar^2\beta}\right)^{1/2} L \tag{20.80}$$

where L is the (infinite) 1-dimensional volume of the system. The q_b, q_a matrix element of the maximum-entropy density operator is

$$\langle q_b|\rho|q_a\rangle = \frac{e^{-m(\boldsymbol{q}_b-\boldsymbol{q}_a)^2/(2\hbar^2\beta)}}{L}. \tag{20.81}$$

For N particles in 3 dimensions, equations (20.7 and 20.80) are

$$\begin{aligned} \langle \{\boldsymbol{q}\}_b | e^{-\beta H} | \{\boldsymbol{q}\}_a \rangle &= \left(\frac{mkT}{2\pi\hbar^2} \right)^{3N/2} e^{-m(\boldsymbol{q}_{jb} - \boldsymbol{q}_{ja})^2/(2\hbar^2\beta)} \\ Z(\beta) &= \left(\frac{mkT}{2\pi\hbar^2} \right)^{3N/2} L^{3N}. \end{aligned} \tag{20.82}$$

□

Example 20.8 (Partition function at high temperatures) At high temperatures, the product $\hbar\beta = \hbar/(kT)$ is very small, and the particles are essentially free. So the path integral reduces to the product of the free-particle partition function (20.82) with L^{3N} replaced by an integral of $\langle \{\boldsymbol{q}\}_0 | e^{-\beta V/\hbar} | \{\boldsymbol{q}\}_0 \rangle$

$$\begin{aligned} Z(\beta) &= \int e^{-\beta V(\{\boldsymbol{q}\}_0)} \exp\left[-\frac{1}{\hbar} \int_0^{\hbar\beta} \frac{m\dot{\boldsymbol{q}}_j^2(u)}{2}\, du \right] D\{\boldsymbol{q}\} \qquad (20.83) \\ &= \left(\frac{mkT}{2\pi\hbar^2} \right)^{3N/2} \int e^{-\beta V(\{q\}_0)}\, d\{\boldsymbol{q}\}_0. \end{aligned}$$

□

20.6 Boltzmann path integrals for quadratic actions

Apart from the factor $Dq \equiv (n\, m/2\pi\, \hbar^2 \beta)^{n/2}\, dq_{n-1} \ldots dq_1$, the euclidian path integral

$$\langle q_b | e^{-\beta H} | q_a \rangle = \int \exp\left[-\frac{1}{\hbar} \int_0^{\hbar\beta} \frac{m\dot{q}^2(u)}{2} + V(q(u))\, du \right] Dq \tag{20.84}$$

is a sum of positive terms $e^{-S_e[q]/\hbar}$ one for each path from $q_a, 0$ to q_b, β. If a path from $q_a, 0$ to q_b, β obeys the euclidian classical equation of motion

$$m\, \frac{d^2 q_{ec}}{du^2} = m\, \ddot{q}_{ec} = V'(q_{ec}) \tag{20.85}$$

then its euclidian action

$$S_e[q] = \int_0^{\hbar\beta} \frac{m\, \dot{q}^2(u)}{2} + V(u)\, du \tag{20.86}$$

is stationary and may be minimal. So we can approximate the euclidian action $S_e[q_{ec} + x]$ as we approximated the action $S[q_c + x]$ in section 20.4. The euclidian action $S_e[q_{ec} + x]$ of an arbitrary path from $q_a, 0$ to q_b, β is the stationary euclidian action $S_e[q_{ec}]$ plus a u-integral of quadratic and higher powers of the detour x which goes from $x(0) = 0$ to $x(\hbar\beta) = 0$

$$
\begin{aligned}
S_e[q_{ec} + x] = & \int_0^{\hbar\beta} \left[\frac{m}{2}\dot{q}_{ec}^2 + V(q_{ec})\right] du + \int_0^{\hbar\beta} \left[\frac{m}{2}\dot{x}^2 + \frac{V''(q_{ec})}{2}x^2 \right. \\
& \left. + \frac{V'''(q_{ec})}{6}\, x^3 + \frac{V''''(q_{ec})}{24}\, x^4 + \dots \right] du \\
= & \, S_e[q_{ec}] + \Delta S_e[q_{ec}, x],
\end{aligned}
\tag{20.87}
$$

and the path integral for the matrix element $\langle q_b | e^{-\beta H} | q_a \rangle$ is

$$
\langle q_b | e^{-\beta H} | q_a \rangle = e^{-S_e[q_{ec}]/\hbar} \int e^{-\Delta S_e[q_{ec}, x]/\hbar} Dx \tag{20.88}
$$

as $n \to \infty$ where $Dx = (n\, m/2\pi\, \hbar^2 \beta)^{n/2}\, dq_{n-1} \dots dq_1$ in the limit $n \to \infty$.

If the action is quadratic in q and $\dot{q}$, then the action $\Delta S_e[q_{ec}, x]$ of the detour x is independent of the euclidian classical path q_{ec}, and so the path integral over x is a function f only of the parameters β, m, $\hbar$, and V''

$$
\langle q_b | e^{-\beta H} | q_a \rangle = e^{-S_e[q_{ec}]/\hbar} \int e^{-\Delta S_e[x]/\hbar} Dx = f(\beta, \hbar, m, V'')\; e^{-S_e[q_{ec}]/\hbar} \tag{20.89}
$$

in which with $x_n = 0 = x_0$ the function f is

$$
\begin{aligned}
f(\beta, \hbar, m, V'') &= \left[\frac{mn}{2\pi\hbar^2\beta}\right]^{n/2} \int e^{-\Delta S_e[x]/\hbar} dx_{n-1} \dots dx_1, \\
\Delta S_e[x] &= \frac{\hbar\beta}{n} \sum_{j=1}^{n} \frac{m}{2\hbar^2} \frac{(x_j - x_{j-1})^2}{(\beta/n)^2} + \frac{1}{2} V''\, x_j^2.
\end{aligned}
\tag{20.90}
$$

Example 20.9 (Density operator for the harmonic oscillator) The path $q_{ec}(\beta)$ that satisfies the euclidian classical equation of motion (20.85)

$$
\ddot{q}_{ec}(u) = \frac{d^2 q_{ec}(u)}{du^2} = \omega^2 q_{ec}(u) \tag{20.91}
$$

and goes from $q_a, 0$ to $q_b, \hbar\beta$ is

$$
q_{ec}(u) = \frac{\sinh(\omega u)\, q_b + \sinh[\omega(\hbar\beta - u)]\, q_a}{\sinh(\hbar\omega\beta)}. \tag{20.92}
$$

Its euclidian action is (exercise 20.20)

$$
\begin{aligned}
S_e[q_{ec}] &= \int_0^{\hbar\beta} \frac{m\dot{q}_{ec}^2(u)}{2} + \frac{m\omega^2 q_{ec}^2(u))}{2}\, du \\
&= \frac{m\omega}{2\hbar\sinh(\hbar\omega\beta)} \left[\cosh(\hbar\omega\beta)(q_a^2 + q_b^2) - 2q_a q_b\right].
\end{aligned}
\tag{20.93}
$$

Since $V'' = m\omega^2$, our formulas (20.89 & 20.90) for quadratic actions give as the matrix element

$$
\langle q_b | e^{-\beta H} | q_a \rangle = f(\beta, \hbar, m, m\omega^2)\; e^{-S_e[q_{ec}]/\hbar}
\tag{20.94}
$$

in which

$$
\begin{aligned}
f(\beta, \hbar, m, m\omega^2) &= \left[\frac{mn}{2\pi\hbar^2\beta}\right]^{n/2} \int e^{-\Delta S_e[x]/\hbar)}\, dx_{n-1} \dots dx_1, \\
\Delta S_e[x] &= \frac{\hbar\beta}{n} \sum_{j=1}^{n} \frac{m}{2\hbar^2} \frac{(x_j - x_{j-1})^2}{(\beta/n)^2} + \frac{m\omega^2\, x_j^2}{2},
\end{aligned}
\tag{20.95}
$$

and $x_n = 0 = x_0$. We can do this integral by using the formula (20.4) for a many variable real gaussian integral

$$
f = \left[\frac{mn}{2\pi\hbar^2 B}\right]^{n/2} \int e^{-a_{jk}x_j x_k} dx_{n-1} \dots dx_1 = \left[\frac{mn}{2\pi\hbar^2 B}\right]^{n/2} \sqrt{\frac{(\pi)^{n-1}}{\det a}}
\tag{20.96}
$$

in which the positive quadratic form $a_{jk}x_j x_k$ is

$$
\frac{nm}{2\hbar^2 B} \sum_{j=1}^{n} \left[-2x_j x_{j-1} + x_j^2 + x_{j-1}^2 + \frac{(\hbar\omega B)^2}{n^2} x_j^2 \right]
\tag{20.97}
$$

which has no linear term because $x_0 = x_n = 0$.

The matrix a is $(nm/(2\hbar^2 B))\, C_{n-1}(y)$ in which $C_{n-1}(y)$ is a square, tridiagonal, $(n-1)$-dimensional matrix whose off-diagonal elements are -1 and whose diagonal elements are $y = 2 + (\hbar\omega\beta)^2/n^2$. The determinants $|C_n(y)|$ obey the recursion relation $|C_{n+1}(y)| = y\,|C_n(y)| - |C_{n-1}(y)|$ and have the initial values $C_1(y) = y$ and $C_2(y) = y^2 - 1$. So do the hyperbolic functions $\sinh(n+1)\theta/\sinh\theta$ with $y = 2\cosh\theta$. So we set $C_n(y) = \sinh(n+1)\theta/\sinh\theta$ with $\theta = \operatorname{arccosh}(y/2)$. We then get as the matrix element (20.94)

$$
\langle q_b | e^{-\beta H} | q_a \rangle = \sqrt{\frac{m\omega}{2\pi\hbar\sinh(\hbar\omega\beta)}} \exp\left[-\frac{m\omega[\cosh(\hbar\omega\beta)(q_a^2 + q_b^2) - 2q_a q_b]}{2\hbar\sinh(\hbar\omega\beta)} \right].
\tag{20.98}
$$

The partition function is the integral over q_a of this matrix element for

$q_b = q_a$

$$Z(\beta) = \sqrt{\frac{m\omega}{2\pi\hbar \sinh(\hbar\omega\beta)}} \int \exp\left[- \frac{m\omega[\cosh(\hbar\omega\beta) - 1]q_a^2}{\hbar \sinh(\hbar\omega\beta)}\right] dq_a$$
$$= \frac{1}{\sqrt{2[\cosh(\hbar\omega\beta) - 1]}}. \tag{20.99}$$

The matrix elements of the maximum-entropy density operator (20.75) are

$$\langle q_b|\rho|q_a\rangle = \frac{\langle q_b|e^{-\beta H}|q_a\rangle}{Z(\beta)} \tag{20.100}$$
$$= \sqrt{\frac{m\omega[\cosh(\hbar\omega\beta) - 1]}{\pi\hbar \sinh(\hbar\omega\beta)}} \exp\left[- \frac{m\omega[\cosh(\hbar\omega\beta)(q_a^2 + q_b^2) - 2q_a q_b]}{2\hbar \sinh(\hbar\omega\beta)}\right]$$

which reveals the ground-state wave functions

$$\lim_{\beta\to\infty} \langle q_b|\rho|q_a\rangle = \langle q_b|0\rangle\langle 0|q_a\rangle = \sqrt{\frac{m\omega}{\pi\hbar}}\; e^{-m\omega(q_a^2+q_b^2)/(2\hbar)}. \tag{20.101}$$

The partition function gives us the ground-state energy

$$\lim_{\beta\to\infty} Z(\beta) = \lim_{\beta\to\infty} \frac{1}{\sqrt{2[\cosh(\hbar\omega\beta) - 1]}} = e^{-\beta E_0} = e^{-\beta\hbar\omega/2}. \tag{20.102}$$

□

20.7 Mean values of time-ordered products

In the Heisenberg picture, the position operator at time t is

$$q(t) = e^{itH/\hbar} q\, e^{-itH/\hbar} \tag{20.103}$$

in which $q = q(0)$ is the position operator at time $t = 0$ or equivalently the position operator in the Schrödinger picture. The time-ordered product of two position operators is

$$\mathcal{T}[q(t_1)q(t_2)] = \left\{ \begin{array}{ll} q(t_1)\, q(t_2) & \text{if } t_1 \ge t_2 \\ q(t_2)\, q(t_1) & \text{if } t_2 \ge t_1 \end{array} \right\} = q(t_>)\, q(t_<) \tag{20.104}$$

in which $t_>$ is the later and $t_<$ the earlier of the two times t_1 and t_2.

The position operator q at the imaginary time $t = -iu = -i\hbar\beta = -i\hbar/(kT)$ is the euclidian position operator

$$q_e(u) = q_e(\hbar\beta) = e^{uH/\hbar} q\, e^{-uH/\hbar}. \tag{20.105}$$

The time-ordered product of two euclidian position operators at euclidian times $u_1 = \hbar\beta_1$ and $u_2 = \hbar\beta_2$ is

$$\mathcal{T}[q_e(u_1)q_e(u_2)] = \left\{ \begin{array}{ll} q_e(u_1)\, q_e(u_2) & \text{if } u_1 \geq u_2 \\ q_e(u_2)\, q_e(u_1) & \text{if } u_2 \geq u_1 \end{array} \right\} = q_e(u_>)\, q_e(u_<). \tag{20.106}$$

The matrix element of the time-ordered product (20.104) of two position operators and two exponentials $e^{-itH/\hbar}$ between states $|a\rangle$ and $|b\rangle$ is

$$\begin{aligned} \langle b|e^{-itH/\hbar}\mathcal{T}[q(t_1)q(t_2)]e^{-itH/\hbar}|a\rangle &= \langle b|e^{-itH/\hbar}q(t_>)q(t_<)e^{-itH/\hbar}|a\rangle \quad (20.107) \\ &= \langle b|e^{-i(t-t_>)H/\hbar}q\, e^{-i(t_>-t_<)H/\hbar}q\, e^{-i(t+t_<)H/\hbar}|a\rangle. \end{aligned}$$

Using the path-integral formula (20.20) for each of the exponentials on the right-hand side of this equation, we find (exercise 20.13)

$$\langle b|e^{-itH/\hbar}\mathcal{T}[q(t_1)q(t_2)]e^{-itH/\hbar}|a\rangle = \int \langle b|q_b\rangle q(t_1)q(t_2)e^{iS[q]/\hbar}\langle q_a|a\rangle Dq \tag{20.108}$$

in which the integral is over all paths that run from $-t$ to t. This equation is simpler when the states $|a\rangle$ and $|b\rangle$ are eigenstates of H with eigenvalues E_m and E_n

$$e^{-it(E_n+E_m)/\hbar}\langle n|\mathcal{T}[q(t_1)q(t_2)]|m\rangle = \int \langle n|q_b\rangle q(t_1)q(t_2)e^{iS[q]/\hbar}\langle q_a|m\rangle Dq. \tag{20.109}$$

By setting $n = m$ and omitting $q(t_1)q(t_2)$, we get

$$e^{-2itE_n/\hbar} = \int \langle n|q_b\rangle e^{iS[q]/\hbar}\langle q_a|n\rangle Dq. \tag{20.110}$$

The ratio of (20.109) with $n = m$ to (20.110) is

$$\langle n|\mathcal{T}[q(t_1)q(t_2)]|n\rangle = \frac{\int \langle n|q_b\rangle q(t_1)q(t_2)e^{iS[q]/\hbar}\langle q_a|n\rangle\, Dq}{\int \langle n|q_b\rangle e^{iS[q]/\hbar}\langle q_a|n\rangle\, Dq} \tag{20.111}$$

in which the integrations are over all paths that go from $-t \leq t_2$ to $t \geq t_1$. The mean value of the time-ordered product of k position operators is

$$\langle n|\mathcal{T}[q(t_1)\cdots q(t_k)]|n\rangle = \frac{\int \langle n|q_b\rangle q(t_1)\cdots q(t_k)e^{iS[q]/\hbar}\langle q_a|n\rangle\, Dq}{\int \langle n|q_b\rangle e^{iS[q]/\hbar}\langle q_a|n\rangle\, Dq} \tag{20.112}$$

in which the integrations are over all paths that go from some time before $t_1, \ldots, t_k$ to some time after them.

We may perform the same operations on the euclidian position operators by replacing t by $-iu = -i\hbar\beta$. A matrix element of the euclidian time-ordered product (20.106) between two states is

$$\begin{aligned} \langle b|e^{-uH/\hbar}\mathcal{T}[q_e(u_1)q_e(u_2)]e^{-uH/\hbar}|a\rangle &= \langle b|e^{-uH/\hbar}q_e(u_>)q_e(u_<)e^{-uH/\hbar}|a\rangle \\ &= \langle b|e^{-(u-u_>)H/\hbar}q\, e^{-(u_>-u_<)H/\hbar}q\, e^{-(u+u_<)H/\hbar}|a\rangle. \end{aligned} \tag{20.113}$$

As $u \to \infty$, the exponential $e^{-uH/\hbar}$ projects (20.74) states in onto the ground state $|0\rangle$ which is an eigenstate of H with energy E_0. So we replace the arbitrary states in (20.113) with the ground state and use the path-integral formula (20.72) for the last three exponentials of (20.113)

$$e^{-2uE_0/\hbar}\langle 0|\mathcal{T}[q_e(u_1)q_e(u_2)]|0\rangle = \int \langle 0|q_b\rangle q(u_1)q(u_2)e^{-S_e[q]/\hbar}\langle q_a|0\rangle Dq. \tag{20.114}$$

The same equation without the time-ordered product is

$$e^{-2uE_0/\hbar}\langle 0|0\rangle = e^{-2uE_0/\hbar} = \int \langle 0|q_b\rangle e^{-S_e[q]/\hbar}\langle q_a|0\rangle Dq. \tag{20.115}$$

The ratio of the last two equations is

$$\langle 0|\mathcal{T}[q_e(u_1)q_e(u_2)]|0\rangle = \frac{\displaystyle\int \langle 0|q_b\rangle q(u_1)q(u_2)e^{-S_e[q]/\hbar}\langle q_a|0\rangle Dq}{\displaystyle\int \langle 0|q_b\rangle e^{-S_e[q]/\hbar}\langle q_a|0\rangle Dq} \tag{20.116}$$

in which the integration is over all paths from $u = -\infty$ to $u = \infty$. The mean value in the ground state of the time-ordered product of k euclidian position operators is

$$\langle 0|\mathcal{T}[q_e(u_1)\cdots q_e(u_k)]|0\rangle = \frac{\displaystyle\int \langle 0|q_b\rangle\, q(u_1)\cdots q(u_k)\, e^{-S_e[q]/\hbar}\langle q_a|0\rangle Dq}{\displaystyle\int \langle 0|q_b\rangle e^{-S_e[q]/\hbar}\langle q_a|0\rangle Dq}. \tag{20.117}$$

20.8 Quantum field theory on a lattice

Quantum mechanics imposes upon n coordinates q_i and conjugate momenta p_k the equal-time commutation relations

$$[q_i, p_k] = i\,\hbar\,\delta_{i,k} \quad \text{and} \quad [q_i, q_k] = [p_i, p_k] = 0. \tag{20.118}$$

In a theory of a single spinless quantum field, a coordinate $q_{\boldsymbol{x}} \equiv \phi(\boldsymbol{x})$ and a conjugate momentum $p_{\boldsymbol{x}} \equiv \pi(\boldsymbol{x})$ are associated with each point $\boldsymbol{x}$ of space. The operators $\phi(\boldsymbol{x}, t)$ and $\pi(\boldsymbol{x}, t)$ obey the equal-time commutation relations

$$\begin{aligned} [\phi(\boldsymbol{x}, t), \pi(\boldsymbol{x}', t)] &= i\,\hbar\,\delta(\boldsymbol{x} - \boldsymbol{x}') \\ [\phi(\boldsymbol{x}, t), \phi(\boldsymbol{x}', t)] &= [\pi(\boldsymbol{x}, t), \pi(\boldsymbol{x}', t)] = 0 \end{aligned} \tag{20.119}$$

inherited from quantum mechanics.

To make path integrals, we replace space by a 3-dimensional lattice of points $\boldsymbol{x} = a(i, j, k) = (ai, aj, ak)$ and eventually let the distance a between adjacent points go to zero. On this lattice and at equal times, e.g., $t = 0$, the field operator $\phi(\boldsymbol{x}, t) \equiv \phi(a(i, j, k), t)$ and its conjugate momentum $\pi(\boldsymbol{x}, t) \equiv \pi(a(i, j, k), t)$ obey discrete forms of the commutation relations (20.119)

$$\begin{aligned} [\phi(\boldsymbol{x}), \pi(\boldsymbol{x}')] &= [\phi(a(i, j, k)), \pi(a(\ell, m, n))] = i\,\frac{\hbar}{a^3}\,\delta_{i,\ell}\,\delta_{j,m}\,\delta_{k,n} \\ [\phi(\boldsymbol{x}), \phi(\boldsymbol{x}')] &= [\phi(a(i, j, k)), \phi(a(\ell, m, n))] = 0 \\ [\pi(\boldsymbol{x}), \pi(\boldsymbol{x}')] &= [\pi(a(i, j, k)), \pi(a(\ell, m, n))] = 0. \end{aligned} \tag{20.120}$$

The vanishing commutators imply that the field and the momenta have compatible eigenvalues for all lattice points $\boldsymbol{x} = a(i, j, k)$

$$\phi(\boldsymbol{x})|\phi'\rangle = \phi'(\boldsymbol{x})|\phi'\rangle \;\text{ and }\; \pi(\boldsymbol{x})|\pi'\rangle = \pi'(\boldsymbol{x})|\pi'\rangle. \tag{20.121}$$

Their inner products are

$$\langle\phi'|\pi'\rangle = \left(\prod_{\boldsymbol{x}} \sqrt{\frac{a^3}{2\pi\hbar}}\right) \exp\left[i\frac{a^3}{\hbar}\sum_{\boldsymbol{x}} \phi'(\boldsymbol{x})\pi'(\boldsymbol{x})\right]. \tag{20.122}$$

These states are complete

$$\int |\phi'\rangle\langle\phi'| \prod_{\boldsymbol{x}} d\phi'(\boldsymbol{x}) = I = \int |\pi'\rangle\langle\pi'| \prod_{\boldsymbol{x}} d\pi'(\boldsymbol{x}) \tag{20.123}$$

and orthonormal

$$\langle\phi'|\phi''\rangle = \prod_{\boldsymbol{x}} \delta(\phi'(\boldsymbol{x}) - \phi''(\boldsymbol{x})) \tag{20.124}$$

with a similar equation for $\langle\pi'|\pi''\rangle$.

The hamiltonian for a free field of mass m

$$H = \frac{1}{2} \int \left[\pi^2 + c^2 (\nabla \phi)^2 + \frac{m^2 c^4}{\hbar^2} \phi^2 \right] d^3 x \tag{20.125}$$

is approximated as

$$H = \frac{a^3}{2} \sum_{\boldsymbol{x}} \left[\pi(\boldsymbol{x})^2 + c^2 (\nabla \phi(\boldsymbol{x}))^2 + \frac{m^2 c^4}{\hbar^2} \phi(\boldsymbol{x})^2 \right] \tag{20.126}$$

where $\boldsymbol{x} = a(i,j,k)$, $\pi(\boldsymbol{x}) = \pi(a(i,j,k))$, $\phi(\boldsymbol{x}) = \phi(a(i,j,k))$, and the square of the lattice gradient is

$$\begin{aligned} (\nabla \phi(\boldsymbol{x}))^2 = \frac{1}{a^2} \Big[& (\phi(a(i+1,j,k)) - \phi(a(i,j,k)))^2 \\ & + (\phi(a(i,j+1,k)) - \phi(a(i,j,k)))^2 \\ & + (\phi(a(i,j,k+1)) - \phi(a(i,j,k)))^2 \Big]. \end{aligned} \tag{20.127}$$

Other interactions, such as $c^3 \phi^4/\hbar$, can be added to this hamiltonian.

To simplify the appearance of the equations in the rest of this chapter, I will often use **natural units** (Chapter 23) in which $\hbar = c = 1$. To convert the value of a physical quantity from natural units to universal units, one multiplies or divides its natural-unit value by suitable factors of $\hbar$ and c until one gets the right dimensions.

We set $K = K(\pi) = (a^3/2) \sum_{\boldsymbol{x}} \pi^2(\boldsymbol{x})$ and $V = V(\phi) = (a^3/2) \sum_{\boldsymbol{x}} \big((\nabla \phi(\boldsymbol{x}))^2 + m^2 \phi^2(\boldsymbol{x}) + P(\phi(\boldsymbol{x})) \big)$ in which $P(\phi(\boldsymbol{x}))$ represents the self-interactions of the field. With $\epsilon = (t_b - t_a)/n$, Trotter's product formula (20.6) is the $n \to \infty$ limit of

$$e^{-i(t_b - t_a)(K+V)} = \left(e^{-i(t_b - t_a)K/n} e^{-i(t_b - t_a)V/n} \right)^n = \left(e^{-i\epsilon K} e^{-i\epsilon V} \right)^n . \tag{20.128}$$

We insert I in the form (20.123) between $e^{-i\epsilon K}$ and $e^{-i\epsilon V}$

$$\langle \phi_1 | e^{-i\epsilon K} \, e^{-i\epsilon V} | \phi_a \rangle = \langle \phi_1 | e^{-i\epsilon K} \int |\pi' \rangle \langle \pi' | \prod_{\boldsymbol{x}} d\pi'(\boldsymbol{x}) e^{-i\epsilon V} | \phi_a \rangle \tag{20.129}$$

and use the eigenstate formula (20.121)

$$\langle \phi_1 | e^{-i\epsilon K} \, e^{-i\epsilon V} | \phi_a \rangle = e^{-i\epsilon V(\phi_a)} \int e^{-i\epsilon K(\pi')} \langle \phi_1 | \pi' \rangle \langle \pi' | \phi_a \rangle \prod_{\boldsymbol{x}} d\pi'(\boldsymbol{x}) \tag{20.130}$$

and the inner-product formula (20.122)

$$\langle\phi_1|e^{-i\epsilon K}e^{-i\epsilon V}|\phi_a\rangle \tag{20.131}$$
$$= e^{-i\epsilon V(\phi_a)}\prod_{\boldsymbol{x}}\left[\int \frac{a^3 d\pi'(\boldsymbol{x})}{2\pi} e^{a^3[-i\epsilon\pi'^2(\boldsymbol{x})/2+i(\phi_1(\boldsymbol{x})-\phi_a(\boldsymbol{x}))\pi'(\boldsymbol{x})]}\right].$$

Using the gaussian integral (20.1), we set $\dot{\phi}_a(\boldsymbol{x}) = (\phi_1(\boldsymbol{x}) - \phi_a(\boldsymbol{x}))/\epsilon$ and get

$$\langle\phi_1|e^{-i\epsilon K}e^{-i\epsilon V}|\phi_a\rangle = \prod_{\boldsymbol{x}}\left[\left(\frac{a^3}{2\pi i\epsilon}\right)^{1/2} e^{i\frac{\epsilon a^3}{2}[\dot{\phi}_a^2(\boldsymbol{x})-(\nabla\phi_a(\boldsymbol{x}))^2-m^2\phi_a^2(\boldsymbol{x})-P(\phi_a(\boldsymbol{x}))]}\right]. \tag{20.132}$$

The product of $n = (t_b - t_a)/\epsilon$ such time intervals is

$$\langle\phi_b|e^{-i(t_b-t_a)H}|\phi_a\rangle = \prod_{\boldsymbol{x}}\left[\left(\frac{a^3 n}{2\pi i(t_b-t_a)}\right)^{n/2}\int e^{iS_{\boldsymbol{x}}}D\phi_{\boldsymbol{x}}\right] \tag{20.133}$$

in which

$$S_{\boldsymbol{x}} = \frac{t_b-t_a}{n}\frac{a^3}{2}\sum_{j=0}^{n-1}\left[\dot{\phi}_j^2(\boldsymbol{x}) - (\nabla\phi_j(\boldsymbol{x}))^2 - m^2\phi_j^2(\boldsymbol{x}) - P(\phi_j(\boldsymbol{x}))\right], \tag{20.134}$$

$\dot{\phi}_j(\boldsymbol{x}) = n(\phi_{j+1}(\boldsymbol{x}) - \phi_j(\boldsymbol{x}))/(t_b - t_a)$, and $D\phi_{\boldsymbol{x}} = d\phi_{n-1}(\boldsymbol{x})\cdots d\phi_1(\boldsymbol{x})$.

The amplitude $\langle\phi_b|e^{-i(t_b-t_a)H}|\phi_a\rangle$ is the integral over all fields that go from $\phi_a(\boldsymbol{x})$ at t_a to $\phi_b(\boldsymbol{x})$ at t_b each weighted by an exponential

$$\langle\phi_b|e^{-i(t_b-t_a)H}|\phi_a\rangle = \int e^{iS[\phi]}\,D\phi \tag{20.135}$$

of its action

$$S[\phi] = \int_{t_a}^{t_b} dt \int d^3x\,\frac{1}{2}\left[\dot{\phi}^2 - (\nabla\phi)^2 - m^2\phi^2 - P(\phi)\right] \tag{20.136}$$

in which $D\phi$ is the $n \to \infty$ limit of the product over all spatial vertices $\boldsymbol{x}$

$$D\phi = \prod_{\boldsymbol{x}}\left[\left(\frac{a^3 n}{2\pi i(t_b-t_a)}\right)^{n/2} d\phi_{n-1}(\boldsymbol{x})\cdots d\phi_1(\boldsymbol{x})\right]. \tag{20.137}$$

Equivalently, the time-evolution operator is

$$e^{-i(t_b-t_a)H} = \int |\phi_b\rangle e^{iS[\phi]}\,\langle\phi_a|\,D\phi\,D\phi_a D\phi_b \tag{20.138}$$

in which $D\phi_a D\phi_b = \prod_v d\phi_{a,v} d\phi_{b,v}$ is an integral over the initial and final states.

As in quantum mechanics (section 20.4), the path integral for an action that is quadratic in the fields is an exponential of the action of a classical process $S[\phi_c]$ times a function of the times t_a, t_b and of other parameters

$$\langle \phi_b | e^{-i(t_b - t_a)H} | \phi_a \rangle = \int e^{iS[\phi]} \, D\phi = f(t_a, t_b, \dots) \, e^{iS[\phi_c]} \tag{20.139}$$

in which $S[\phi_c]$ is the action of the process that goes from $\phi(\boldsymbol{x}, t_a) = \phi_a(\boldsymbol{x})$ to $\phi(\boldsymbol{x}, t_b) = \phi_b(\boldsymbol{x})$ and obeys the classical equations of motion, and the function f is a path integral over all fields that go from $\phi(\boldsymbol{x}, t_a) = 0$ to $\phi(\boldsymbol{x}, t_b) = 0$.

Example 20.10 (Classical processes) The field

$$\phi(\boldsymbol{x}, t) = \int e^{i\boldsymbol{k}\cdot\boldsymbol{x}} [a(\boldsymbol{k}) \, \cos\omega t \, + b(\boldsymbol{k}) \, \sin\omega t] \, d^3k \tag{20.140}$$

with $\omega = \sqrt{\boldsymbol{k}^2 + m^2}$ makes the action (20.136) for $P = 0$ stationary because it is a solution of the equation of motion $\nabla^2\phi - \ddot{\phi} - m^2\phi = 0$. In terms of the Fourier transforms

$$\tilde{\phi}(\boldsymbol{k}, t_a) = \int e^{-i\boldsymbol{k}\cdot\boldsymbol{x}} \, \phi(\boldsymbol{x}, t_a) \, \frac{d^3x}{(2\pi)^3} \quad \text{and} \quad \tilde{\phi}(\boldsymbol{k}, t_b) = \int e^{-i\boldsymbol{k}\cdot\boldsymbol{x}} \, \phi(\boldsymbol{x}, t_b) \, \frac{d^3x}{(2\pi)^3}, \tag{20.141}$$

the solution that goes from $\phi(\boldsymbol{x}, t_a)$ to $\phi(\boldsymbol{x}, t_b)$ is

$$\phi(\boldsymbol{x}, t) = \int e^{i\boldsymbol{k}\cdot\boldsymbol{x}} \, \frac{\sin\omega(t_b - t) \, \tilde{\phi}(\boldsymbol{k}, t_a) + \sin\omega(t - t_a) \, \tilde{\phi}(\boldsymbol{k}, t_b)}{\sin\omega(t_b - t_a)} \, d^3k. \tag{20.142}$$

The solution that evolves from $\phi(\boldsymbol{x}, t_a)$ and $\dot{\phi}(\boldsymbol{x}, t_a)$ is

$$\phi(\boldsymbol{x}, t) = \int e^{i\boldsymbol{k}\cdot\boldsymbol{x}} \left[\cos\omega(t - t_a) \, \tilde{\phi}(\boldsymbol{k}, t_a) + \frac{\sin\omega(t - t_a)}{\omega} \, \tilde{\dot{\phi}}(\boldsymbol{k}, t_a) \right] d^3k \tag{20.143}$$

in which the Fourier transform $\tilde{\dot{\phi}}(\boldsymbol{k}, t_a)$ is defined as in (20.141). □

Like a position operator (20.103), a field at time t is defined as

$$\phi(\boldsymbol{x}, t) = e^{itH/\hbar} \phi(\boldsymbol{x}, 0) e^{-itH/\hbar} \tag{20.144}$$

in which $\phi(\boldsymbol{x}) = \phi(\boldsymbol{x}, 0)$ is the field at time zero, which obeys the commutation relations (20.119). The time-ordered product of several fields is their product with newer (later time) fields standing to the left of older (earlier time) fields as in the definition (20.104). The logic (20.107–20.111) of the derivation of the path-formulas for time-ordered products of position operators also applies to field operators. One finds (exercise 20.14) for the mean value of the time-ordered product of two fields in an energy eigenstate $|n\rangle$

$$\langle n|\mathcal{T}[\phi(x_1)\phi(x_2)]|n\rangle = \frac{\displaystyle\int \langle n|\phi_b\rangle \phi(x_1)\phi(x_2) e^{iS[\phi]/\hbar} \langle \phi_a|n\rangle \, D\phi}{\displaystyle\int \langle n|\phi_b\rangle e^{iS[\phi]/\hbar} \langle \phi_a|n\rangle \, D\phi} \tag{20.145}$$

in which the integrations are over all paths that go from before t_1 and t_2 to after both times. The analogous result for several fields is (exercise 20.15)

$$\langle n|\mathcal{T}[\phi(x_1)\cdots\phi(x_k)]|n\rangle = \frac{\displaystyle\int \langle n|\phi_b\rangle \phi(x_1)\cdots\phi(x_k) e^{iS[\phi]/\hbar} \langle \phi_a|n\rangle \, D\phi}{\displaystyle\int \langle n|\phi_b\rangle e^{iS[\phi]/\hbar} \langle \phi_a|n\rangle \, D\phi} \tag{20.146}$$

in which the integrations are over all paths that go from before the times $t_1, \ldots, t_k$ to after them.

20.9 Finite-temperature field theory

Since the Boltzmann operator $e^{-\beta H} = e^{-H/(kT)}$ is the time evolution operator $e^{-itH/\hbar}$ at the imaginary time $t = -i\hbar\beta = -i\hbar/(kT)$, the formulas of finite-temperature field theory are those of quantum field theory with t replaced by $-iu = -i\hbar\beta = -i\hbar/(kT)$.

As in section 20.8, we use as our hamiltonian $H = k + v$ where k and v are sums over all lattice vertices $v = a(i, j, k) = (ai, aj, ak)$ of the cubes of volume a^3 times the squared momentum and the potential energy

$$H = k + v = \frac{a^3}{2}\sum_v \pi_v^2 + \frac{a^3}{2}\sum_v (\nabla\phi_v)^2 + m^2\phi_v^2 + P(\phi_v). \tag{20.147}$$

A matrix element of the first term of the Trotter product formula (20.7)

$$e^{-\beta(k+v)} = \lim_{n\to\infty}\left(e^{-\beta k/n}\, e^{-\beta v/n}\right)^n \tag{20.148}$$

is the imaginary-time version of (20.131) with $\epsilon = \hbar\beta/n$

$$\langle\phi_1|e^{-\epsilon k}\, e^{-\epsilon v}|\phi_a\rangle = e^{-\epsilon v(\phi_a)} \prod_v \left[\int \frac{a^3 d\pi'_v}{2\pi} e^{a^3[-\epsilon\pi_v^2/2 + i(\phi_{1v} - \phi_{av})\pi'_v]}\right]. \tag{20.149}$$

Setting $\dot\phi_{av} = (\phi_{1v} - \phi_{av})/\epsilon$, we find, instead of (20.132)

$$\langle \phi_1 | e^{-\epsilon k} \, e^{-\epsilon v} | \phi_a \rangle = \prod_v \left[\left(\frac{a^3}{2\pi\epsilon} \right)^{1/2} e^{-\epsilon a^3 [\dot\phi_{av}^2 + (\nabla\phi_{av})^2 + m^2 \phi_{av}^2 + P(\phi_v)]/2} \right]. \tag{20.150}$$

The product of $n = \hbar\beta/\epsilon$ such inverse-temperature intervals is

$$\langle \phi_b | e^{-\beta H} | \phi_a \rangle = \prod_v \left[\left(\frac{a^3 n}{2\pi\beta} \right)^{n/2} \int e^{-S_{ev}} D\phi_v \right] \tag{20.151}$$

in which the euclidian action is

$$S_{ev} = \frac{\beta}{n} \frac{a^3}{2} \sum_{j=0}^{n-1} \left[\dot\phi_{jv}^2 + (\nabla\phi_{jv})^2 + m^2 \phi_{jv}^2 + P(\phi_v) \right] \tag{20.152}$$

where $\dot\phi_{jv} = n(\phi_{j+1,v} - \phi_{j,v})/\beta$ and $D\phi_v = d\phi_{n-1,v} \cdots d\phi_{1,v}$.

The amplitude $\langle \phi_b | e^{-(\beta_b - \beta_a)H} | \phi_a \rangle$ is the integral over all fields that go from $\phi_a(\boldsymbol{x})$ at β_a to $\phi_b(\boldsymbol{x})$ at β_b each weighted by an exponential

$$\langle \phi_b | e^{-(\beta_b - \beta_a)H} | \phi_a \rangle = \int e^{-S_e[\phi]} \, D\phi \tag{20.153}$$

of its euclidian action

$$S_e[\phi] = \int_{\beta_a}^{\beta_b} du \int d^3x \, \frac{1}{2} \left[\dot\phi^2 + (\nabla\phi)^2 + m^2\phi^2 + P(\phi) \right] \tag{20.154}$$

in which $D\phi$ is the $n \to \infty$ limit of the product over all spatial vertices v

$$D\phi = \prod_v \left[\left(\frac{a^3 n}{2\pi(\beta_b - \beta_a)} \right)^{n/2} d\phi_{n-1,v} \cdots d\phi_{1,v} \right]. \tag{20.155}$$

Equivalently, the Boltzmann operator is

$$e^{-(\beta_b - \beta_a)H} = \int |\phi_b\rangle e^{-S_e[\phi]} \, \langle \phi_a | \, D\phi \, D\phi_a D\phi_b \tag{20.156}$$

in which $D\phi_a D\phi_b = \prod_v d\phi_{a,v} d\phi_{b,v}$ is an integral over the initial and final states.

The trace of the Boltzmann operator is the partition function

$$Z(\beta) = \mathrm{Tr}(e^{-\beta H}) = \int e^{-S_e[\phi]} \, \langle \phi_a | \phi_b \rangle \, D\phi \, D\phi_a D\phi_b = \int e^{-S_e[\phi]} \; D\phi \, D\phi_a \tag{20.157}$$

which is an integral over all fields that go back to themselves in euclidian time β.

Like a position operator (20.105), a field at an imaginary time $t = -iu = -i\hbar\beta$ is defined as

$$\phi_e(\boldsymbol{x}, u) = \phi_e(\boldsymbol{x}, \hbar\beta) = e^{uH/\hbar}\phi(\boldsymbol{x}, 0)\, e^{-uH/\hbar} \tag{20.158}$$

in which $\phi(\boldsymbol{x}) = \phi(\boldsymbol{x}, 0) = \phi_e(\boldsymbol{x}, 0)$ is the field at time zero, which obeys the commutation relations (20.119). The euclidian-time-ordered product of several fields is their product with newer (higher $u = \hbar\beta$) fields standing to the left of older (lower $u = \hbar\beta$) fields as in the definition (20.106).

The euclidian path integrals for the mean values of euclidian-time-ordered-products of fields are similar to those (20.145 & 20.146) for ordinary time-ordered-products. The euclidian-time-ordered-product of the fields $\phi(x_j) = \phi(\boldsymbol{x}_j, u_j)$ is the path integral

$$\langle n|\mathcal{T}[\phi_e(x_1)\phi_e(x_2)]|n\rangle = \frac{\displaystyle\int \langle n|\phi_b\rangle \phi(x_1)\phi(x_2) e^{-S_e[\phi]/\hbar}\langle\phi_a|n\rangle\, D\phi}{\displaystyle\int \langle n|\phi_b\rangle e^{-S_e[\phi]/\hbar}\langle\phi_a|n\rangle\, D\phi} \tag{20.159}$$

in which the integrations are over all paths that go from before u_1 and u_2 to after both euclidian times. The analogous result for several fields is

$$\langle n|\mathcal{T}[\phi_e(x_1)\cdots\phi_e(x_k)]|n\rangle = \frac{\displaystyle\int \langle n|\phi_b\rangle \phi(x_1)\cdots\phi(x_k) e^{-S_e[\phi]/\hbar}\langle\phi_a|n\rangle\, D\phi}{\displaystyle\int \langle n|\phi_b\rangle e^{-S_e[\phi]/\hbar}\langle\phi_a|n\rangle\, D\phi} \tag{20.160}$$

in which the integrations are over all paths that go from before the times $u_1, \ldots, u_k$ to after them.

In the low-temperature $\beta = 1/(kT) \to \infty$ limit, the Boltzmann operator is proportional to the outer product $|0\rangle\langle 0|$ of the ground-state kets, $e^{-\beta H} \to e^{-\beta E_0}|0\rangle\langle 0|$. In this limit, the integrations are over all fields that run from $u = -\infty$ to $u = \infty$, and the only energy eigenstate $|n\rangle$ that contributes is the ground state $|0\rangle$ of the theory

$$\langle 0|\mathcal{T}[\phi_e(x_1)\cdots\phi_e(x_k)]|0\rangle = \frac{\displaystyle\int \langle 0|\phi_b\rangle \phi(x_1)\cdots\phi(x_k) e^{-S_e[q]/\hbar}\langle\phi_a|0\rangle\, D\phi}{\displaystyle\int \langle 0|\phi_b\rangle e^{-S_e[q]/\hbar}\langle\phi_a|0\rangle\, D\phi}. \tag{20.161}$$

Formulas like this one are used in lattice gauge theory.

20.10 Perturbation theory

Field theories with hamiltonians that are quadratic in their fields like

$$H_0 = \int \tfrac{1}{2} \left[\pi^2(x) + (\nabla\phi(x))^2 + m^2 \phi^2(x) \right] d^3x \tag{20.162}$$

are soluble. Their fields evolve in time as

$$\phi(\boldsymbol{x}, t) = e^{itH_0} \phi(\boldsymbol{x}, 0) e^{-itH_0}. \tag{20.163}$$

The mean value in the ground state of H_0 of a time-ordered product of these fields is a ratio (20.146) of path integrals

$$\langle 0 | \mathcal{T} \left[\phi(x_1) \cdots \phi(x_k) \right] | 0 \rangle = \frac{\displaystyle\int \langle 0|\phi_b\rangle \, \phi(x_1) \cdots \phi(x_n) \, e^{iS_0[\phi]} \langle \phi_a | 0 \rangle \, D\phi}{\displaystyle\int \langle 0|\phi_b\rangle \, e^{iS_0[\phi]} \langle \phi_a | 0 \rangle \, D\phi} \tag{20.164}$$

in which the action $S_0[\phi]$ is quadratic in the field ϕ

$$S_0[\phi] = \tfrac{1}{2} \int - \partial_a \phi(x) \partial^a \phi(x) - m^2 \phi^2(x) \; d^4x. \tag{20.165}$$

Here $-\partial_a \, \phi \partial^a \phi = \dot{\phi}^2 - (\nabla\phi)^2$, and the integrations are over all fields that run from ϕ_a at a time before the times $t_1, \dots, t_k$ to ϕ_b at a time after $t_1, \dots, t_k$. The path integrals in the ratio (20.164) are gaussian and doable.

The Fourier transforms

$$\tilde{\phi}(p) = \int e^{-ipx} \phi(x) \, d^4x \quad \text{and} \quad \phi(x) = \int e^{ipx} \tilde{\phi}(p) \, \frac{d^4p}{(2\pi)^4} \tag{20.166}$$

turn the spacetime derivatives in the action into a quadratic form

$$S_0[\phi] = -\tfrac{1}{2} \int |\tilde{\phi}(p)|^2 \, (p^2 + m^2) \, \frac{d^4p}{(2\pi)^4} \tag{20.167}$$

in which $p^2 = \boldsymbol{p}^2 - p^{02}$ and $\tilde{\phi}(-p) = \tilde{\phi}^*(p)$ by (4.28) since the field ϕ is real.

The initial $\langle \phi_a | 0 \rangle$ and final $\langle 0 | \phi_b \rangle$ wave functions produce the $i\epsilon$ in the Feynman propagator (7.64). Although its exact form doesn't matter here, the wave function $\langle \phi | 0 \rangle$ of the ground state of H_0 is the exponential (19.53)

$$\langle \phi | 0 \rangle = c \exp \left[-\frac{1}{2} \int |\tilde{\phi}(\boldsymbol{p})|^2 \, \sqrt{\boldsymbol{p}^2 + m^2} \, \frac{d^3p}{(2\pi)^3} \right] \tag{20.168}$$

in which $\tilde{\phi}(\boldsymbol{p})$ is the spatial Fourier transform of the eigenvalue $\phi(\boldsymbol{x})$

$$\tilde{\phi}(\boldsymbol{p}) = \int e^{-i\boldsymbol{p}\cdot\boldsymbol{x}} \, \phi(\boldsymbol{x}) \, d^3x \tag{20.169}$$

and c is a normalization factor that will cancel in ratios of path integrals.

Apart from $-2i \log c$ which we will not keep track of, the wave functions $\langle \phi_a | 0 \rangle$ and $\langle 0 | \phi_b \rangle$ add to the action $S_0[\phi]$ the term

$$\Delta S_0[\phi] = \frac{i}{2} \int \sqrt{\boldsymbol{p}^2 + m^2} \left(|\tilde{\phi}(\boldsymbol{p}, t)|^2 + |\tilde{\phi}(\boldsymbol{p}, -t)|^2 \right) \frac{d^3 p}{(2\pi)^3} \tag{20.170}$$

in which we envision taking the limit $t \to \infty$ with $\phi(\boldsymbol{x}, t) = \phi_b(\boldsymbol{x})$ and $\phi(\boldsymbol{x}, -t) = \phi_a(\boldsymbol{x})$. The identity (Weinberg, 1995, pp. 386–388)

$$f(+\infty) + f(-\infty) = \lim_{\epsilon \to 0+} \epsilon \int_{-\infty}^{\infty} f(t)\, e^{-\epsilon |t|}\, dt \tag{20.171}$$

(exercise 20.22) allows us to write $\Delta S_0[\phi]$ as

$$\Delta S_0[\phi] = \lim_{\epsilon \to 0+} \frac{i\epsilon}{2} \int \sqrt{\boldsymbol{p}^2 + m^2} \int_{-\infty}^{\infty} |\tilde{\phi}(\boldsymbol{p}, t)|^2\, e^{-\epsilon |t|}\, dt\, \frac{d^3 p}{(2\pi)^3}. \tag{20.172}$$

So to first order in ϵ, the change in the action is (exercise 20.23)

$$\begin{aligned} \Delta S_0[\phi] &= \lim_{\epsilon \to 0+} \frac{i\epsilon}{2} \int \sqrt{\boldsymbol{p}^2 + m^2} \int_{-\infty}^{\infty} |\tilde{\phi}(\boldsymbol{p}, t)|^2\, dt\, \frac{d^3 p}{(2\pi)^3} \\ &= \lim_{\epsilon \to 0+} \frac{i\epsilon}{2} \int \sqrt{\boldsymbol{p}^2 + m^2}\, |\tilde{\phi}(p)|^2\, \frac{d^4 p}{(2\pi)^4}. \end{aligned} \tag{20.173}$$

Thus the modified action is

$$\begin{aligned} S_0[\phi, \epsilon] = S_0[\phi] + \Delta S_0[\phi] &= -\frac{1}{2} \int |\tilde{\phi}(p)|^2 \left(p^2 + m^2 - i\epsilon \sqrt{\boldsymbol{p}^2 + m^2} \right) \frac{d^4 p}{(2\pi)^4} \\ &= -\frac{1}{2} \int |\tilde{\phi}(p)|^2 \left(p^2 + m^2 - i\epsilon \right) \frac{d^4 p}{(2\pi)^4} \end{aligned} \tag{20.174}$$

since the square root is positive. In terms of the modified action, our formula (20.164) for the time-ordered product is the ratio

$$\langle 0 | \mathcal{T} \left[\phi(x_1) \cdots \phi(x_n) \right] | 0 \rangle = \frac{\displaystyle\int \phi(x_1) \cdots \phi(x_n)\, e^{iS_0[\phi, \epsilon]}\, D\phi}{\displaystyle\int e^{iS_0[\phi, \epsilon]}\, D\phi}. \tag{20.175}$$

We can use this formula (20.175) to express the mean value in the vacuum $|0\rangle$ of the time-ordered exponential of a spacetime integral of $j(x)\phi(x)$, in which $j(x)$ is a classical (c-number, external) current, as the ratio

$$\begin{aligned} Z_0[j] &\equiv \langle 0|\,\mathcal{T}\left\{\exp\left[i\int j(x)\,\phi(x)\,d^4x\right]\right\}|0\rangle \\ &= \frac{\displaystyle\int \exp\left[i\int j(x)\,\phi(x)\,d^4x\right] e^{iS_0[\phi,\epsilon]}\,D\phi}{\displaystyle\int e^{iS_0[\phi,\epsilon]}\,D\phi}. \end{aligned} \tag{20.176}$$

Since the state $|0\rangle$ is normalized, the mean value $Z_0[0]$ is unity, $Z_0[0] = 1$. If we absorb the current into the action

$$S_0[\phi, \epsilon, j] = S_0[\phi, \epsilon] + \int j(x)\,\phi(x)\,d^4x \tag{20.177}$$

then in terms of the current's Fourier transform

$$\tilde{j}(p) = \int e^{-ipx}\,j(x)\,d^4x \tag{20.178}$$

the modified action $S_0[\phi, \epsilon, j]$ is (exercise 20.24)

$$S_0[\phi, \epsilon, j] = -\tfrac{1}{2}\int \left[|\tilde{\phi}(p)|^2\left(p^2 + m^2 - i\epsilon\right) - \tilde{j}^*(p)\tilde{\phi}(p) - \tilde{\phi}^*(p)\tilde{j}(p)\right]\frac{d^4p}{(2\pi)^4}. \tag{20.179}$$

Changing variables to $\tilde{\psi}(p) = \tilde{\phi}(p) - \tilde{j}(p)/(p^2 + m^2 - i\epsilon)$, we can write the action $S_0[\phi, \epsilon, j]$ as (exercise 20.25)

$$\begin{aligned} S_0[\phi, \epsilon, j] &= -\tfrac{1}{2}\int \left[|\tilde{\psi}(p)|^2\,\left(p^2 + m^2 - i\epsilon\right) - \frac{\tilde{j}^*(p)\tilde{j}(p)}{(p^2 + m^2 - i\epsilon)}\right]\frac{d^4p}{(2\pi)^4} \\ &= S_0[\psi, \epsilon] + \tfrac{1}{2}\int \left[\frac{\tilde{j}^*(p)\tilde{j}(p)}{(p^2 + m^2 - i\epsilon)}\right]\frac{d^4p}{(2\pi)^4}. \end{aligned} \tag{20.180}$$

And since $D\phi = D\psi$, our formula (20.176) gives simply (exercise 20.26)

$$Z_0[j] = \exp\left(\frac{i}{2}\int \frac{|\tilde{j}(p)|^2}{p^2 + m^2 - i\epsilon}\frac{d^4p}{(2\pi)^4}\right). \tag{20.181}$$

Going back to position space, one finds (exercise 20.27)

$$Z_0[j] = \exp\left[\frac{i}{2}\int j(x)\,\Delta(x - x')\,j(x')\,d^4x\,d^4x'\right] \tag{20.182}$$

in which $\Delta(x - x')$ is Feynman's **propagator** (7.64)

$$\Delta(x - x') = \Delta_F(x - x') = \int \frac{e^{ip(x - x')}}{p^2 + m^2 - i\epsilon}\frac{d^4p}{(2\pi)^4}. \tag{20.183}$$

The functional derivative (chapter 19) of $Z_0[j]$, defined by (20.176), is

$$\frac{1}{i}\frac{\delta Z_0[j]}{\delta j(x)} = \langle 0|\,\mathcal{T}\left[\phi(x)\exp\left(i\int j(x')\phi(x')d^4x'\right)\right]|0\rangle \tag{20.184}$$

while that of equation (20.182) is

$$\frac{1}{i}\frac{\delta Z_0[j]}{\delta j(x)} = Z_0[j]\int \Delta(x-x')\,j(x')\,d^4x'. \tag{20.185}$$

Thus the second functional derivative of $Z_0[j]$ evaluated at $j=0$ gives

$$\langle 0|\,\mathcal{T}\left[\phi(x)\phi(x')\right]|0\rangle = \frac{1}{i^2}\frac{\delta^2 Z_0[j]}{\delta j(x)\delta j(x')}\bigg|_{j=0} = -i\,\Delta(x-x'). \tag{20.186}$$

Similarly, one may show (exercise 20.28) that

$$\begin{aligned}\langle 0|\,\mathcal{T}\big[\phi(x_1)\phi(x_2)\phi(x_3)\phi(x_4)\big]|0\rangle = {} & \frac{1}{i^4}\frac{\delta^4 Z_0[j]}{\delta j(x_1)\delta j(x_2)\delta j(x_3)\delta j(x_4)}\bigg|_{j=0}\\ = {} & -\Delta(x_1-x_2)\Delta(x_3-x_4)-\Delta(x_1-x_3)\Delta(x_2-x_4)\\ & -\Delta(x_1-x_4)\Delta(x_2-x_3).\end{aligned} \tag{20.187}$$

Suppose now that we add a potential $V(\phi)$ to the free hamiltonian (20.162). Scattering amplitudes are matrix elements of the time-ordered exponential $\mathcal{T}\exp\left[-i\int V(\phi)\,d^4x\right]$ (Weinberg, 1995, p. 260) Our formula (20.175) for the mean value in the ground state $|0\rangle$ of the free hamiltonian H_0 of any time-ordered product of fields leads us to

$$\langle 0|\mathcal{T}\left\{\exp\left[-i\int V(\phi)\,d^4x\right]\right\}|0\rangle = \frac{\int \exp\left[-i\int V(\phi)\,d^4x\right]\,e^{iS_0[\phi,\epsilon]}\,D\phi}{\int e^{iS_0[\phi,\epsilon]}\,D\phi}. \tag{20.188}$$

Using (20.186 & 20.187), we can cast this expression into the magical form

$$\langle 0|\mathcal{T}\left\{\exp\left[-i\int V(\phi)\,d^4x\right]\right\}|0\rangle = \exp\left[-i\int V\left(\frac{\delta}{i\delta j(x)}\right)\,d^4x\right]Z_0[j]\bigg|_{j=0}. \tag{20.189}$$

The generalization of the path-integral formula (20.175) to the ground state $|\Omega\rangle$ of an interacting theory with action S is

$$\langle\Omega|\mathcal{T}\left[\phi(x_1)\cdots\phi(x_n)\right]|\Omega\rangle = \frac{\int \phi(x_1)\cdots\phi(x_n)\,e^{iS[\phi,\epsilon]}\,D\phi}{\int e^{iS[\phi,\epsilon]}\,D\phi} \tag{20.190}$$

in which a term like $i\epsilon\phi^2$ is added to make the modified action $S[\phi, \epsilon]$.

These are some of the techniques one uses to make states of incoming and outgoing particles and to compute scattering amplitudes (Weinberg, 1995, 1996; Srednicki, 2007; Zee, 2010).

20.11 Application to quantum electrodynamics

In the Coulomb gauge $\nabla \cdot \boldsymbol{A} = 0$, the QED hamiltonian is

$$H = H_m + \int \left[\tfrac{1}{2}\boldsymbol{\pi}^2 + \tfrac{1}{2}(\nabla \times \boldsymbol{A})^2 - \boldsymbol{A} \cdot \boldsymbol{j}\right] d^3x + V_C \tag{20.191}$$

in which H_m is the matter hamiltonian, and V_C is the Coulomb term

$$V_C = \frac{1}{2} \int \frac{j^0(\boldsymbol{x}, t)\, j^0(\boldsymbol{y}, t)}{4\pi|\boldsymbol{x} - \boldsymbol{y}|}\, d^3x\, d^3y. \tag{20.192}$$

The operators $\boldsymbol{A}$ and $\boldsymbol{\pi}$ are canonically conjugate, but they satisfy the Coulomb-gauge conditions $\nabla \cdot \boldsymbol{A} = 0$ and $\nabla \cdot \boldsymbol{\pi} = 0$.

One may show (Weinberg, 1995, pp. 413–418) that in this theory, the analog of equation (20.190) is

$$\langle\Omega|\mathcal{T}\left[\mathcal{O}_1 \cdots \mathcal{O}_n\right]|\Omega\rangle = \frac{\displaystyle\int \mathcal{O}_1 \cdots \mathcal{O}_n\, e^{iS_C}\, \delta[\nabla \cdot \boldsymbol{A}]\, D\boldsymbol{A}\, D\psi}{\displaystyle\int e^{iS_C}\, \delta[\nabla \cdot \boldsymbol{A}]\, D\boldsymbol{A}\, D\psi} \tag{20.193}$$

in which the Coulomb-gauge action is

$$S_C = \int \tfrac{1}{2}\dot{\boldsymbol{A}}^2 - \tfrac{1}{2}(\nabla \times \boldsymbol{A})^2 + \boldsymbol{A} \cdot \boldsymbol{j} + \mathcal{L}_m\, d^4x - \int V_C\, dt \tag{20.194}$$

and the functional delta function

$$\delta[\nabla \cdot \boldsymbol{A}] = \prod_x \delta(\nabla \cdot \boldsymbol{A}(x)) \tag{20.195}$$

enforces the Coulomb-gauge condition. The term $\mathcal{L}_m$ is the action density of the matter field ψ.

Tricks are available. We introduce a new field $A^0(x)$ and consider the factor

$$F = \int \exp\left[i \int \frac{1}{2}\left(\nabla A^0 + \nabla \triangle^{-1} j^0\right)^2 d^4x\right] DA^0 \tag{20.196}$$

which is just a *number* independent of the charge density j^0 since we can cancel the j^0 term by shifting A^0. By $\triangle^{-1}$, we mean $-1/4\pi|\boldsymbol{x}-\boldsymbol{y}|$. By integrating by parts, we can write the number F as (exercise 20.29)

$$\begin{aligned} F &= \int \exp\left[i\int \tfrac{1}{2}\left(\boldsymbol{\nabla}A^0\right)^2 - A^0 j^0 - \tfrac{1}{2}\, j^0 \triangle^{-1} j^0 \; d^4x\right] DA^0 \\ &= \int \exp\left[i\int \tfrac{1}{2}\left(\boldsymbol{\nabla}A^0\right)^2 - A^0 j^0 \; d^4x + i\int V_C\, dt\right] DA^0. \end{aligned} \tag{20.197}$$

So when we multiply the numerator and denominator of the amplitude (20.193) by F, the awkward Coulomb term V_C cancels, and we get

$$\langle\Omega|\mathcal{T}\left[\mathcal{O}_1\cdots\mathcal{O}_n\right]|\Omega\rangle = \frac{\displaystyle\int \mathcal{O}_1\cdots\mathcal{O}_n\, e^{iS'}\,\delta[\boldsymbol{\nabla}\cdot\boldsymbol{A}]\, DA\, D\psi}{\displaystyle\int e^{iS'}\,\delta[\boldsymbol{\nabla}\cdot\boldsymbol{A}]\, DA\, D\psi} \tag{20.198}$$

where now DA includes all four components A^μ and

$$S' = \int \tfrac{1}{2}\,\dot{\boldsymbol{A}}^2 - \tfrac{1}{2}\,(\boldsymbol{\nabla}\times\boldsymbol{A})^2 + \tfrac{1}{2}\left(\boldsymbol{\nabla}A^0\right)^2 + \boldsymbol{A}\cdot\boldsymbol{j} - A^0 j^0 + \mathcal{L}_m\, d^4x. \tag{20.199}$$

Since the delta-functional $\delta[\boldsymbol{\nabla}\cdot\boldsymbol{A}]$ enforces the Coulomb-gauge condition, we can add to the action S' the term $(\boldsymbol{\nabla}\cdot\dot{\boldsymbol{A}})\,A^0$ which is $-\dot{\boldsymbol{A}}\cdot\boldsymbol{\nabla}A^0$ after we integrate by parts and drop the surface term. This extra term makes the action gauge invariant

$$\begin{aligned} S &= \int \tfrac{1}{2}\,(\dot{\boldsymbol{A}} - \boldsymbol{\nabla}\boldsymbol{A^0})^2 - \tfrac{1}{2}\,(\boldsymbol{\nabla}\times\boldsymbol{A})^2 + \boldsymbol{A}\cdot\boldsymbol{j} - A^0 j^0 + \mathcal{L}_m\, d^4x \\ &= \int -\tfrac{1}{4}\, F_{ab}\, F^{ab} + A^b j_b + \mathcal{L}_m \; d^4x. \end{aligned} \tag{20.200}$$

Thus at this point we have

$$\langle\Omega|\mathcal{T}\left[\mathcal{O}_1\cdots\mathcal{O}_n\right]|\Omega\rangle = \frac{\displaystyle\int \mathcal{O}_1\cdots\mathcal{O}_n\, e^{iS}\,\delta[\boldsymbol{\nabla}\cdot\boldsymbol{A}]\, DA\, D\psi}{\displaystyle\int e^{iS}\,\delta[\boldsymbol{\nabla}\cdot\boldsymbol{A}]\, DA\, D\psi} \tag{20.201}$$

in which S is the gauge-invariant action (20.200), and the integral is over all fields. The only relic of the Coulomb gauge is the gauge-fixing delta functional $\delta[\boldsymbol{\nabla}\cdot\boldsymbol{A}]$.

We now make the gauge transformations $A'_b(x) = A_b(x) + \partial_b\Lambda(x)$ and $\psi'(x) = e^{iq\Lambda(x)}\psi(x)$ in the numerator and also, using a different gauge transformation Λ', in the denominator of the ratio (20.201) of path integrals. Since we are integrating over all gauge fields, these gauge transformations merely change the order of integration in the numerator and denominator of that ratio. They are like replacing $\int_{-\infty}^{\infty} f(x)\,dx$ by $\int_{-\infty}^{\infty} f(y)\,dy$. They change nothing, and so $\langle\Omega|\mathcal{T}\left[\mathcal{O}_1\cdots\mathcal{O}_n\right]|\Omega\rangle = \langle\Omega|\mathcal{T}\left[\mathcal{O}_1\cdots\mathcal{O}_n\right]|\Omega\rangle'$ in which the prime refers to the gauge transformations Λ and Λ'.

We've seen that the action S is gauge invariant. So is the measure $DA\,D\psi$. We now restrict ourselves to operators $\mathcal{O}_1\cdots\mathcal{O}_n$ that are **gauge invariant**. So in $\langle\Omega|\mathcal{T}\left[\mathcal{O}_1\cdots\mathcal{O}_n\right]|\Omega\rangle'$, the replacement of the fields by their gauge transforms affects only the Coulomb-gauge term $\delta[\boldsymbol{\nabla}\cdot\boldsymbol{A}]$

$$\langle\Omega|\mathcal{T}\left[\mathcal{O}_1\cdots\mathcal{O}_n\right]|\Omega\rangle = \frac{\displaystyle\int \mathcal{O}_1\cdots\mathcal{O}_n\, e^{iS}\,\delta[\boldsymbol{\nabla}\cdot\boldsymbol{A}+\triangle\Lambda]\,DA\,D\psi}{\displaystyle\int e^{iS}\,\delta[\boldsymbol{\nabla}\cdot\boldsymbol{A}+\triangle\Lambda']\,DA\,D\psi}. \tag{20.202}$$

We now have two choices. If we integrate over all gauge functions $\Lambda(x)$ and $\Lambda'(x)$ in both the numerator and the denominator of this ratio (20.202), then apart from over-all constants that cancel, the mean value in the vacuum of the time-ordered product is the ratio

$$\langle\Omega|\mathcal{T}\left[\mathcal{O}_1\cdots\mathcal{O}_n\right]|\Omega\rangle = \frac{\displaystyle\int \mathcal{O}_1\cdots\mathcal{O}_n\, e^{iS}\,DA\,D\psi}{\displaystyle\int e^{iS}\,DA\,D\psi} \tag{20.203}$$

in which we integrate over all matter fields, gauge fields, and gauges. That is, **we do not fix the gauge**.

The analogous formula for the euclidian time-ordered product is

$$\langle\Omega|\mathcal{T}\left[\mathcal{O}_{e,1}\cdots\mathcal{O}_{e,n}\right]|\Omega\rangle = \frac{\displaystyle\int \mathcal{O}_1\cdots\mathcal{O}_n\, e^{-S_e}\,DA\,D\psi}{\displaystyle\int e^{-S_e}\,DA\,D\psi} \tag{20.204}$$

in which the euclidian action S_e is the spacetime integral of the energy density. This formula is quite general; it holds in nonabelian gauge theories and is important in lattice gauge theory.

Our second choice is to multiply the numerator and the denominator of the ratio (20.202) by the exponential $\exp[-i\frac{1}{2}\alpha\int(\triangle\Lambda)^2\,d^4x]$ and then integrate over $\Lambda(x)$ in the numerator and over $\Lambda'(x)$ in the denominator. This operation just multiplies the numerator and denominator by the same constant factor, which cancels. But if before integrating over all gauge transformations, we shift Λ so that $\triangle\Lambda$ changes to $\triangle\Lambda - \dot{A}^0$, then the exponential factor is $\exp[-i\frac{1}{2}\alpha\int(\dot{A}^0-\triangle\Lambda)^2\,d^4x]$. Now when we integrate over $\Lambda(x)$, the delta function $\delta(\boldsymbol{\nabla}\cdot\boldsymbol{A}+\triangle\Lambda)$ replaces $\triangle\Lambda$ by $-\boldsymbol{\nabla}\cdot\boldsymbol{A}$ in the inserted exponential, converting it to $\exp[-i\frac{1}{2}\alpha\int(\dot{A}^0+\boldsymbol{\nabla}\cdot\boldsymbol{A})^2\,d^4x]$. This term changes the gauge-invariant action (20.200) to the gauge-fixed action

$$S_\alpha = \int -\frac{1}{4} F_{ab}\, F^{ab} - \frac{\alpha}{2}(\partial_b A^b)^2 + A^b j_b + \mathcal{L}_m \; d^4x. \tag{20.205}$$

This Lorentz-invariant, gauge-fixed action is much easier to use than the Coulomb-gauge action (20.194) with the Coulomb potential (20.192). We can use it to compute scattering amplitudes perturbatively. The mean value of a time-ordered product of operators in the ground state $|0\rangle$ of the free theory is

$$\langle 0| \mathcal{T} \left[\mathcal{O}_1 \cdots \mathcal{O}_n \right] |0\rangle = \frac{\displaystyle\int \mathcal{O}_1 \cdots \mathcal{O}_n \, e^{iS_\alpha} \, DA \, D\psi}{\displaystyle\int e^{iS_\alpha} \, DA \, D\psi}. \tag{20.206}$$

By following steps analogous to those that led to (20.183), one may show (exercise 20.30) that in Feynman's gauge, $\alpha = 1$, the photon propagator is

$$\langle 0| \mathcal{T} \left[A_\mu(x) A_\nu(y) \right] |0\rangle = -i \triangle_{\mu\nu}(x-y) = -i \int \frac{\eta_{\mu\nu}}{q^2 - i\epsilon} \, e^{iq\cdot(x-y)} \, \frac{d^4q}{(2\pi)^4}. \tag{20.207}$$

20.12 Fermionic Path Integrals

In our brief introduction (1.11–1.12) and (1.48–1.50), to Grassmann variables, we learned that because $\theta^2 = 0$ the most general function $f(\theta)$ of a single Grassmann variable θ is $f(\theta) = a + b\,\theta$. So a complete integral table consists of the integral of this linear function

$$\int f(\theta)\, d\theta = \int a + b\,\theta\, d\theta = a \int d\theta + b \int \theta\, d\theta. \tag{20.208}$$

This equation has two unknowns, the integral $\int d\theta$ of unity and the integral $\int \theta\, d\theta$ of θ. We choose them so that the integral of $f(\theta + \zeta)$

$$\int f(\theta + \zeta)\, d\theta = \int a + b\,(\theta + \zeta)\, d\theta = (a + b\,\zeta) \int d\theta + b \int \theta\, d\theta \tag{20.209}$$

is the same as the integral (20.208) of $f(\theta)$. Thus the integral $\int d\theta$ of unity must vanish, while the integral $\int \theta\, d\theta$ of θ can be any constant, which we choose to be unity. Our complete table of integrals is then

$$\int d\theta = 0 \quad \text{and} \quad \int \theta\, d\theta = 1. \tag{20.210}$$

This table of integrals is true for all Grassmann variables. So if $\theta' = c\,\theta$ is a complex multiple of θ, then we must set $d\theta' = c^{-1}\,d\theta$ in order to have

$$\int d\theta' = 0 \quad \text{and} \quad \int \theta'\,d\theta' = \int c\,\theta\,d\theta' = \int c\,\theta\,c^{-1}\,d\theta = 1. \tag{20.211}$$

The anticommutation relations for a fermionic degree of freedom ψ are

$$\{\psi, \psi^\dagger\} \equiv \psi\,\psi^\dagger + \psi^\dagger\psi = 1 \quad \text{and} \quad \{\psi, \psi\} = \{\psi^\dagger, \psi^\dagger\} = 0. \tag{20.212}$$

Because ψ has $\psi^\dagger$, it is conventional to introduce a variable $\theta^* = \theta^\dagger$ that anti-commutes with itself and with θ

$$\{\theta^*, \theta^*\} = \{\theta^*, \theta\} = \{\theta, \theta\} = 0. \tag{20.213}$$

The logic that led to (20.210) now gives

$$\int d\theta^* = 0 \quad \text{and} \quad \int \theta^*\,d\theta^* = 1. \tag{20.214}$$

We define the reference state $|0\rangle$ as $|0\rangle \equiv \psi|s\rangle$ for a state $|s\rangle$ that is not annihilated by ψ. Since $\psi^2 = 0$, the operator ψ annihilates the state $|0\rangle$

$$\psi|0\rangle = \psi^2|s\rangle = 0. \tag{20.215}$$

The effect of the operator ψ on the state

$$|\theta\rangle = \exp\left(\psi^\dagger\theta - \tfrac{1}{2}\theta^*\theta\right)|0\rangle = \left(1 + \psi^\dagger\theta - \tfrac{1}{2}\theta^*\theta\right)|0\rangle \tag{20.216}$$

is

$$\psi|\theta\rangle = \psi(1 + \psi^\dagger\theta - \tfrac{1}{2}\theta^*\theta)|0\rangle = \psi\psi^\dagger\theta|0\rangle = (1 - \psi^\dagger\psi)\theta|0\rangle = \theta|0\rangle \tag{20.217}$$

while that of θ on $|\theta\rangle$ is

$$\theta|\theta\rangle = \theta(1 + \psi^\dagger\theta - \tfrac{1}{2}\theta^*\theta)|0\rangle = \theta|0\rangle. \tag{20.218}$$

The state $|\theta\rangle$ therefore is an eigenstate of ψ with eigenvalue θ

$$\psi|\theta\rangle = \theta|\theta\rangle. \tag{20.219}$$

The bra corresponding to the ket $|\zeta\rangle$

$$\langle\zeta| = \langle 0|\left(1 + \zeta^*\psi - \frac{1}{2}\zeta^*\zeta\right) \tag{20.220}$$

is a left eigenstate of $\psi^\dagger$

$$\langle\zeta|\psi^\dagger = \langle\zeta|\zeta^* = \zeta^*\langle\zeta| \tag{20.221}$$

and the inner product $\langle\zeta|\theta\rangle$ is (exercise 20.31)

$$\begin{aligned}\langle\zeta|\theta\rangle &= \langle 0|\left(1+\zeta^*\psi-\frac{1}{2}\zeta^*\zeta\right)\left(1+\psi^\dagger\theta-\frac{1}{2}\theta^*\theta\right)|0\rangle \\ &= \langle 0|1+\zeta^*\theta-\frac{1}{2}\zeta^*\zeta-\frac{1}{2}\theta^*\theta+\frac{1}{4}\zeta^*\zeta\theta^*\theta|0\rangle \\ &= \exp\left[\zeta^*\theta-\frac{1}{2}\left(\zeta^*\zeta+\theta^*\theta\right)\right]. \end{aligned} \tag{20.222}$$

Example 20.11 (A gaussian integral) For any number c, we can compute the integral of $\exp(c\,\theta^*\theta)$ by expanding the exponential

$$\int e^{c\,\theta^*\theta}\,d\theta^*d\theta=\int(1+c\,\theta^*\theta)\,d\theta^*d\theta=\int(1-c\,\theta\,\theta^*)\,d\theta^*d\theta=-c. \tag{20.223}$$

□

The identity operator for the space of states

$$c|0\rangle+d|1\rangle\equiv c|0\rangle+d\psi^\dagger|0\rangle \tag{20.224}$$

is (exercise 20.32) the integral

$$I=\int|\theta\rangle\langle\theta|\,d\theta^*d\theta=|0\rangle\langle 0|+|1\rangle\langle 1| \tag{20.225}$$

in which the differentials anti-commute with each other and with other fermionic variables: $\{d\theta,d\theta^*\}=0$, $\{d\theta,\theta\}=0$, $\{d\theta,\psi\}=0$, and so forth.

The case of several Grassmann variables $\theta_1,\theta_2,\ldots,\theta_n$ and several Fermi operators $\psi_1,\psi_2,\ldots,\psi_n$ is similar. The θ_k anticommute among themselves and with the Fermi operators

$$\{\theta_i,\theta_j\}=\{\theta_i,\theta_j^*\}=\{\theta_i^*,\theta_j^*\}=0 \quad\text{and}\quad \{\theta_i,\psi_k\}=\{\theta_i^*,\psi_k\}=0 \tag{20.226}$$

while the ψ_k satisfy

$$\{\psi_k,\psi_\ell^\dagger\}=\delta_{k\ell} \quad\text{and}\quad \{\psi_k,\psi_l\}=\{\psi_k^\dagger,\psi_\ell^\dagger\}=0. \tag{20.227}$$

The reference state $|0\rangle$ is

$$|0\rangle=\left(\prod_{k=1}^n\psi_k\right)|s\rangle \tag{20.228}$$

in which $|s\rangle$ is any state not annihilated by any ψ_k (so the resulting $|0\rangle$ isn't zero). The direct-product state

$$|\theta\rangle\equiv\exp\left(\sum_{k=1}^n\psi_k^\dagger\theta_k-\frac{1}{2}\theta_k^*\theta_k\right)|0\rangle=\left[\prod_{k=1}^n\left(1+\psi_k^\dagger\theta_k-\frac{1}{2}\theta_k^*\theta_k\right)\right]|0\rangle \tag{20.229}$$

is (exercise 20.33) a simultaneous eigenstate $\psi_k|\theta\rangle = \theta_k|\theta\rangle$ of each ψ_k. It follows that

$$\psi_\ell\psi_k|\theta\rangle = \psi_\ell\theta_k|\theta\rangle = -\theta_k\psi_\ell|\theta\rangle = -\theta_k\theta_\ell|\theta\rangle = \theta_\ell\theta_k|\theta\rangle \tag{20.230}$$

and so too $\psi_k\psi_\ell|\theta\rangle = \theta_k\theta_\ell|\theta\rangle$. Since the ψ's anticommute, their eigenvalues must also

$$\theta_\ell\theta_k|\theta\rangle = \psi_\ell\psi_k|\theta\rangle = -\psi_k\psi_\ell|\theta\rangle = -\theta_k\theta_\ell|\theta\rangle. \tag{20.231}$$

The inner product $\langle\zeta|\theta\rangle$ is

$$\begin{aligned}\langle\zeta|\theta\rangle &= \langle 0| \left[\prod_{k=1}^{n}(1+\zeta_k^*\psi_k - \frac{1}{2}\zeta_k^*\zeta_k)\right] \left[\prod_{\ell=1}^{n}(1+\psi_\ell^\dagger\theta_\ell - \frac{1}{2}\theta_\ell^*\theta_\ell)\right] |0\rangle \\ &= \exp\left[\sum_{k=1}^{n}\zeta_k^*\theta_k - \frac{1}{2}\left(\zeta_k^*\zeta_k + \theta_k^*\theta_k\right)\right] = e^{\zeta^\dagger\theta - (\zeta^\dagger\zeta + \theta^\dagger\theta)/2}. \end{aligned} \tag{20.232}$$

The identity operator is

$$I = \int |\theta\rangle\langle\theta| \prod_{k=1}^{n} d\theta_k^* d\theta_k. \tag{20.233}$$

Example 20.12 (Gaussian Grassmann integral) For any 2×2 matrix A, we may compute the gaussian integral

$$g(A) = \int e^{-\theta^\dagger A\theta}\, d\theta_1^* d\theta_1 d\theta_2^* d\theta_2 \tag{20.234}$$

by expanding the exponential. The only terms that survive are the ones that have exactly one of each of the four variables θ_1, θ_2, θ_1^*, and θ_2^*. Thus the integral is the determinant of the matrix A

$$\begin{aligned} g(A) &= \int \frac{1}{2}\left(\theta_k^* A_{k\ell}\theta_\ell\right)^2\, d\theta_1^* d\theta_1 d\theta_2^* d\theta_2 \\ &= \int \left(\theta_1^* A_{11}\theta_1\, \theta_2^* A_{22}\theta_2 + \theta_1^* A_{12}\theta_2\, \theta_2^* A_{21}\theta_1\right)\, d\theta_1^* d\theta_1 d\theta_2^* d\theta_2 \\ &= A_{11}A_{22} - A_{12}A_{21} = \det A. \end{aligned} \tag{20.235}$$

The natural generalization to n dimensions is

$$\int e^{-\theta^\dagger A\theta} \prod_{k=1}^{n} d\theta_k^* d\theta_k = \det A \tag{20.236}$$

and is true for any $n\times n$ matrix A. If A is invertible, then the invariance of

Grassmann integrals under translations implies that

$$\begin{aligned}\int e^{-\theta^\dagger A\theta+\theta^\dagger\zeta+\zeta^\dagger\theta}\prod_{k=1}^{n}d\theta_k^* d\theta_k &= \int e^{-\theta^\dagger A(\theta+A^{-1}\zeta)+\theta^\dagger\zeta+\zeta^\dagger(\theta+A^{-1}\zeta)}\prod_{k=1}^{n}d\theta_k^* d\theta_k\\ &= \int e^{-\theta^\dagger A\theta+\zeta^\dagger\theta+\zeta^\dagger A^{-1}\zeta}\prod_{k=1}^{n}d\theta_k^* d\theta_k\\ &= \int e^{-(\theta^\dagger+\zeta^\dagger A^{-1})A\theta+\zeta^\dagger\theta+\zeta^\dagger A^{-1}\zeta}\prod_{k=1}^{n}d\theta_k^* d\theta_k\\ &= \int e^{-\theta^\dagger A\theta+\zeta^\dagger A^{-1}\zeta}\prod_{k=1}^{n}d\theta_k^* d\theta_k\\ &= \det A\; e^{\zeta^\dagger A^{-1}\zeta}. \end{aligned} \tag{20.237}$$

The values of θ and $\theta^\dagger$ that make the argument $-\theta^\dagger A\theta + \theta^\dagger\zeta + \zeta^\dagger\theta$ of the exponential stationary are $\overline{\theta} = A^{-1}\zeta$ and $\overline{\theta^\dagger} = \zeta^\dagger A^{-1}$. So a gaussian Grassmann integral is equal to its exponential evaluated at its stationary point, apart from a prefactor involving the determinant $\det A$. Exercises (20.2 & 20.4) are about the bosonic versions (20.3 & 20.4) of this result. □

One may further extend these definitions to a Grassmann field $\chi_m(x)$ and an associated Dirac field $\psi_m(x)$. The $\chi_m(x)$'s anticommute among themselves and with all fermionic variables at all points of spacetime

$$\{\chi_m(x),\chi_n(x')\} = \{\chi_m^*(x),\chi_n(x')\} = \{\chi_m^*(x),\chi_n^*(x')\} = 0 \tag{20.238}$$

and the Dirac field $\psi_m(x)$ obeys the equal-time anticommutation relations

$$\begin{aligned}&\{\psi_m(\boldsymbol{x},t),\psi_n^\dagger(\boldsymbol{x}',t)\} = \delta_{mn}\,\delta(\boldsymbol{x}-\boldsymbol{x}') \quad (n,m=1,\dots,4)\\ &\{\psi_m(\boldsymbol{x},t),\psi_n(\boldsymbol{x}',t)\} = \{\psi_m^\dagger(\boldsymbol{x},t),\psi_n^\dagger(\boldsymbol{x}',t)\} = 0.\end{aligned} \tag{20.239}$$

As in (20.228), we use eigenstates of the field ψ at $t=0$. If $|0\rangle$ is defined in terms of a state $|s\rangle$ that is not annihilated by any $\psi_m(\boldsymbol{x},0)$ as

$$|0\rangle = \left[\prod_{m,\boldsymbol{x}}\psi_m(\boldsymbol{x},0)\right]|s\rangle \tag{20.240}$$

then (exercise 20.34) the state

$$\begin{aligned}|\chi\rangle &= \exp\left(\int\sum_m \psi_m^\dagger(\boldsymbol{x},0)\,\chi_m(\boldsymbol{x}) - \frac{1}{2}\chi_m^*(\boldsymbol{x})\chi_m(\boldsymbol{x})\,d^3x\right)|0\rangle\\ &= \exp\left(\int \psi^\dagger\chi - \tfrac{1}{2}\chi^\dagger\chi\,d^3x\right)|0\rangle\end{aligned} \tag{20.241}$$

is an eigenstate of the operator $\psi_m(\boldsymbol{x},0)$ with eigenvalue $\chi_m(\boldsymbol{x})$

$$\psi_m(\boldsymbol{x},0)|\chi\rangle = \chi_m(\boldsymbol{x})|\chi\rangle. \tag{20.242}$$

The inner product of two such states is (exercise 20.35)

$$\langle\chi'|\chi\rangle = \exp\left[\int \chi'^\dagger\chi - \frac{1}{2}\chi'^\dagger\chi' - \frac{1}{2}\chi^\dagger\chi \; d^3x\right]. \tag{20.243}$$

The identity operator is the integral

$$I = \int |\chi\rangle\langle\chi| \, D\chi^* D\chi \tag{20.244}$$

in which

$$D\chi^* D\chi \equiv \prod_{m,\boldsymbol{x}} d\chi_m^*(\boldsymbol{x}) d\chi_m(\boldsymbol{x}). \tag{20.245}$$

The hamiltonian for a free Dirac field ψ of mass m is the spatial integral

$$H_0 = \int \overline{\psi}\,(\boldsymbol{\gamma}\cdot\boldsymbol{\nabla} + m)\,\psi \; d^3x \tag{20.246}$$

in which $\overline{\psi} \equiv i\psi^\dagger\gamma^0$ and the gamma matrices (11.340) satisfy

$$\{\gamma^a, \gamma^b\} = 2\,\eta^{ab} \tag{20.247}$$

where η is the 4×4 diagonal matrix with entries $(-1,1,1,1)$. Since $\psi|\chi\rangle = \chi|\chi\rangle$ and $\langle\chi'|\psi^\dagger = \langle\chi'|\chi'^\dagger$, the quantity $\langle\chi'|\exp(-i\epsilon H_0)|\chi\rangle$ is by (20.243)

$$\begin{aligned}\langle\chi'|e^{-i\epsilon H_0}|\chi\rangle &= \langle\chi'|\chi\rangle \exp\left[-i\epsilon\int \overline{\chi}'\,(\boldsymbol{\gamma}\cdot\boldsymbol{\nabla} + m)\,\chi \; d^3x\right] \\ &= \exp\left[\int \tfrac{1}{2}(\chi'^\dagger - \chi^\dagger)\chi - \tfrac{1}{2}\chi'^\dagger(\chi' - \chi) - i\epsilon\overline{\chi}'(\boldsymbol{\gamma}\cdot\boldsymbol{\nabla} + m)\chi d^3x\right] \\ &= \exp\left\{\epsilon\int\left[\tfrac{1}{2}\dot{\chi}^\dagger\chi - \tfrac{1}{2}\chi'^\dagger\dot{\chi} - i\overline{\chi}'\,(\boldsymbol{\gamma}\cdot\boldsymbol{\nabla} + m)\,\chi\right]\; d^3x\right\}\end{aligned} \tag{20.248}$$

in which $\chi'^\dagger - \chi^\dagger = \epsilon\dot{\chi}^\dagger$ and $\chi' - \chi = \epsilon\dot{\chi}$. Everything within the square brackets is multiplied by ϵ, so we may replace $\chi'^\dagger$ by $\chi^\dagger$ and $\overline{\chi}'$ by $\overline{\chi}$ so as to write to first order in ϵ

$$\langle\chi'|e^{-i\epsilon H_0}|\chi\rangle = \exp\left[\epsilon\int \tfrac{1}{2}\dot{\chi}^\dagger\chi - \tfrac{1}{2}\chi^\dagger\dot{\chi} - i\overline{\chi}\,(\boldsymbol{\gamma}\cdot\boldsymbol{\nabla} + m)\,\chi \; d^3x\right] \tag{20.249}$$

in which the dependence upon χ' is through the time derivatives.

Putting together $n = 2t/\epsilon$ such matrix elements, integrating over all intermediate-state dyadics $|\chi\rangle\langle\chi|$, and using our formula (20.244), we find

$$\langle\chi_t|e^{-2itH_0}|\chi_{-t}\rangle = \int \exp\left[\int \tfrac{1}{2}\dot{\chi}^\dagger\chi - \tfrac{1}{2}\chi^\dagger\dot{\chi} - i\overline{\chi}\left(\boldsymbol{\gamma}\cdot\boldsymbol{\nabla} + m\right)\chi d^4x\right] D\chi^* D\chi. \tag{20.250}$$

Integrating $\dot{\chi}^\dagger\chi$ by parts and dropping the surface term, we get

$$\langle\chi_t|e^{-2itH_0}|\chi_{-t}\rangle = \int \exp\left[\int - \chi^\dagger\dot{\chi} - i\overline{\chi}\left(\boldsymbol{\gamma}\cdot\boldsymbol{\nabla} + m\right)\chi\, d^4x\right] D\chi^* D\chi. \tag{20.251}$$

Since $-\chi^\dagger\dot{\chi} = -i\overline{\chi}\gamma^0\dot{\chi}$, the argument of the exponential is

$$i\int - \overline{\chi}\gamma^0\dot{\chi} - \overline{\chi}\left(\boldsymbol{\gamma}\cdot\boldsymbol{\nabla} + m\right)\chi\ d^4x = i\int - \overline{\chi}\left(\gamma^\mu\partial_\mu + m\right)\chi\ d^4x. \tag{20.252}$$

We then have

$$\langle\chi_t|e^{-2itH_0}|\chi_{-t}\rangle = \int \exp\left(i\int \mathcal{L}_0(\chi)\, d^4x\right) D\chi^* D\chi \tag{20.253}$$

in which $\mathcal{L}_0(\chi) = -\overline{\chi}\left(\gamma^\mu\partial_\mu + m\right)\chi$ is the action density (11.342) for a free Dirac field. Thus the amplitude is a path integral with phases given by the classical action $S_0[\chi]$

$$\langle\chi_t|e^{-2itH_0}|\chi_{-t}\rangle = \int e^{i\int \mathcal{L}_0(\chi)\, d^4x} D\chi^* D\chi = \int e^{iS_0[\chi]} D\chi^* D\chi \tag{20.254}$$

and the integral is over all fields that go from $\chi(\boldsymbol{x}, -t) = \chi_{-t}(\boldsymbol{x})$ to $\chi(\boldsymbol{x}, t) = \chi_t(\boldsymbol{x})$. Any normalization factor will cancel in ratios of such integrals.

Since Fermi fields anticommute, their time-ordered product has an extra minus sign

$$\mathcal{T}\left[\overline{\psi}(x_1)\psi(x_2)\right] = \theta(x_1^0 - x_2^0)\,\overline{\psi}(x_1)\,\psi(x_2) - \theta(x_2^0 - x_1^0)\,\psi(x_2)\,\overline{\psi}(x_1). \tag{20.255}$$

The logic behind our formulas (20.146) and (20.164) for the time-ordered product of bosonic fields now leads to an expression for the time-ordered product of $2n$ Dirac fields (with $D\chi''$ and $D\chi'$ suppressed)

$$\langle 0|\mathcal{T}\left[\overline{\psi}(x_1)\cdots\psi(x_{2n})\right]|0\rangle = \frac{\displaystyle\int \langle 0|\chi''\rangle\,\overline{\chi}(x_1)\cdots\chi(x_{2n})\, e^{iS_0[\chi]}\langle\chi'|0\rangle\, D\chi^* D\chi}{\displaystyle\int \langle 0|\chi''\rangle\, e^{iS_0[\chi]}\langle\chi'|0\rangle\, D\chi^* D\chi}. \tag{20.256}$$

As in (20.175), the effect of the inner products $\langle 0|\chi''\rangle$ and $\langle\chi'|0\rangle$ is to insert

ϵ-terms which modify the Dirac propagators

$$\langle 0|\mathcal{T}\left[\overline{\psi}(x_1)\cdots\psi(x_{2n})\right]|0\rangle = \frac{\displaystyle\int \overline{\chi}(x_1)\cdots\chi(x_{2n})\, e^{iS_0[\chi,\epsilon]}\, D\chi^* D\chi}{\displaystyle\int e^{iS_0[\chi,\epsilon]}\, D\chi^* D\chi}. \quad (20.257)$$

Imitating (20.176), we introduce a Grassmann external current $\zeta(x)$ and define a fermionic analog of $Z_0[j]$

$$Z_0[\zeta] \equiv \langle 0|\,\mathcal{T}\left[e^{\int \overline{\zeta}\psi + \overline{\psi}\zeta\, d^4x}\right]|0\rangle = \frac{\displaystyle\int e^{\int \overline{\zeta}\chi+\overline{\chi}\zeta\, d^4x} e^{iS_0[\chi,\epsilon]} D\chi^* D\chi}{\displaystyle\int e^{iS_0[\chi,\epsilon]} D\chi^* D\chi}. \quad (20.258)$$

Example 20.13 (Feynman's fermion propagator) Since

$$\begin{aligned} i\left(\gamma^\mu\partial_\mu + m\right)\Delta(x-y) &\equiv i\left(\gamma^\mu\partial_\mu + m\right)\int \frac{d^4p}{(2\pi)^4} e^{ip(x-y)}\frac{-i\left(-i\gamma^\nu p_\nu + m\right)}{p^2+m^2-i\epsilon} \\ &= \int \frac{d^4p}{(2\pi)^4} e^{ip(x-y)}\left(i\gamma^\mu p_\mu + m\right)\frac{\left(-i\gamma^\nu p_\nu + m\right)}{p^2+m^2-i\epsilon} \\ &= \int \frac{d^4p}{(2\pi)^4} e^{ip(x-y)}\frac{p^2+m^2}{p^2+m^2-i\epsilon} = \delta^4(x-y), \end{aligned} \quad (20.259)$$

the function $\Delta(x-y)$ is the inverse of the differential operator $i(\gamma^\mu\partial_\mu + m)$. Thus the Grassmann identity (20.237) implies that $Z_0[\zeta]$ is

$$\begin{aligned} \langle 0|\,\mathcal{T}\left[e^{\int \overline{\zeta}\psi+\overline{\psi}\zeta\, d^4x}\right]|0\rangle &= \frac{\displaystyle\int e^{\int [\overline{\zeta}\chi+\overline{\chi}\zeta - i\,\overline{\chi}(\gamma^\mu\partial_\mu+m)\chi]d^4x} D\chi^* D\chi}{\displaystyle\int e^{iS_0[\chi,\epsilon]} D\chi^* D\chi} \\ &= \exp\left[\int \overline{\zeta}(x)\Delta(x-y)\zeta(y)\, d^4x d^4y\right]. \end{aligned} \quad (20.260)$$

Differentiating we get

$$\langle 0|\mathcal{T}\left[\psi(x)\overline{\psi}(y)\right]|0\rangle = \Delta(x-y) = -i\int \frac{d^4p}{(2\pi)^4} e^{ip(x-y)}\frac{-i\gamma^\nu p_\nu + m}{p^2+m^2-i\epsilon}. \quad (20.261)$$

□

20.13 Application to nonabelian gauge theories

The action of a generic nonabelian gauge theory is

$$S = \int - \tfrac{1}{4} F_{a\mu\nu} F_a^{\mu\nu} - \overline{\psi} \left(\gamma^\mu D_\mu + m \right) \psi \; d^4x \tag{20.262}$$

in which the Maxwell field is

$$F_{a\mu\nu} \equiv \partial_\mu A_{a\nu} - \partial_\nu A_{a\mu} + g \, f_{abc} \, A_{b\mu} \, A_{c\nu} \tag{20.263}$$

and the covariant derivative is

$$D_\mu \psi \equiv \partial_\mu \psi - i g \, t_a \, A_{a\mu} \, \psi. \tag{20.264}$$

Here g is a coupling constant, f_{abc} is a structure constant (11.69), and t_a is a generator (11.58) of the Lie algebra (section 11.16) of the gauge group.

One may show (Weinberg, 1996, pp. 14–18) that the analog of equation (20.201) for quantum electrodynamics is

$$\langle \Omega | \mathcal{T} \left[\mathcal{O}_1 \cdots \mathcal{O}_n \right] | \Omega \rangle = \frac{\displaystyle\int \mathcal{O}_1 \cdots \mathcal{O}_n \, e^{iS} \, \delta[A_{a3}] \, DA \, D\psi}{\displaystyle\int e^{iS} \, \delta[A_{a3}] \, DA \, D\psi} \tag{20.265}$$

in which the functional delta function

$$\delta[A_{a3}] \equiv \prod_x \delta(A_{a3}(x)) \tag{20.266}$$

enforces the axial-gauge condition, and $D\psi$ stands for $D\psi^* D\psi$.

Initially, physicists had trouble computing nonabelian amplitudes beyond the lowest order of perturbation theory. Then DeWitt showed how to compute to second order (DeWitt, 1967), and Faddeev and Popov, using path integrals, showed how to compute to all orders (Faddeev and Popov, 1967).

20.14 Faddeev-Popov tricks

The path-integral methods of Faddeev and Popov are described in (Weinberg, 1996, pp. 19–27). We will use gauge-fixing functions $G_a(x)$ to impose a gauge condition on our nonabelian gauge fields $A^a_\mu(x)$. For instance, we can use $G_a(x) = A^3_a(x)$ to impose an axial gauge or $G_a(x) = i\partial_\mu A^\mu_a(x)$ to impose a Lorentz-invariant gauge.

Under an infinitesimal gauge transformation (13.415)

$$A^\lambda_{a\mu} = A_{a\mu} - \partial_\mu \lambda_a - g \, f_{abc} \, A_{b\mu} \, \lambda_c \tag{20.267}$$

the gauge fields change, and so the gauge-fixing functions $G_b(x)$, which depend upon them, also change. The jacobian J of that change at $\lambda = 0$ is

$$J = \det\left(\frac{\delta G_a^\lambda(x)}{\delta\lambda_b(y)}\right)\bigg|_{\lambda=0} \equiv \frac{DG^\lambda}{D\lambda}\bigg|_{\lambda=0} \tag{20.268}$$

and it typically involves the delta function $\delta^4(x-y)$.

Let $B[G]$ be any functional of the gauge-fixing functions $G_b(x)$ such as

$$B[G] = \prod_{x,a} \delta(G_a(x)) = \prod_{x,a} \delta(A_a^3(x)) \tag{20.269}$$

in an axial gauge or

$$B[G] = \exp\left[\frac{i}{2}\int (G_a(x))^2 \, d^4x\right] = \exp\left[-\frac{i}{2}\int (\partial_\mu A_a^\mu(x))^2 \, d^4x\right] \tag{20.270}$$

in a Lorentz-invariant gauge.

We want to understand functional integrals like (20.265)

$$\langle\Omega|\mathcal{T}\left[\mathcal{O}_1\cdots\mathcal{O}_n\right]|\Omega\rangle = \frac{\displaystyle\int \mathcal{O}_1\cdots\mathcal{O}_n \, e^{iS} \, B[G] \, J \, DA \, D\psi}{\displaystyle\int e^{iS} \, B[G] \, J \, DA \, D\psi} \tag{20.271}$$

in which the operators $\mathcal{O}_k$, the action functional $S[A]$, and the differentials $DAD\psi$ (but not the gauge-fixing functional $B[G]$ or the Jacobian J) are gauge invariant. The axial-gauge formula (20.265) is a simple example in which $B[G] = \delta[A_{a3}]$ enforces the axial-gauge condition $A_{a3}(x) = 0$ and the determinant $J = \det\left(\delta_{ab}\partial_3\delta(x-y)\right)$ is a constant that cancels.

If we translate the gauge fields by gauge transformations Λ and Λ', then the ratio (20.271) does not change

$$\langle\Omega|\mathcal{T}\left[\mathcal{O}_1\cdots\mathcal{O}_n\right]|\Omega\rangle = \frac{\displaystyle\int \mathcal{O}_1^\Lambda\cdots\mathcal{O}_n^\Lambda \, e^{iS^\Lambda} \, B[G^\Lambda] \, J^\Lambda \, DA^\Lambda \, D\psi^\Lambda}{\displaystyle\int e^{iS^{\Lambda'}} \, B[G^{\Lambda'}] \, J^{\Lambda'} \, DA^{\Lambda'} \, D\psi^{\Lambda'}} \tag{20.272}$$

any more than $\int f(y)\,dy$ is different from $\int f(x)\,dx$. Since the operators $\mathcal{O}_k$, the action functional $S[A]$, and the differentials $DAD\psi$ are gauge invariant, most of the Λ-dependence goes away

$$\langle\Omega|\mathcal{T}\left[\mathcal{O}_1\cdots\mathcal{O}_n\right]|\Omega\rangle = \frac{\displaystyle\int \mathcal{O}_1\cdots\mathcal{O}_n \, e^{iS} \, B[G^\Lambda] \, J^\Lambda \, DA \, D\psi}{\displaystyle\int e^{iS} \, B[G^{\Lambda'}] \, J^{\Lambda'} \, DA \, D\psi}. \tag{20.273}$$

Let $\Lambda\lambda$ be a gauge transformation Λ followed by an infinitesimal gauge transformation λ. The jacobian J^Λ is a determinant of a product of matrices which is a product of their determinants

$$\begin{aligned} J^\Lambda &= \det\left(\frac{\delta G_a^{\Lambda\lambda}(x)}{\delta\lambda_b(y)}\right)\Bigg|_{\lambda=0} = \det\left(\int \frac{\delta G_a^{\Lambda\lambda}(x)}{\delta\Lambda\lambda_c(z)}\frac{\delta\Lambda\lambda_c(z)}{\delta\lambda_b(y)}\,d^4z\right)\Bigg|_{\lambda=0} \\ &= \det\left(\frac{\delta G_a^{\Lambda\lambda}(x)}{\delta\Lambda\lambda_c(z)}\right)\Bigg|_{\lambda=0} \det\left(\frac{\delta\Lambda\lambda_c(z)}{\delta\lambda_b(y)}\right)\Bigg|_{\lambda=0} \\ &= \det\left(\frac{\delta G_a^{\Lambda}(x)}{\delta\Lambda_c(z)}\right) \det\left(\frac{\delta\Lambda\lambda_c(z)}{\delta\lambda_b(y)}\right)\Bigg|_{\lambda=0} \equiv \frac{DG^\Lambda}{D\Lambda}\frac{D\Lambda\lambda}{D\lambda}\Bigg|_{\lambda=0}. \end{aligned} \tag{20.274}$$

Now we integrate over the gauge transformation Λ with weight function $\rho(\Lambda) = (\,D\Lambda\lambda/D\lambda|_{\lambda=0})^{-1}$ and find, since the ratio (20.273) is Λ-independent

$$\begin{aligned} \langle\Omega|\mathcal{T}\left[\mathcal{O}_1\cdots\mathcal{O}_n\right]|\Omega\rangle &= \frac{\displaystyle\int \mathcal{O}_1\cdots\mathcal{O}_n\, e^{iS}\, B[G^\Lambda]\,\frac{DG^\Lambda}{D\Lambda}\,D\Lambda\,DA\,D\psi}{\displaystyle\int e^{iS}\, B[G^\Lambda]\,\frac{DG^\Lambda}{D\Lambda}\,D\Lambda\,DA\,D\psi} \\ &= \frac{\displaystyle\int \mathcal{O}_1\cdots\mathcal{O}_n\, e^{iS}\, B[G^\Lambda]\,DG^\Lambda\,DA\,D\psi}{\displaystyle\int e^{iS}\, B[G^\Lambda]\,DG^\Lambda\,DA\,D\psi} \\ &= \frac{\displaystyle\int \mathcal{O}_1\cdots\mathcal{O}_n\, e^{iS}\;DA\,D\psi}{\displaystyle\int e^{iS}\;DA\,D\psi}. \end{aligned} \tag{20.275}$$

Thus the mean-value in the vacuum of a time-ordered product of gauge-invariant operators is a ratio of path integrals over all gauge fields without any gauge fixing. No matter what gauge condition G or gauge-fixing functional $B[G]$ we use, the resulting gauge-fixed ratio (20.271) is equal to the ratio (20.275) of path integrals over all gauge fields without any gauge fixing. All gauge-fixed ratios (20.271) give the same time-ordered products, and so we can use whatever gauge condition G or gauge-fixing functional $B[G]$ is most convenient.

The analogous formula for the euclidian time-ordered product is

$$\langle\Omega|\mathcal{T}_e\left[\mathcal{O}_1\cdots\mathcal{O}_n\right]|\Omega\rangle = \frac{\displaystyle\int \mathcal{O}_1\cdots\mathcal{O}_n\, e^{-S_e}\,DA\,D\psi}{\displaystyle\int e^{-S_e}\,DA\,D\psi} \tag{20.276}$$

where the euclidian action S_e is the spacetime integral of the energy density. This formula is the basis for lattice gauge theory.

The path-integral formulas (20.203 & 20.204) derived for quantum electrodynamics therefore also apply to nonabelian gauge theories.

20.15 Ghosts

Faddeev, Popov, and DeWitt showed how to do perturbative calculations in which one does fix the gauge. To continue our description of their tricks, we return to the gauge-fixed expression (20.271) for the time-ordered product

$$\langle\Omega|\mathcal{T}\left[\mathcal{O}_1\cdots\mathcal{O}_n\right]|\Omega\rangle = \frac{\displaystyle\int \mathcal{O}_1\cdots\mathcal{O}_n\, e^{iS}\, B[G]\, J\, DA\, D\psi}{\displaystyle\int e^{iS}\, B[G]\, J\, DA\, D\psi} \tag{20.277}$$

set $G_b(x) = -i\partial_\mu A^\mu_b(x)$ and use (20.270) as the gauge-fixing functional $B[G]$

$$B[G] = \exp\left[\frac{i}{2}\int (G_a(x))^2\, d^4x\right] = \exp\left[-\frac{i}{2}\int (\partial_\mu A^\mu_a(x))^2\, d^4x\right]. \tag{20.278}$$

This functional adds to the action density the term $-(\partial_\mu A^\mu_a)^2/2$ which leads to a gauge-field propagator like the photon's (20.207)

$$\langle 0|\mathcal{T}\left[A^a_\mu(x)A^b_\nu(y)\right]|0\rangle = -i\delta_{ab}\triangle_{\mu\nu}(x-y) = -i\int \frac{\eta_{\mu\nu}\delta_{ab}}{q^2-i\epsilon}\, e^{iq\cdot(x-y)}\,\frac{d^4q}{(2\pi)^4}. \tag{20.279}$$

What about the determinant J? Under an infinitesimal gauge transformation (20.267), the gauge field becomes

$$A^\lambda_{a\mu} = A_{a\mu} - \partial_\mu\lambda_a - g\, f_{abc}\, A_{b\mu}\,\lambda_c \tag{20.280}$$

and so $G^\lambda_a(x) = i\partial^\mu A^\lambda_{a\mu}(x)$ is

$$G^\lambda_a(x) = i\partial^\mu A_{a\mu}(x) + i\partial^\mu\int[-\delta_{ac}\partial_\mu - g\, f_{abc}A_{b\mu}(x)]\,\delta^4(x-y)\lambda_c(y)\, d^4y. \tag{20.281}$$

The jacobian J then is the determinant (20.268) of the matrix

$$\left(\frac{\delta G^\lambda_a(x)}{\delta\lambda_c(y)}\right)\bigg|_{\lambda=0} = -i\delta_{ac}\,\Box\,\delta^4(x-y) - ig\, f_{abc}\,\frac{\partial}{\partial x^\mu}\left[A^\mu_b(x)\delta^4(x-y)\right] \tag{20.282}$$

that is

$$J = \det\left(-i\delta_{ac}\,\Box\,\delta^4(x-y) - ig\, f_{abc}\,\frac{\partial}{\partial x^\mu}\left[A^\mu_b(x)\delta^4(x-y)\right]\right). \tag{20.283}$$

But we've seen (20.236) that a determinant can be written as a fermionic path integral

$$\det A = \int e^{-\theta^\dagger A\,\theta} \prod_{k=1}^{n} d\theta_k^* d\theta_k. \tag{20.284}$$

So we can write the jacobian J as

$$J = \int \exp\left[\int i\omega_a^* \Box \omega_a + ig f_{abc} \omega_a^* \partial_\mu (A_b^\mu \omega_c)\, d^4x\right] D\omega^* D\omega \tag{20.285}$$

which contributes the terms $-\partial_\mu \omega_a^* \partial^\mu \omega_a$ and

$$-\partial_\mu \omega_a^*\, g\, f_{abc}\, A_b^\mu \omega_c = \partial_\mu \omega_a^*\, g\, f_{abc}\, A_c^\mu \omega_b \tag{20.286}$$

to the action density.

Thus we can do perturbation theory by using the modified action density

$$\mathcal{L}' = -\tfrac{1}{4} F_{a\mu\nu} F_a^{\mu\nu} - \tfrac{1}{2}\left(\partial_\mu A_a^\mu\right)^2 - \partial_\mu \omega_a^* \partial^\mu \omega_a + \partial_\mu \omega_a^*\, g\, f_{abc}\, A_c^\mu \omega_b - \overline{\psi}\,(\not{D} + m)\,\psi \tag{20.287}$$

in which $\not{D} \equiv \gamma^\mu D_\mu = \gamma^\mu(\partial_\mu - igt^a A_{a\mu})$. The **ghost** field ω is a mathematical device, not a physical field describing real particles, which would be spinless fermions violating the spin-statistics theorem (example 11.25).

20.16 Effective field theories

Suppose a field ϕ whose mass M is huge compared to accessible energies interacts with a field ψ of a low-energy theory such as the standard model

$$L_\phi = -\tfrac{1}{2}\partial_a \phi(x)\, \partial^a \phi(x) - \tfrac{1}{2} M^2 \phi^2(x) + g\, \overline{\psi}(x) \psi(x) \phi(x). \tag{20.288}$$

Compared to the mass term M^2, the derivative terms $\partial_a \phi\, \partial^a \phi$ contribute little to the action. So we represent the effect of the heavy field ϕ as $L_{\phi 0} = -\frac{1}{2} M^2 \phi^2 + g\overline{\psi}\psi\phi$. Completing the square

$$L_{\phi 0} = -\tfrac{1}{2} M^2 \left(\phi - \frac{g}{M^2}\overline{\psi}\psi\right)^2 + \frac{g^2}{2M^2}\left(\overline{\psi}\psi\right)^2 \tag{20.289}$$

and shifting ϕ by $g\overline{\psi}\psi/M^2$, we see that the gaussian path integral is

$$\int \exp\left[i \int -\tfrac{1}{2} M^2 \phi^2 + \frac{g^2}{2M^2} (\overline{\psi}\psi)^2\, d^4x\right] D\phi = \exp\left[i \int \frac{g^2}{2M^2} (\overline{\psi}\psi)^2\, d^4x\right]$$

apart from a field-independent factor. The net effect of heavy field ϕ is thus to add to the low-energy theory a new interaction

$$L_\psi = \frac{g^2}{2M^2}\left(\overline{\psi}\psi\right)^2 \tag{20.290}$$

which is small because M^2 is large. If a gauge boson Y_a of huge mass M interacts as $L_{Y0} = -\frac{1}{2}M^2 Y_a Y^a + ig\overline{\psi}\gamma^a\psi Y_a$ with a spin-one-half field ψ, then $L_\psi = -\left(g^2/(2M^2)\right)\overline{\psi}\gamma^a\psi\,\overline{\psi}\gamma_a\psi$ is the new low-energy interaction.

20.17 Complex path integrals

In this chapter, it has been tacitly assumed that the action is quadratic in the time derivatives of the fields. This assumption makes the hamiltonian quadratic in the momenta and the path integral over them gaussian. In general, however, the partition function is a path integral over fields and momenta

$$Z(\beta) = \int \exp\left\{\int_0^\beta \int \left[i\dot{\phi}(x)\pi(x) - H(\phi,\pi)\right] dt d^3x\right\} D\phi\, D\pi \qquad (20.291)$$

in which the exponential is not gaussian or positive. To study such theories, one may numerically integrate over the momenta, make a look-up table, and use the Monte Carlo methods of Section 16.6 (Amdahl and Cahill, 2016). Programs that do this are in the repository Path_integrals at `github.com/kevinecahill`.

Further reading

"Space-Time Approach to Non-relativistic Quantum Mechanics" (Feynman, 1948), *Quantum Mechanics and Path Integrals* (Feynman et al., 2010), *Statistical Mechanics* (Feynman, 1972), *The Quantum Theory of Fields I, II, & III* (Weinberg, 1995, 1996, 2005), *Quantum Field Theory in a Nutshell* (Zee, 2010), and *Quantum Field Theory* (Srednicki, 2007) all provide excellent treatments of path integrals. Some applications are described in *Path Integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets* (Kleinert, 2009).

Exercises

20.1 From (20.1), derive the multiple gaussian integral for real a_j and b_j

$$\int_{-\infty}^{\infty} \exp\left(\sum_{j=1}^{n} i a_j x_j^2 + 2 i b_j x_j\right) \prod_{j=1}^{n} dx_j = \prod_{j=1}^{n} \sqrt{\frac{i\pi}{a_j}}\, e^{-ib_j^2/a_j}. \qquad (20.292)$$

20.2 Use (20.292) to derive the multiple imaginary gaussian integral (20.3).

Hint: Any real symmetric matrix s can be diagonalized by an orthogonal transformation $a = oso^{\mathsf{T}}$. Let $y = ox$.

20.3 Use (20.2) to show that for positive a_j

$$\int_{-\infty}^{\infty} \exp\left(\sum_j -a_j x_j^2 + 2ib_j x_j\right) \prod_{j=1}^{n} dx_j = \prod_{j=1}^{n} \sqrt{\frac{\pi}{a_j}}\, e^{-b_j^2/a_j}. \quad (20.293)$$

20.4 Use (20.293) to derive the many variable real gaussian integral (20.4). Same hint as for exercise 20.2.

20.5 Do the q_2 integral (20.27).

20.6 Insert the identity operator in the form of an integral (20.10) of outer products $|p\rangle\langle p|$ of eigenstates of the momentum operator p between the exponential and the state $|q_a\rangle$ in the matrix element (20.25) and so derive for that matrix element $\langle q_b|\exp(-i(t_b - t_a)H/\hbar)|q_a\rangle$ the formula (20.28). Hint: use the inner product $\langle q|p\rangle = \exp(iqp/\hbar)/\sqrt{2\pi\hbar}$, and do the resulting Fourier transform.

20.7 Derive the path-integral formula (20.39) for the quadratic action (20.38).

20.8 Show that for the simple harmonic oscillator (20.47) the action $S[q_c]$ of the classical path from q_a, t_a to q_b, t_b is (20.49).

20.9 Show that the determinants $|C_n(y)| = \det C_n(y)$ of the tridiagonal matrices (20.57) satisfy the recursion relation (20.58) and have the initial values $|C_1(y)| = y$ and $|C_2(y)| = y^2 - 1$. Incidentally, the Chebyshev polynomials (9.68) of the second kind $U_n(y/2)$ obey the same recursion relation and have the same initial values, so $|C_n(y)| = U_n(y/2)$.

20.10 (a) Show that the functions $S_n(y) = \sin(n+1)\theta/\sin\theta$ with $y = 2\cos\theta$ satisfy the Toeplitz recursion relation (20.58) which after a cancellation simplifies to $\sin(n+2)\theta = 2\cos\theta\,\sin(n+1)\theta - \sin n\theta$. (b) Derive the initial conditions $S_0(y) = 1$, $S_1(y) = y$, and $S_2(y) = y^2 - 1$.

20.11 Do the q_2 integral (20.79).

20.12 Show that the euclidian action (20.93) is stationary if the path $q_{ec}(u)$ obeys the euclidian equation of motion $\ddot{q}_{ec}(u) = \omega^2 q_{ec}(u)$.

20.13 By using (20.20) for each of the three exponentials in (20.107), derive (20.108) from (20.107). Hint: From (20.20), one has

$$q e^{-i\,(t_b - t_a)\,H/\hbar} q = \int q_b |q_b\rangle\, e^{iS[q]/\hbar}\, \langle q_a| q_a\, Dq\, dq_a\, dq_b \quad (20.294)$$

in which $q_a = q(t_a)$ and $q_b = q(t_b)$.

20.14 Derive the path-integral formula (20.145) from (20.135–20.138).

20.15 Derive the path-integral formula (20.159) from (20.153–20.156).

20.16 Show that the vector $\overline{Y}$ that makes the argument $-iY^{\mathsf{T}}SY + iD^{\mathsf{T}}Y$ of the multiple gaussian integral

$$\int_{-\infty}^{\infty} \exp\big(-iY^{\mathsf{T}}SY + iD^{\mathsf{T}}Y\big) \prod_{i=1}^{n} dy_i = \sqrt{\frac{\pi^n}{\det(iS)}}\, \exp\left(\frac{i}{4}\, D^{\mathsf{T}}S^{-1}D\right) \tag{20.295}$$

stationary is $\overline{Y} = S^{-1}D/2$, and that the multiple gaussian integral (20.295) is equal to its exponential $\exp(-iY^{\mathsf{T}}SY + iD^{\mathsf{T}}Y)$ evaluated at its stationary point $Y = \overline{Y}$ apart from a prefactor involving $\det iS$.

20.17 Show that the vector $\overline{Y}$ that makes the argument $-Y^{\mathsf{T}}SY + D^{\mathsf{T}}Y$ of the multiple gaussian integral

$$\int_{-\infty}^{\infty} \exp\big(-Y^{\mathsf{T}}SY + D^{\mathsf{T}}Y\big) \prod_{i=1}^{n} dy_i = \sqrt{\frac{\pi^n}{\det(S)}}\, \exp\left(\frac{1}{4}\, D^{\mathsf{T}}S^{-1}D\right) \tag{20.296}$$

stationary is $\overline{Y} = S^{-1}D/2$, and that the multiple gaussian integral (20.296) is equal to its exponential $\exp(-Y^{\mathsf{T}}SY + D^{\mathsf{T}}Y)$ evaluated at its stationary point $Y = \overline{Y}$ apart from a prefactor involving $\det S$.

20.18 By taking the nonrelativistic limit of the formula (12.70) for the action of a relativistic particle of mass m and charge q, derive the expression (20.44) for the action of a nonrelativistic particle in an electromagnetic field with no scalar potential.

20.19 Work out the path-integral formula for the amplitude for a mass m initially at rest to fall to the ground from height h in a gravitational field of local acceleration g to lowest order and then including loops up to an overall constant. Hint: use the technique of section 20.4.

20.20 Show that the euclidian action of the stationary solution (20.92) is (20.93).

20.21 Derive formula (20.167) for the action $S_0[\phi]$ from (20.165 & 20.166).

20.22 Derive identity (20.171). Split the time integral at $t = 0$ into two halves, use $\epsilon\, e^{\pm\epsilon t} = \pm\, d\, e^{\pm\epsilon t}/dt$ and then integrate each half by parts.

20.23 Derive the third term in equation (20.173) from the second term.

20.24 Use (20.177) and the Fourier transform (20.178) of the external current j to derive the formula (20.179) for the modified action $S_0[\phi, \epsilon, j]$.

20.25 Derive equation (20.180) from equation (20.179).

20.26 Derive the formula (20.181) for $Z_0[j]$ from the formula for $S_0[\phi, \epsilon, j]$.

20.27 Derive equations (20.182 & 20.183) from formula (20.181).

20.28 Derive equation (20.187) from the formula (20.182) for $Z_0[j]$.

20.29 Show that the time integral of the Coulomb term (20.192) is the term that is quadratic in j^0 in the number F defined by (20.196).

20.30 By following steps analogous to those that led to (20.183), derive the formula (20.207) for the photon propagator in Feynman's gauge.

20.31 Derive expression (20.222) for the inner product $\langle\zeta|\theta\rangle$.

20.32 Derive the representation (20.225) of the identity operator I for a single fermionic degree of freedom from the rules (20.210 & 20.214) for Grassmann integration and the anticommutation relations (20.213).

20.33 Derive the eigenvalue equation $\psi_k|\theta\rangle = \theta_k|\theta\rangle$ from the definitions (20.228 & 20.229) of the eigenstate $|\theta\rangle$.

20.34 Derive the eigenvalue relation (20.242) for the Fermi field $\psi_m(\boldsymbol{x}, t)$ from the anticommutation relations (20.238 & 20.239) and the definitions (20.240 & 20.241).

20.35 Derive the formula (20.243) for the inner product $\langle\chi'|\chi\rangle$ from the definition (20.241) of the ket $|\chi\rangle$.

20.36 Imitate the derivation of the path-integral formula (20.70) and derive its three-dimensional version (20.77).

20.37 Differentials $d\zeta_i$ of complex linear combinations $\zeta_i = A_{i\ell}\,\theta_\ell$ of Grassmann variables are defined as $d\zeta_i = d\theta_\ell\,(A^{-1})_{\ell i}$ and as $d\zeta_1 \cdots d\zeta_n = \det(A^{-1})\,d\theta_1 \cdots d\theta_n$. Show that the ζ's inherit the rules of integration of the θ's:

$$\delta_{ik} = \int \theta_i\,d\theta_k \implies \delta_{ik} = \int \zeta_i\,d\zeta_k. \tag{20.297}$$