2. Quantization with Path Integral Methods

In the previous chapter we learned about operators occurring in quantum mechanics. In this chapter we demonstrate that it is also possible to describe quantum mechanics using integrals in the space of functions, namely functional integrals and path integrals, instead of using operators.

2.1 Single-Particle Quantum Mechanics and Path Integrals

Everybody who learnt quantum mechanics should have heard about the interference experiment of electron waves through slits. Figure 2.1 shows the principle. Electrons emitted from an electron gun pass either through slit A or slit B of a shield and finally illuminate a screen. Because it is possible to avoid more than one electron reaching the screen at the same time by adjusting the intensity of the electron gun to be small enough, it is clear that electrons can indeed be interpreted as propagating "particles". However, when this kind of experiment is performed over a long period, the observed distribution of electrons at all points of the screen becomes the interference pattern of a wave.

In quantum mechanics, this interference pattern is explained as follows. We call the paths from the electron gun through slit A or slit B to the point P on the screen P_{A} or P_{B}, respectively. P_{A} and P_{B} each corresponds to a complex amplitude a_{A} and a_{B} of a quantum mechanical wave. Then, the phase difference φ of the complex functions a_{A} and a_{B} ($a_{\mathrm{A}}/a_{\mathrm{B}} \propto \mathrm{e}^{\mathrm{i}\varphi}$) equals the phase difference of the waves. The complex amplitude corresponding to the process that an electron started from the electron gun and reached the point P, without asking whether the electron passed through slit A or slit B is given by the sum of the amplitudes P_{A} and P_{B}. The intensity of the wave reaching P (in quantum mechanics the probability of reaching P) is given by the absolute value of the square of the complex amplitude

$$|a_{\mathrm{A}} + a_{\mathrm{B}}|^2 = |a_{\mathrm{A}}|^2 + |a_{\mathrm{B}}|^2 + 2|a_{\mathrm{A}}||a_{\mathrm{B}}|\cos\varphi \quad .$$

This expression varies periodically depending on φ.

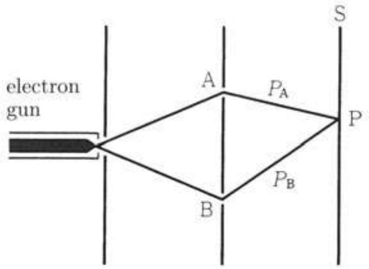

Fig. 2.1. Interference experiment with electron waves. The waves that passed through slits A and B interfere on the screen S

Next, we generalize this approach as shown in Fig. 2.2. Different from Fig. 2.1, there is not just one screening shield, but many, and there are not two slits in each, but a large number (Fig. 2.2a).

Depending on the way at each screen, many different combinations c for passing through the slits are possible, each corresponding to an amplitude a_c, the total amplitude a is given by $\sum_c a_c$. By increasing the number of screening layers and slits more and more, and finally reaching an infinite number, each screening layer will have many slits and finally will disappear. The interval between the gun and the screen will become a continuous space (Fig. 2.2b), and depending on the "combination of slits" the path will mutate to an arbitrary path from the gun to the screen, and "the sum of all amplitudes of possible ways" will mutate to an integral over the paths, that is, the path integral. That is to say, the principle that "the amplitude corresponding to a transition from a starting point to an end point corresponds to an integral over the amplitudes of all possible paths linking these two points" can be regarded as the principle of quantum mechanics.

When considering quantum mechanics, one might have in mind the wave function, and the Schrödinger equation of the wave function, all describing wave properties of the particle. It should be possible to link this description with the picture of the path integral described above by using the superposition principle of waves. However, it required the genius of Feynman to make this discovery.

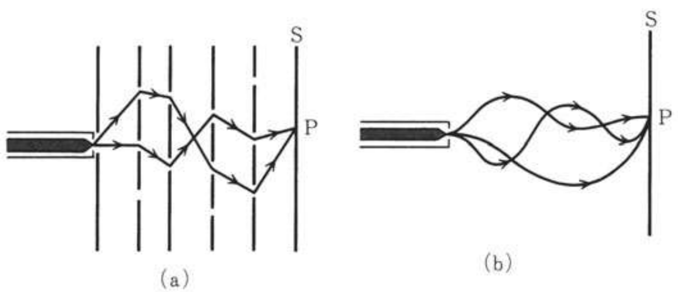

Fig. 2.2a, b. Generalization of the interference experiment of Fig. 2.1. The number of screens and the number of slits in the screen is increased

We now turn to exact mathematics. We start from the Schrödinger equation

$$
\begin{aligned}
\mathrm{i}\hbar\frac{\partial\psi(x,t)}{\partial t} &= -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi(x,t)}{\mathrm{d}x^2} + V(x)\psi(x,t) \\
&= H\psi(x,t) \quad . \qquad (2.1.1)
\end{aligned}
$$

For a moment, we restrict the motion of the particle to a one-dimensional space with space coordinate x.

As shown in (1.1.3), it is possible to integrate (2.1.1) formally

$$
|\psi(t')\rangle = U(t',t)|\psi(t)\rangle = \mathrm{e}^{-(\mathrm{i}/\hbar)H(t'-t)}|\psi(t)\rangle \quad . \qquad (2.1.2)
$$

We choose $t' > t$. Equation (2.1.2) describes the time evolution of the state $|\psi(t)\rangle$ occurring at t through $U(t',t)$ during the time $t'-t$, leading to the state $|\psi(t')\rangle$. Not the wave function can be expressed with the path integral mentioned before, but the operator $U(t,t')$ describing the time evolution. In (2.1.2), the label x has been omitted intentionally, because $|\psi(t)\rangle$ should be regarded as a continuous infinite dimensional vector with components $\psi(x,t)$ labelled by x, and $U(t',t)$ should be regarded as a matrix with components $U(x',t';x,t)$.

In x-representation, we obtain

$$
\psi(x',t') = \int \mathrm{d}x\, U(x',t';x,t)\psi(x,t) \quad . \qquad (2.1.3)
$$

We decompose $t'-t$ into small time intervals. We write $t'-t = N\Delta t$ and $t_k = t + k\Delta t$. The time evolution corresponding to these steps can be expressed as

$$
U(t',t) = U(t',t_{N-1})U(t_{N-1},t_{N-2})\ldots U(t_2,t_1)U(t_1,t) \qquad (2.1.4)
$$

using matrix multiplication of $U(t_{k+1},t_k)$. In components, we obtain

$$
\begin{aligned}
U(x',t';x,t) = \int &\mathrm{d}x\,(N-1)\,\mathrm{d}x\,(N-2)\ldots\mathrm{d}x\,(1) \\
&\times U(x',t';x(N-1),t_{N-1}) \\
&\times U(x(N-1),t_{N-1};x(N-2),t_{N-2}) \\
&\times\ldots U(x(1),t_1;x,t) \quad . \qquad (2.1.5)
\end{aligned}
$$

Here, the matrix components are given by the "bra- and ket-sandwich"

$$
U(x(k+1),t_{k+1};x(k),t_k) = \langle x(k+1)|\,\mathrm{e}^{-(\mathrm{i}/\hbar)H\Delta t}|x(k)\rangle \quad . \qquad (2.1.6)
$$

When Δt is small enough, the exponential can be expanded:

$$
\langle x(k+1)|\,\mathrm{e}^{-(\mathrm{i}/\hbar)H\Delta t}|x(k)\rangle \cong \langle x(k+1)|\left(1-\frac{\mathrm{i}}{\hbar}\Delta t H\right)|x(k)\rangle \quad . \qquad (2.1.7)
$$

Using the momentum eigenstates introduced in (1.1.34) and below, by inserting the completeness relations (1.1.37) we obtain

$$\langle x(k+1)|H|x(k)\rangle = \int \mathrm{d}p\,(k)\langle x(k+1)|p(k)\rangle\langle p(k)|H|x(k)\rangle \quad . \tag{2.1.8}$$

Because the Hamiltonian (2.1.1) is expressed in terms of $\hat{p}$ and $\hat{x}$, we obtain

$$\langle p(k)|H(\hat{p},\hat{x})|x(k)\rangle = H(p(k),x(k))\langle p(k)|x(k)\rangle \quad .$$

Here, $\hat{p} = (\hbar/\mathrm{i})\,\mathrm{d}/\mathrm{d}x$, and for $\hat{x}$ the hat has been written to stress that it is an operator.

Using this, (2.1.6) and (2.1.7) can be written as

$$\begin{aligned} &U(x(k+1),t_{k+1};x(k),t_k) \\ &\quad\cong \int \mathrm{d}p\,(k)\langle x(k+1)|p(k)\rangle\langle p(k)|x(k)\rangle\left(1-\frac{\mathrm{i}}{\hbar}\Delta t H(p(k),x(k))\right) \\ &\quad\cong \int \frac{\mathrm{d}p\,(k)}{2\pi\hbar}\exp\left[\mathrm{i}\frac{p(k)}{\hbar}(x(k+1)-x(k))-\frac{\mathrm{i}}{\hbar}\Delta t H(p(k),x(k))\right] . \end{aligned} \tag{2.1.9}$$

Inserting this for each term in (2.1.5), we obtain for $U(x',t';x,t)$

$$\begin{aligned} U(x',t';x,t) &= \int \frac{\mathrm{d}p\,(N-1)}{2\pi\hbar}\cdots\int\frac{\mathrm{d}p\,(0)}{2\pi\hbar}\int \mathrm{d}x\,(N-1)\cdots\int\mathrm{d}x\,(1) \\ &\quad\times\exp\left[\frac{\mathrm{i}}{\hbar}\sum_{k=0}^{N-1}\left[p(k)(x(k+1)-x(k))-\Delta t H(p(k),x(k))\right]\right] \quad . \end{aligned} \tag{2.1.10}$$

By performing the limit $N\to\infty$ and $\Delta t\to 0$, we obtain

$$x(k+1)-x(k)\to\dot{x}(t)\Delta t$$
$$\sum_{k=0}^{N-1}\Delta t\to\int_t^{t'}\mathrm{d}t \quad ,$$

and writing $\mathcal{D}p(t)$ and $\mathcal{D}x(t)$ for the multiple integrals over $p(k)$ and $x(k)$ in (2.1.10), respectively, the result is

$$\begin{aligned} U(x',t';x,t) &= \int_{\substack{x(t)=x\\ x(t')=x'}}\mathcal{D}p(t'')\mathcal{D}x(t'') \\ &\quad\times\exp\left[\frac{\mathrm{i}}{\hbar}\int_t^{t'}\left[p(t'')\dot{x}(t'')-H(p(t''),x(t''))\right]\mathrm{d}t''\right] \quad . \end{aligned} \tag{2.1.11}$$

Recalling the definition (1.3.3) and (1.3.4) of the action S, we notice that the expression in the exponent of (2.1.11) is exactly $(\mathrm{i}/\hbar)S$. We conclude that the amplitude corresponding to the path $x(t'')$ and $p(t'')$ ($t\le t''\le t'$) is given by $\exp[\mathrm{i}S(x(t''),p(t''))]$. The action is defined for every arbitrary path $x(t'')$ and $p(t'')$, and the relation $p(t'')=m\dot{x}(t'')$ need not necessarily be valid.

Because the dependence on $p(t'')$ in S is given by

$$\begin{aligned}\int_t^{t'} \left[p(t'')\dot{x}(t'') - \frac{p(t'')^2}{2m}\right] \mathrm{d}t'' \\ = \int_t^{t'} \left\{-\frac{1}{2m}\left(p(t'') - m\dot{x}(t'')\right)^2 + \frac{m\dot{x}(t'')^2}{2}\right\} \mathrm{d}t'' \quad , \end{aligned} \tag{2.1.12}$$

it is possible to perform the integral in $p(t'')$ obtaining

$$\begin{aligned} U(x', t'; x, t) &= \int_{\substack{x(t)=x \\ x(t')=x'}} \mathcal{D}x(t'') \exp\left[\frac{\mathrm{i}}{\hbar} S(\{x(t'')\})\right] \\ &= \int_{\substack{x(t)=x \\ x(t')=x'}} \mathcal{D}x(t'') \exp\left[\frac{\mathrm{i}}{\hbar}\int_t^{t'} \left\{\frac{m\dot{x}(t')^2}{2} - V(x(t''))\right\} \mathrm{d}t''\right] . \end{aligned} \tag{2.1.13}$$

The equation (2.1.13) corresponds to the Lagrangian in the sense that L is given as a function of $\dot{x}$ and x, and (2.1.11) corresponds to the canonical (Hamiltonian) formalism. In textbooks, equation (2.1.13) is often presented; however, (2.1.11) is the more basic equation. This is due to the fact that both canonical coordinates x and p appear in the equation, and that the term $\mathrm{i}p\dot{x}$ has the important interpretation of the Berry phase, as will be explained in Sect. 2.5. In the above case, it has been possible to integrate out the momentum; however, in general this is not always the case.

Next, as a repetition of (1.3.5) of the previous chapter, let us take the variation of $S(x(t''), p(t''))$ appearing in (2.1.11) and $S(x(t''))$ in (2.1.13):

$$\begin{aligned} \delta S(\{x(t'')\}, \{p(t'')\}) &= \delta \int_t^{t'} \mathrm{d}t'' \left[p(t'')\dot{x}(t'') - \frac{p(t'')^2}{2m} - V(x(t''))\right] \\ &= \int_t^{t'} \mathrm{d}t'' \left\{\delta p(t'') \left[\dot{x}(t'') - \frac{p(t'')}{m}\right]\right. \\ &\quad \left. + \delta x(t'')\left[-\dot{p}(t'') - V'(x(t''))\right]\right\} \quad , \end{aligned} \tag{2.1.14}$$

$$\begin{aligned} \delta S(\{x(t'')\}) &= \delta \int_t^{t'} \mathrm{d}t'' \left[\frac{m\dot{x}(t'')^2}{2} - V(x(t''))\right] \\ &= \int_t^{t'} \mathrm{d}t''\, \delta x(t'')\left[-m\ddot{x}(t'') - V'(x(t''))\right] \quad . \end{aligned} \tag{2.1.15}$$

Here we used $\delta x(t) = \delta x(t') = 0$ for partial integration.

$\delta S = 0$ in (2.1.14) and (2.1.15) leads to the classical equations of motion. From the point of view of classical dynamics, this is the well-known variation principle, but what will be the meaning from the point of view of the path integral? The meaning of equations (2.1.11) and (2.1.13) is that the transition amplitude from x, t to x', t' is given by integrating over all amplitudes:

$$\exp\left[\frac{\mathrm{i}}{\hbar}S(\{x(t'')\},\{p(t'')\})\right] \ , \qquad \exp\left[\frac{\mathrm{i}}{\hbar}S(\{x(t'')\})\right]$$

of every single path $x(t'')$ and $p(t'')$. However, even when all paths have to be taken into account, not every path is equally important. Especially, considering the fact that $\hbar$ is "small" (in the classical limit, this is a good approximation), we see that even a small change of the path will alter drastically the phase in $\exp[(\mathrm{i}/\hbar)S]$. Taking the sum, the contribution of the phase average will therefore be extremely small. An exception is a path where a small change does no affect S, that is, the path satisfying $\delta S = 0$.

In summary, we have just learnt that quantum mechanics can be formulated without the use of operators, only with c-numbers. The price we pay is that we have to perform an infinite dimensional integral in paths (being in the present case functions of time). The largest contribution to this integral is given by the classical path.

Next, we discuss the term $\mathrm{i}p\dot{x}$. We consider the following path integral of the functional $F(x(t'), p(t'))$ of $x(t'), p(t')$:

$$\begin{aligned} &\langle F(\{x(t')\},\{p(t')\})\rangle \\ &\quad = \int \mathcal{D}x(t')\mathcal{D}p(t')F(\{x(t')\},\{p(t')\})\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(\{x(t')\},\{p(t')\})} \ . \end{aligned} \tag{2.1.16}$$

We split the time intervals as done starting from (2.1.4):

$$\begin{aligned} F(\{x(t')\},\{p(t')\}) &\to F(x(1),\ldots,x(N-1);p(0),p(1),\ldots,p(N-1)) \\ &= F(x(k),p(k)) \ , \end{aligned} \tag{2.1.17}$$

$$\int \mathcal{D}x(t')\mathcal{D}p(t') = \prod_k \int \mathrm{d}x\,(k)\mathrm{d}p\,(k) \ . \tag{2.1.18}$$

We perform now a transformation of the integration measure by introducing the infinitesimal variables $\eta(k)$ and $\xi(k)$:

$$x(k) = \tilde{x}(k) + \eta(k) \quad \text{and} \quad p(k) = \tilde{p}(k) + \zeta(k) \tag{2.1.19}$$

and write the integral in the $\tilde{x}(k)$ and $\tilde{p}(k)$ variables introduced in this manner. Then, the integral becomes

$$\begin{aligned} &\langle F(x(k)), p(k))\rangle \\ &= \int \prod_{k'} \mathrm{d}\tilde{x}(k')\,\mathrm{d}\tilde{p}(k')\,F(\tilde{x}(k)+\eta(k),\tilde{p}(k)+\zeta(k)) \\ &\quad \times \exp\left\{\frac{\mathrm{i}}{\hbar}S[\tilde{x}(k)+\eta(k);\tilde{p}(k)+\zeta(k)]\right\} \end{aligned}$$

$$= \int \prod_{k'} \mathrm{d}x(k')\,\mathrm{d}p(k') \left(F + \sum_k \eta(k) \frac{\partial F}{\partial x(k)} + \sum_k \zeta(k) \frac{\partial F}{\partial p(k)} \right)$$
$$\times \left(1 + \frac{\mathrm{i}}{\hbar} \sum_k \eta(k) \frac{\partial S}{\partial x(k)} + \frac{\mathrm{i}}{\hbar} \sum \zeta(k) \frac{\partial S}{\partial p(k)} \right) \mathrm{e}^{\mathrm{i}S/\hbar}$$
$$= \langle F(x(k), p(k)) \rangle + \sum_k \eta(k) \left\langle \frac{\partial F}{\partial x(k)} + \frac{\mathrm{i}}{\hbar} F \frac{\partial S}{\partial x(k)} \right\rangle$$
$$+ \sum_k \zeta(k) \left\langle \frac{\partial F}{\partial p(k)} + \frac{\mathrm{i}}{\hbar} F \frac{\partial S}{\partial p(k)} \right\rangle \quad . \tag{2.1.20}$$

We expanded the expression up to first order in $\eta(k)$ and $\xi(k)$. Equation (2.1.10) holds for every $\eta(k)$ and $\xi(k)$, therefore

$$\left\langle \frac{\partial F}{\partial x(k)} \right\rangle = -\frac{\mathrm{i}}{\hbar} \left\langle F \frac{\partial S}{\partial x(k)} \right\rangle \quad ,$$
$$\left\langle \frac{\partial F}{\partial p(k)} \right\rangle = -\frac{\mathrm{i}}{\hbar} \left\langle F \frac{\partial S}{\partial p(k)} \right\rangle \tag{2.1.21}$$

hold. By setting $F(x(k), p(k)) = p(k_0)$, (2.1.21) reads

$$1 = -\frac{\mathrm{i}}{\hbar} \left\langle p(k_0) \frac{\partial S}{\partial p(k_0)} \right\rangle \quad . \tag{2.1.22}$$

On the other hand, because of

$$S = \sum_k p(k)(x(k+1) - x(k)) - \Delta t \sum_k H(p(k), x(k)) \tag{2.1.23}$$

we obtain

$$\frac{\partial S}{\partial p(k_0)} = x(k_0 + 1) - x(k_0) - \Delta t \frac{\partial H(p(k_0), x(k_0))}{\partial p(k_0)} \tag{2.1.24}$$

and for $\Delta t \to 0$ the third term disappears. Therefore, (2.1.22) becomes

$$\mathrm{i}\hbar = \langle p(k_0)[x(k_0 + 1) - x(k_0)] \rangle \quad . \tag{2.1.25}$$

To the expectation value of which operator does the right-hand side of this equation correspond? As is clear from the discussion in (2.1.7)–(2.1.10), the order of the operators is important:

$$\langle \hat{x}\hat{p} \rangle_{t=t_0} \to \langle x(k_0 + 1) p(k_0) \rangle \quad ,$$
$$\langle \hat{p}\hat{x} \rangle_{t=t_0} \to \langle p(k_0) x(k_0) \rangle \quad . \tag{2.1.26}$$

Therefore, the right-hand side of (2.1.25) corresponds to the expectation value of the equal time commutator of $\hat{x}$ and $\hat{p}$:

$$[\hat{x}, \hat{p}] = \mathrm{i}\hbar \ . \tag{2.1.27}$$

In this manner, $\mathrm{i}p\dot{x}$ shows that $\hat{x}$ and $\hat{p}$ are canonical conjugate operators, and the ordering of these operators is represented in the path integral as time ordering.

Next, we consider the formalism in imaginary time. As is clear from (2.1.2), we used the operator $\exp[(-\mathrm{i}/\hbar)Ht]$ for the discussion. Writing $-\mathrm{i}\tau$ instead of t, and redoing the steps as before, we obtain

$$\begin{aligned}\langle x'|\,\mathrm{e}^{-H\tau/\hbar}|x\rangle &= \int_{\substack{x(0)=x\\ x(\tau)=x'}} \mathcal{D}x(\tau') \int \mathcal{D}p(\tau') \exp\left[-\frac{1}{\hbar}S(\{x(\tau')\},\{p(\tau')\})\right] \\ &= \int_{\substack{x(0)=x\\ x(\tau)=x'}} \mathcal{D}x(\tau') \int \mathcal{D}p(\tau') \\ &\quad \times \exp\left[-\frac{1}{\hbar}\int_0^\tau \left\{-\mathrm{i}p(\tau')\dot{x}(\tau') + \frac{p(\tau')^2}{2m} + V(x(\tau'))\right\}\mathrm{d}\tau'\right] , \end{aligned} \tag{2.1.28}$$

$$\begin{aligned}\langle x'|\,\mathrm{e}^{-H\tau/\hbar}|x\rangle &= \int_{\substack{x(0)=x\\ x(\tau)=x'}} \mathcal{D}x(\tau') \exp\left[-\frac{1}{\hbar}S(\{x(\tau')\})\right] \\ &= \int_{\substack{x(0)=x\\ x(\tau)=x'}} \mathcal{D}x(\tau') \exp\left[-\frac{1}{\hbar}\int_0^\tau \left\{\frac{m\dot{x}(\tau')^2}{2} + V(x(\tau'))\right\}\mathrm{d}\tau'\right] . \end{aligned} \tag{2.1.29}$$

Here, we replaced

$$\int \mathrm{d}t'' \to -\mathrm{i}\int \mathrm{d}\tau' \quad \text{and} \quad \dot{x}(t'') \to \mathrm{i}\dot{x}(\tau') \ .$$

In particular, when setting $\tau = \beta\hbar$ and $x' = x$ and integrating in x (see Appendix C)

$$Z = \mathrm{Tr}\,\mathrm{e}^{-\beta H} = \int \mathrm{d}x \langle x|\,\mathrm{e}^{-\beta H}|x\rangle \ , \tag{2.1.30}$$

we obtain the partition function of the system. Using the path integral formalism in imaginary time, it is therefore also possible to apply it to statistical physics.

Notice that the factor i in (2.1.28) does not disappear in the term $\mathrm{i}p(\tau')\dot{x}(\tau')$ in the complex-time formalism. This term indicates the phase (Berry phase). On the other hand, after the $p(\tau')$-integration, no complex term is present in (2.1.29), and the exponent is positive as usual. In such a case, the partition function (2.1.30) corresponds to that of one string $x(\tau')$ in classical statistical mechanics. In general, a d-dimensional system in quantum physics can be associated with a $(d+1)$-dimensional classical system in such a manner. However, for the case that the phase factor mentioned above remains, no equivalent classical model exists.

Next, we determine the path with the largest contribution to (2.1.29), as was done for (2.1.13). Taking the variation, we obtain

$$\delta \int_0^\beta \left\{ \frac{m\dot{x}(\tau')^2}{2} + V(x(\tau')) \right\} \mathrm{d}\tau' = \int_0^\beta [-m\ddot{x}(\tau') + V'(x(\tau'))]\delta x(\tau')\mathrm{d}\tau'$$
$$= 0 \ . \qquad (2.1.31)$$

This path obeys the equation $m\ddot{x}(\tau') = V'(x(\tau'))$. This is a classical equation of motion, corresponding to the classical motion of a particle in a potential with reversed sign, that is, where up and down are reversed. For example, a potential $V(x)$ as shown in Fig. 2.3 with two valleys becomes the potential $-V(x)$ with two mountains. In this case, possible motions are the way from the top of one mountain to the other, falling down in the valley, or climbing up in the valley.

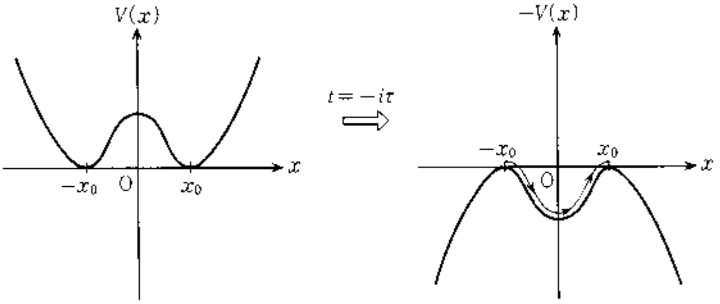

Fig. 2.3. Classical movement in the complex-time formalism. When the real time is changed to complex time, the potential is reversed, and therefore classical movement in regions that has been forbidden before becomes possible

The classical solution for a path in the imaginary-time formalism is called the instanton, and has the physical meaning of tunnelling within the framework of quantum mechanics. Because the potential is reversed, motion in classical forbidden regions becomes possible, and in contrast to the normal description of tunnelling, where the wave number becomes imaginary and the wave is damped, in this case the imaginary time represents the damping of the wave.

In order to confirm that the instanton is indeed responsible for the tunnelling, we perform the following calculation. We set $\hbar = 1$, and for T large enough, we want to calculate in (2.1.29) the amplitude of the transition from $\pm x_0$ to $\pm x_0$:

$$\langle x_0 | \, \mathrm{e}^{-HT} | x_0 \rangle = \langle -x_0 | \, \mathrm{e}^{-HT} | -x_0 \rangle \ , \qquad (2.1.32)$$

and from $\pm x_0$ to $\mp x_0$:

$$\langle x_0 | \, \mathrm{e}^{-HT} | -x_0 \rangle = \langle -x_0 | \, \mathrm{e}^{-HT} | x_0 \rangle \ . \qquad (2.1.33)$$

Writing τ ($0 \le \tau \le T$) on the x axis and $x(\tau)$ on the y axis, one type of path rests at $x(\tau) = \pm x_0$ and the second type connects the points x_0 and $-x_0$, corresponding to the instanton (anti-instanton) described above. With the boundary condition $x(0) = \pm x(T)$, the number of instantons and anti-instantons in (2.1.32) is equal; in (2.1.33) the numbers differ by one.

In the vicinity of the top of the mountain, $V(x)$ can be written approximately as

$$-V(x) = -V(x_0) - \frac{m\omega^2}{2}(x - x_0)^2$$

and we obtain the equation of motion $m\ddot{x}(\tau) = \omega^2(x - x_0)$. The instanton solution behaves as $x - x_0 \propto \mathrm{e}^{-\omega\tau}$. In the case when the distance between the instanton and anti-instanton is large compared with the width of the instanton solution itself, the instantons can be regarded as a dilute free gas living on the τ axis, assigned to distinct places $0 \le \tau_1 \le \tau_2 \ldots \le \tau_n \le T$ (the dilute gas approximation). If no instanton is present, then we obtain

$$V(x) = \frac{m\omega^2}{2}(x \pm x_0)^2$$

as the solution of the harmonic oscillator problem

$$\begin{aligned}\langle x_0|\,\mathrm{e}^{-HT}|x_0\rangle &= \langle -x_0|\,\mathrm{e}^{-HT}|-x_0\rangle \\ &= \left(\frac{m\omega}{\pi}\right)^{1/2}\mathrm{e}^{-\omega T/2} \quad .\end{aligned} \tag{2.1.34}$$

Recall that the ground state of the harmonic oscillator with energy $\omega/2$ is given by

$$\varphi_0(x) = \left(\frac{m\omega}{\pi}\right)^{1/4}\mathrm{e}^{-m\omega(x\pm x_0)^2/2} \quad .$$

For the case when n instantons and anti-instantons are present, the answer will become

$$\int_0^T \mathrm{d}\tau_n \int_0^{\tau_n} \mathrm{d}\tau_{n-1} \ldots \int_0^{\tau_2} \mathrm{d}\tau_1 \left(\frac{m\omega}{\pi}\right)^{1/2}\mathrm{e}^{-\omega T/2}K^n\,\mathrm{e}^{-nS_0} \quad . \tag{2.1.35}$$

Here, S_0 is the action of the one-instanton solution $S(x(\tau))$, and K is the ratio of the Gauss integral with and without the instanton. More detailed discussions can be found in the literature [G.6]. Here, it is sufficient to assume that K is just a number. It is important to notice that the term $(K\,\mathrm{e}^{-S_0})^n$ appears in the dilute gas approximation. The imaginary time integral in (2.1.35) can be performed easily, with the result $T^n/n!$, and taking the sum over n, we obtain

$$\begin{aligned}\langle x_0|\,\mathrm{e}^{-HT}|x_0\rangle &= \langle -x_0|\,\mathrm{e}^{-HT}|-x_0\rangle \\ &= \left(\frac{m\omega}{\pi}\right)^{1/2}\mathrm{e}^{-\omega T/2}\sum_{n=0\ (\text{even})}^{\infty}\frac{(TK\,\mathrm{e}^{-S_0})^n}{n!} \\ &= \left(\frac{m\omega}{\pi}\right)^{1/2}\mathrm{e}^{-\omega T/2}\cosh(TK\,\mathrm{e}^{-S_0})\ , \end{aligned} \tag{2.1.36}$$

$$\begin{aligned}\langle x_0|\,\mathrm{e}^{-HT}|-x_0\rangle &= \langle -x_0|\,\mathrm{e}^{-HT}|x_0\rangle \\ &= \left(\frac{m\omega}{\pi}\right)^{1/2}\mathrm{e}^{-\omega T/2}\sum_{n=1\ (\text{odd})}^{\infty}\frac{(TK\,\mathrm{e}^{-S_0})^n}{n!} \\ &= \left(\frac{m\omega}{\pi}\right)^{1/2}\mathrm{e}^{-\omega T/2}\sinh(TK\,\mathrm{e}^{-S_0})\ . \end{aligned} \tag{2.1.37}$$

On the other hand, using the eigenstates $|n\rangle$ and eigenvalues of the energy E_n in (2.1.29), we obtain

$$\begin{aligned}\langle x'|\,\mathrm{e}^{-HT}|x\rangle &= \sum_n \langle x'|n\rangle\langle n|x\rangle\,\mathrm{e}^{-E_nT} \\ &= \sum_n \phi_n(x')\phi_n^*(x)\,\mathrm{e}^{-E_nT}\ . \end{aligned} \tag{2.1.38}$$

Comparing (2.1.36) with (2.1.37), we obtain two energy levels:

$$E_\pm = \frac{\omega}{2} \pm K\,\mathrm{e}^{-S_0}\ . \tag{2.1.39}$$

This can be interpreted as splitting of the ground state energies around $\pm x_0$ due to the tunnelling contribution $K\,\mathrm{e}^{-S_0}$.

The reader might wonder why such a long-winded method has been presented, whereas the normal WKB method would have been sufficient for the calculation. Indeed, for this simple case of a single particle in one dimension, this is the case; however, when proceeding to many-particle systems, that is, quantum field theory, the generalization of the instanton calculation can be done easily. On the other hand, the WKB method, based on fitting boundary conditions of solutions in different regions of a differential equation, becomes very complicated in a more generalized case.

2.2 The Path Integral for Bosons

In the previous section, we introduced the path integral for a single-particle system. In the present and the following section, the path integral of the many-particle system using second quantization is presented. A more precise discussion can be found in the literature [G.16].

As first step in this section, the bosonic system will be discussed, which is quite analogous to the classical case, so the method will be almost parallel to the previous section. Two points have to be noticed: first observe the correspondence of the operators

$$\hat{x} \leftrightarrow \hat{\psi}(\boldsymbol{r}) \quad \text{and} \quad \hat{p} \leftrightarrow \mathrm{i}\hbar\hat{\psi}^{\dagger}(\boldsymbol{r}) \ , \tag{2.2.1}$$

and next notice that it becomes necessary to perform the sum (integral) in $\boldsymbol{r}$. For simplicity, we set $\hbar = 1$ in this section. Doing so, the partition function in the imaginary time formalism becomes by analogy to (2.1.28)

$$Z = \int \mathcal{D}\bar{\psi}(\boldsymbol{r},\tau)\mathcal{D}\psi(\boldsymbol{r},\tau)\, \mathrm{e}^{-S(\{\bar{\psi}\},\{\psi\})} \ , \tag{2.2.2}$$

$$S = \int_0^{\beta} \mathrm{d}\tau \int \mathrm{d}\boldsymbol{r}\, \bar{\psi}(\boldsymbol{r},\tau)\partial_t\psi(\boldsymbol{r},\tau) + \int_0^{\beta} \mathrm{d}\tau\, H(\tau) \ , \tag{2.2.3}$$

with

$$\begin{aligned} H(\tau) = &\int \mathrm{d}\boldsymbol{r} \left(\frac{1}{2m}\nabla\bar{\psi}(\boldsymbol{r},\tau)\nabla\psi(\boldsymbol{r},\tau) - \mu\bar{\psi}(\boldsymbol{r},\tau)\psi(\boldsymbol{r},\tau) \right) \\ &+ \frac{1}{2}\int \mathrm{d}\boldsymbol{r}\,\mathrm{d}\boldsymbol{r}'\, \bar{\psi}(\boldsymbol{r})\bar{\psi}(\boldsymbol{r}')v(\boldsymbol{r}-\boldsymbol{r}')\psi(\boldsymbol{r}')\psi(\boldsymbol{r}) \ . \end{aligned} \tag{2.2.4}$$

In (2.2.3) and (2.2.4), $\bar{\psi}(\boldsymbol{r},\tau)$ and $\psi(\boldsymbol{r},\tau)$ correspond to the operators $\hat{\psi}^{\dagger}(\boldsymbol{r},\tau)$ and $\hat{\psi}(\boldsymbol{r},\tau)$. However, they are not operators, but c-number functions of $\boldsymbol{r}$ and τ.

Notice that we have chosen the grand canonical ensemble, where instead of a constant particle number, the chemical potential μ has been introduced.

The reader might think that ψ and $\bar{\psi}$ are complex conjugate; however, this must not be the case. When restricting to one $\boldsymbol{r}, t$, we have the line integrals

$$\int \mathrm{d}\bar{\psi}\,(\boldsymbol{r},\tau) \ , \qquad \int \mathrm{d}\psi\,(\boldsymbol{r},\tau) \ ,$$

and since the path on the $\bar{\psi}$-plane and the ψ-plane can be altered independently, in general $\bar{\psi}$ can be independent of ψ. Starting from Chap. 4, the path of this complex contour integral will be chosen by the saddle-point method, where S becomes larger in every direction when the path is deviating from the saddle-point solution.

Next, we introduce by the following equation another important physical function besides the partition function, namely the thermal Green function $\mathcal{G}(\boldsymbol{r},\boldsymbol{r}';\tau,\tau')$:

$$\begin{aligned} \mathcal{G}(\boldsymbol{r},\boldsymbol{r}';\tau,\tau') &= -\langle \mathrm{T}_{\tau}\psi(\boldsymbol{r},\tau)\psi^{\dagger}(\boldsymbol{r}',\tau')\rangle \\ &= \begin{cases} -\langle\psi(\boldsymbol{r},\tau)\psi^{\dagger}(\boldsymbol{r}',\tau')\rangle & (\text{for } \tau > \tau') \\ -\langle\psi^{\dagger}(\boldsymbol{r}',\tau')\psi(\boldsymbol{r},\tau)\rangle & (\text{for } \tau < \tau') \end{cases} \ . \end{aligned} \tag{2.2.5}$$

Here, T_τ is the time ordering operator. In terms of the functional integral, the Green function is given by

$$\mathcal{G}(\boldsymbol{r},\boldsymbol{r}';\tau,\tau') = -\frac{1}{Z}\int \mathcal{D}\bar{\psi}\mathcal{D}\psi\,\psi(\boldsymbol{r},\tau)\bar{\psi}(\boldsymbol{r}',\tau)\,\mathrm{e}^{-S(\{\bar{\psi}\},\{\psi\})} \quad . \tag{2.2.6}$$

The proof proceeds in the same manner as in Sect. 2.1. Notice that in the path integral, the Green function is automatically time ordered. Now, let us consider the Green function explicitly in the case where the interaction is set to zero ($v(\boldsymbol{r}-\boldsymbol{r}')=0$). We perform the Fourier transformation

$$\psi(\boldsymbol{r},\tau) = (\beta V)^{-1/2}\sum_{\boldsymbol{k},\omega}\mathrm{e}^{-\mathrm{i}\omega\tau+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}a(\boldsymbol{k},\omega) \quad , \tag{2.2.7}$$

$$\bar{\psi}(\boldsymbol{r},\tau) = (\beta V)^{-1/2}\sum_{\boldsymbol{k},\omega}\mathrm{e}^{\mathrm{i}\omega\tau-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}\bar{a}(\boldsymbol{k},\omega) \quad . \tag{2.2.8}$$

Imposing the boundary conditions $\psi(\boldsymbol{r},\beta)=\psi(\boldsymbol{r},0)$ and $\bar{\psi}(\boldsymbol{r},\beta)=\bar{\psi}(\boldsymbol{r},0)$, only discrete values $\omega = 2\pi n/\beta$ for ω ($n=$ integer) become possible, which are the so-called Matsubara frequencies. S becomes

$$S_0 = \sum_{\boldsymbol{k},\omega}\left(-\mathrm{i}\omega + \frac{\boldsymbol{k}^2}{2m} - \mu\right)\bar{a}(\boldsymbol{k},\omega)a(\boldsymbol{k},\omega) \tag{2.2.9}$$

and (2.2.5) is equal to

$$\begin{aligned}\mathcal{G}(\boldsymbol{r},\boldsymbol{r}';\tau,\tau') = &-\frac{1}{\beta}\sum_{\boldsymbol{k}_1,\omega_1}\sum_{\boldsymbol{k}_2,\omega_2}\frac{1}{Z}\int\prod_{\boldsymbol{k},\omega}\mathrm{d}a\,(\boldsymbol{k},\omega)\,\mathrm{d}\bar{a}\,(\boldsymbol{k},\omega)\\ &\times a(\boldsymbol{k}_1,\omega_1)\bar{a}(\boldsymbol{k}_2,\omega_2)\\ &\times \exp\left[\sum_{\boldsymbol{k},\omega}\left(\mathrm{i}\omega - \frac{\boldsymbol{k}^2}{2m}+\mu\right)\bar{a}(\boldsymbol{k},\omega)a(\boldsymbol{k},\omega)\right]\\ &\times \exp[\,\mathrm{i}\,(-\omega_1\tau+\boldsymbol{k}_1\cdot\boldsymbol{r})]\exp[\,\mathrm{i}\,(\omega_2\tau'-\boldsymbol{k}_2\cdot\boldsymbol{r}')] \quad .\end{aligned} \tag{2.2.10}$$

Essentially, by setting $\bar{a}(\boldsymbol{k},\omega)=[a(\boldsymbol{k},\omega)]^* = a'(\boldsymbol{k},\omega)-\mathrm{i}a''(\boldsymbol{k},\omega)$ and performing the Gauss integral in a' and a'' from $-\infty$ to $+\infty$, only the term with $\boldsymbol{k}_1=\boldsymbol{k}_2$ and $\omega_1=\omega_2$ contributes. Then, (2.2.10) becomes

$$\mathcal{G}(\boldsymbol{r},\boldsymbol{r}';\tau,\tau') = \frac{1}{\beta V}\sum_{\boldsymbol{k}_1,\omega_1}\frac{1}{\mathrm{i}\omega_1-\boldsymbol{k}_1^2/2m+\mu}\,\mathrm{e}^{-\mathrm{i}\omega_1(\tau-\tau')+\mathrm{i}\boldsymbol{k}_1\cdot(\boldsymbol{r}-\boldsymbol{r}')} \quad . \tag{2.2.11}$$

Writing $\mathcal{G}(\boldsymbol{k},\mathrm{i}\omega_n)$ $[\omega_n = 2\pi kTn]$ for the Fourier transformation of $\mathcal{G}(\boldsymbol{r},\boldsymbol{r}';\tau,\tau')$, we obtain $\mathcal{G}(\boldsymbol{k},\mathrm{i}\omega_n) = (\mathrm{i}\omega_n - \boldsymbol{k}^2/2m+\mu)^{-1}$.

The reader might already know the following direct proof for $\mathcal{G}(\boldsymbol{k},\mathrm{i}\omega_n) = (\mathrm{i}\omega_n - \boldsymbol{k}^2/2m+\mu)^{-1}$ starting from (2.2.5). The Hamiltonian is given by

$$
\begin{aligned}
H &= \sum_{\boldsymbol{k}} \left(\frac{\boldsymbol{k}^2}{2m} - \mu \right) a^\dagger(\boldsymbol{k}) a(\boldsymbol{k}) \\
&\equiv \sum_{\boldsymbol{k}} \xi_{\boldsymbol{k}} a^\dagger(\boldsymbol{k}) a(\boldsymbol{k})
\end{aligned} \tag{2.2.12}
$$

and with

$$
a(\boldsymbol{k},\tau) = \mathrm{e}^{-\xi_{\boldsymbol{k}}\tau} a(\boldsymbol{k}) \ , \qquad a^\dagger(\boldsymbol{k},\tau) = \mathrm{e}^{\xi_{\boldsymbol{k}}\tau} a^\dagger(\boldsymbol{k})
$$

for $0 < \tau < \beta$, we obtain

$$
\begin{aligned}
\mathcal{G}(\boldsymbol{r},\boldsymbol{r}';\tau,0) &= -\frac{1}{V} \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2} \langle a(\boldsymbol{k}_1) a^\dagger(\boldsymbol{k}_2) \rangle \, \mathrm{e}^{-\xi_{\boldsymbol{k}_1}\tau} \, \mathrm{e}^{\mathrm{i}(\boldsymbol{k}_1\cdot\boldsymbol{r} - \boldsymbol{k}_2\cdot\boldsymbol{r}')} \\
&= -\frac{1}{V} \sum_{\boldsymbol{k}_1} [1 + n(\boldsymbol{k}_1)] \, \mathrm{e}^{-\xi_{\boldsymbol{k}_1}\tau} \, \mathrm{e}^{\mathrm{i}\boldsymbol{k}_1\cdot(\boldsymbol{r}-\boldsymbol{r}')} \quad .
\end{aligned} \tag{2.2.13}
$$

Performing the Fourier transformation, we obtain

$$
\begin{aligned}
\mathcal{G}(\boldsymbol{k},\mathrm{i}\omega_n) &= \int_0^\beta \mathrm{d}\tau \, \mathrm{e}^{\mathrm{i}\omega_n\tau} \int \mathrm{d}(\boldsymbol{r}-\boldsymbol{r}') \, \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')} \mathcal{G}(\boldsymbol{r},\boldsymbol{r}';\tau,0) \\
&= -[1 + n(\boldsymbol{k})] \int_0^\beta \mathrm{d}\tau \exp[(\mathrm{i}\omega_n - \xi_{\boldsymbol{k}})\tau] \\
&= -[1 + n(\boldsymbol{k})] \frac{\exp[-\beta\xi_{\boldsymbol{k}}] - 1}{\mathrm{i}\omega_n - \xi_{\boldsymbol{k}}} = \frac{1}{\mathrm{i}\omega_n - \xi_{\boldsymbol{k}}} \quad .
\end{aligned} \tag{2.2.14}
$$

This expression agrees with the result we obtained before. More generally, using the energy eigenvalues and eigenfunctions of the system in (2.2.5), we obtain the spectral decomposition

$$
\begin{aligned}
\mathcal{G}(\boldsymbol{k},\mathrm{i}\omega_n) &= -\int_0^\beta \mathrm{d}\tau \, \mathrm{e}^{\mathrm{i}\omega_n\tau} \langle a(\boldsymbol{k},\tau) a^\dagger(\boldsymbol{k}) \rangle \\
&= -\frac{1}{Z} \int_0^\beta \mathrm{d}\tau \, \mathrm{e}^{\mathrm{i}\omega_n\tau} \sum_{n,m} \mathrm{e}^{-\beta E_n} \langle n|a(\boldsymbol{k})|m\rangle \, \mathrm{e}^{\tau(E_n - E_m)} \langle m|a^\dagger(\boldsymbol{k})|n\rangle \\
&= -\frac{1}{Z} \sum_{n,m} |\langle n|a(\boldsymbol{k})|m\rangle|^2 \int_0^\beta \mathrm{d}\tau \, \mathrm{e}^{\tau(\mathrm{i}\omega_n + E_n - E_m)} \, \mathrm{e}^{-\beta E_n} \\
&= \frac{1}{Z} \sum_{n,m} \frac{|\langle n|a(\boldsymbol{k})|m\rangle|^2}{\mathrm{i}\omega_n - (E_m - E_n)} (\mathrm{e}^{-\beta E_n} - \mathrm{e}^{-\beta E_m}) \quad .
\end{aligned} \tag{2.2.15}
$$

Next, we want to link the imaginary time formalism developed so far with the real-time formalism. For this purpose, we introduce the advanced Green function and the retarded Green function $G^{\mathrm{A}}(\boldsymbol{k},\omega)$, $G^{\mathrm{R}}(\boldsymbol{k},\omega)$

$$
G^{\mathrm{A}}(\boldsymbol{k},\omega) = +\mathrm{i} \int_{-\infty}^0 \langle [a(\boldsymbol{k},t), a^\dagger(\boldsymbol{k})] \rangle \, \mathrm{e}^{\mathrm{i}\omega t + \delta t} \mathrm{d}t \quad , \tag{2.2.16}
$$

$$G^{\mathrm{R}}(\boldsymbol{k},\omega) = -\mathrm{i}\int_0^{\infty} \langle [a(\boldsymbol{k},t), a^{\dagger}(\boldsymbol{k})] \rangle \, \mathrm{e}^{\mathrm{i}\omega t - \delta t} \mathrm{d}t \quad , \tag{2.2.17}$$

where δ is an infinitesimal positive constant introduced to make the t integral converge. The spectral decomposition corresponding to (2.2.15) now reads

$$G^{\mathrm{A,R}}(\boldsymbol{k},\omega) = \frac{1}{Z}\sum_{n,m} \frac{|\langle n|a(\boldsymbol{k})|m\rangle|^2}{\omega \mp \mathrm{i}\delta - (E_m - E_n)} (\mathrm{e}^{-\beta E_n} - \mathrm{e}^{-\beta E_m}) \quad . \tag{2.2.18}$$

Comparing this with (2.2.15), (2.2.16) and (2.2.17), we see that by analytic continuation of $\mathrm{i}\omega_n$ in the thermal Green function to $\omega - \mathrm{i}\delta$ ($\omega + \mathrm{i}\delta$), the advanced Green function (retarded Green function) can be obtained. For a system at finite temperature, this suggests the method to calculate first the thermal Green function in the complex time formalism, and then to obtain by analytic continuation $\mathrm{i}\omega_n \to \pm\omega \mp \mathrm{i}\delta$ the Green functions G^A and G^R in the real-time formalism. This formalism is named after its inventor and is called the Matsubara formalism.

Next, we want to compare the advantages of the path integral method with those of the operator formalism. The advantage is that no operators are present, but only c-numbers (commutators are trivial). However, the price we pay is an infinite-dimensional integral.

In the case when an interaction $v(\boldsymbol{r} - \boldsymbol{r}')$ is present, the most popular technique might be perturbation theory. This means splitting S in (2.2.6) into $S_0 + S_1$, and expanding e^{-S_1}, and because S_1 is a simple c-number function containing no operators, the expansion is possible. In this case the cumulant analysis of the Gauss-integral can be applied; for example,

$$\langle \psi_1 \psi_2 \psi_3^{\dagger} \psi_4^{\dagger} \rangle = \langle \psi_1 \psi_3^{\dagger} \rangle \langle \psi_2 \psi_4^{\dagger} \rangle + \langle \psi_1 \psi_4^{\dagger} \rangle \langle \psi_2 \psi_3^{\dagger} \rangle \quad . \tag{2.2.19}$$

Now, because we are dealing with c-numbers, the variational method can be introduced easily. Splitting S in (2.2.2) into the sum of the "trial action" S_0 and $S - S_0$, we can write

$$Z = Z_0 \langle \mathrm{e}^{-S+S_0} \rangle_{S_0} \quad . \tag{2.2.20}$$

Here, Z_0 is the partition function of the action S_0 and $\langle \ \rangle_{S_0}$ means averaging with respect to e^{-S_0}. Because S and S_0 are in general real, with $\exp[(x_1 + x_2)/2] \le (\mathrm{e}^{x_1} + \mathrm{e}^{x_2})/2$, we obtain $\exp[-\langle S - S_0 \rangle_{S_0}] \le \langle \exp[-S + S_0] \rangle_{S_0}$ and therefore

$$J = -k_{\mathrm{B}} T \ln Z \leqq -k_{\mathrm{B}} T \ln Z_0 + k_{\mathrm{B}} T \langle S - S_0 \rangle_{S_0} \quad . \tag{2.2.21}$$

Here, k_{B} is the Boltzmann's constant and $J = -pV$ is the thermal potential of the grand canonical ensemble. The right-hand side can be calculated when S_0 is determined, and by optimizing the variation parameter in it, it is possible to determine the best S_0 for this framework. In practise, because almost only Gauss integrals can be performed, S_0 is often quadratic in ψ and $\bar{\psi}$, and often this approximation agrees with the mean field approximation.

So far we have discussed the bosonic path integral. Starting from Chap. 1, ψ appeared on the stage and "evolved". This flow is shown in Fig. 2.4, and when we meet ψ, it is important to remember to which step ψ corresponds.

Single-particle quantum mechanics
$\psi(\boldsymbol{r}, t)$: wave function in three-dimensional space

$\Downarrow$

Many-particle quantum mechanics, first quantization
$\psi(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N, t)$: wave function in $3N$-dimensional space

$\Downarrow$

Many-particle quantum mechanics, second quantization
$\hat{\psi}^\dagger(\boldsymbol{r}, t), \hat{\psi}(\boldsymbol{r}, t)$: Annihilation and creation operators of the field in three-dimensional space

$\Downarrow$

Path integral representation of field theory
$\bar{\psi}(\boldsymbol{r}, t), \psi(\boldsymbol{r}, t)$: function of three-dimensional space and of time (integration variable in the functional integral)

Fig. 2.4

2.3 The Path Integral for Fermions

In this section we discuss the case of fermions. Different from the bosonic case, a correspondence to a classical system does not exist. The reader might think that in this case the path integral method is useless; however, this is not the case. At least mathematically, by introducing Grassmann numbers, the description can be given in a manner totally similar to the bosonic case.

Corresponding to the anti-commutation relations of fermions, Grassmann numbers are defined to be anti-commuting, that is $x_i x_j + x_j x_i = 0$. Therefore, $x_i^2 = 0$ holds, and we conclude that every function in $x_1, \ldots, x_n$ can be written as

$$f(x_1 \ldots, x_N) = \sum_{n=0}^{N} \sum_{i_1 < i_2 < \cdots < i_n} C_n(i_1, \ldots, i_n) x_{i_1} \ldots x_{i_n} \quad . \tag{2.3.1}$$

Here $i_1, \ldots, i_n$ is a disjunct set of indices $1 - N$, and we define the order to be $i_1 < i_2 < \cdots < i_n$. The coefficient $C_n(i_1, \ldots, i_n)$ is a simple complex function. We define the "integral" of this function as follows:

$$\int x_{i_1} \dots x_{i_n} \, \mathrm{d}x_{j_n} \dots \mathrm{d}x_{j_1} = \varepsilon \begin{pmatrix} i_1, \dots, i_n \\ j_1, \dots, j_n \end{pmatrix} \quad . \tag{2.3.2}$$

Here, $\varepsilon(\cdots)$ is different from zero only for the case when $(i_1, \dots, i_n)$ equals $(j_1, \dots, j_n)$. Then, it is $+1$ when both sets become identical under an even number of permutations and -1 when both set become identical under an odd number of permutations. We choose N even $(= 2n)$ and split $x_1, \dots, x_N$ into $\psi_1, \dots, \psi_n$ and $\bar{\psi}_1, \dots, \bar{\psi}_n$, with ψ and $\bar{\psi}$ corresponding to the fermionic operators $\hat{\psi}_i$ and $\hat{\psi}_i^\dagger$, respectively. The index i then indicates the space coordinates $\boldsymbol{r}$ and the complex time τ $(i = (\boldsymbol{r}, \tau))$. From (2.3.2), we deduce that for a c-number $n \times n$ matrix A with components A_{ij}

$$\int \exp\left[- \sum_{i,j} \bar{\psi}_i A_{ij} \psi_j \right] \prod_{i=1}^{n} \mathrm{d}\bar{\psi}_i \, \mathrm{d}\psi_i = \det A \tag{2.3.3}$$

holds. (The proof is left as an exercise.) If ψ and $\bar{\psi}$ had been c-numbers, then the result would have been $(\det A)^{-1}$.

As for the case of the bosons, we define the coherent state of one fermion as follows:

$$|\{\psi(\boldsymbol{r})\}\rangle = \prod_{\boldsymbol{r}} (|0_{\boldsymbol{r}}\rangle + |1_{\boldsymbol{r}}\rangle \psi(\boldsymbol{r})) \quad , \tag{2.3.4}$$

$$\langle\{\bar{\psi}(\boldsymbol{r})\}| = \prod_{\boldsymbol{r}} (\langle 0_{\boldsymbol{r}}| + \bar{\psi}(\boldsymbol{r}) \langle 1_{\boldsymbol{r}}|) \quad . \tag{2.3.5}$$

Here, $|0_{\boldsymbol{r}}\rangle, |1_{\boldsymbol{r}}\rangle$ are the states where at $\boldsymbol{r}$ no fermion or one fermion is present, respectively. The completeness relation

$$\int |\{\psi(\boldsymbol{r})\}\rangle \langle \{\bar{\psi}(\boldsymbol{r})\}| \exp\left[- \sum_{\boldsymbol{r}} \bar{\psi}(\boldsymbol{r}) \psi(\boldsymbol{r}) \right] \prod_{\boldsymbol{r}} \mathrm{d}\bar{\psi}(\boldsymbol{r}) \, \mathrm{d}\psi(\boldsymbol{r}) = 1 \tag{2.3.6}$$

holds because at every $\boldsymbol{r}$ the equation

$$\begin{aligned} &\int (|0\rangle + |1\rangle\psi)(\langle 0| + \bar{\psi}\langle 1|) \, e^{-\bar{\psi}\psi} \, \mathrm{d}\bar{\psi} \, \mathrm{d}\psi \\ &\quad = \int (|0\rangle\langle 0|(1 + \psi\bar{\psi}) + |0\rangle\langle 1|\bar{\psi} + |1\rangle\langle 0|\psi + |1\rangle\langle 1|\psi\bar{\psi}) \, \mathrm{d}\bar{\psi} \, \mathrm{d}\psi \\ &\quad = |0\rangle\langle 0| + |1\rangle\langle 1| = 1 \end{aligned} \tag{2.3.7}$$

holds.

Similarly to (2.3.7), for every operator A we obtain

$$\begin{aligned} \int \langle -\bar{\psi}|A|\psi\rangle \, e^{-\bar{\psi}\psi} \, \mathrm{d}\bar{\psi} \, \mathrm{d}\psi &= \int ((\langle 0| - \bar{\psi}\langle 1|) A (|0\rangle + \psi|1\rangle))(1 - \bar{\psi}\psi) \, \mathrm{d}\bar{\psi} \, \mathrm{d}\psi \\ &= \langle 0|A|0\rangle + \langle 1|A|1\rangle = \operatorname{Tr} A \quad . \end{aligned} \tag{2.3.8}$$

Using (2.3.7) and (2.3.8), the partition function becomes

$$
\begin{aligned}
Z &= \operatorname{Tr} e^{-\beta H} \\
&= \int \langle -\bar{\psi}_0 | e^{-\beta H/N} | \psi_{N-1} \rangle \langle \bar{\psi}_{N-1} | e^{-\beta H/N} | \psi_{N-2} \rangle \cdots \langle \bar{\psi}_1 | e^{-\beta H/N} | \psi_0 \rangle \\
&\quad \times \exp\left[-\sum_{i=0}^{N-1} \bar{\psi}_i \psi_i \right] \prod_{i=0}^{N-1} d\bar{\psi}_i \, d\psi_i \\
&= \int \exp\left[-\bar{\psi}_0 \psi_{N-1} - \frac{\beta}{N} H(-\bar{\psi}_0, \psi_{N-1}) \right] \\
&\quad \times \exp\left[\bar{\psi}_{N-1} \psi_{N-2} - \frac{\beta}{N} H(\bar{\psi}_{N-1}, \psi_{N-2}) \right] \\
&\quad \times \cdots \times \exp\left[\bar{\psi}_1 \psi_0 - \frac{\beta}{N} H(\bar{\psi}_1, \psi_0) \right] \exp\left[-\sum_{i=0}^{N-1} \bar{\psi}_i \psi_i \right] \prod_{i=0}^{N-1} d\bar{\psi}_i \, d\psi_i \\
&= \int \exp\Bigg[-\bar{\psi}_0 \psi_{N-1} - \bar{\psi}_0 \psi_0 - \frac{\beta}{N} H(-\bar{\psi}_0, \psi_{N-1}) \\
&\quad - \sum_{i=1}^{N-1} \left\{ \bar{\psi}_i (\psi_i - \psi_{i-1}) + \frac{\beta}{N} H(\bar{\psi}_i, \psi_{i-1}) \right\} \Bigg] \prod_{i=0}^{N-1} d\bar{\psi}_i \, d\psi_i \quad . \qquad (2.3.9)
\end{aligned}
$$

Requiring for $\bar{\psi}_N$ and ψ_N the anti-periodic boundary conditions

$$
\psi_N = -\psi_0 \ , \qquad \bar{\psi}_N = -\bar{\psi}_0 \ , \tag{2.3.10}
$$

the sign in the exponential of (2.3.9) changes, and the action S becomes

$$
S = \sum_{i=1}^{N} \left[\bar{\psi}_i (\psi_i - \psi_{i-1}) + \frac{\beta}{N} H(\bar{\psi}_i, \psi_{i-1}) \right] \ , \tag{2.3.11}
$$

and formally taking the limit $N \to \infty$, we can write

$$
S = \int_0^\beta d\tau \, [\bar{\psi}(\tau) \partial_\tau \psi(\tau) + H(\bar{\psi}(\tau), \psi(\tau))] \ . \tag{2.3.12}
$$

In this case, corresponding to (2.3.10), we write

$$
\psi(\beta) = -\psi(0) \ , \qquad \bar{\psi}(\beta) = -\bar{\psi}(0) \ . \tag{2.3.13}
$$

Therefore, the Fourier transformation of $\bar{\psi}(\tau)$ and $\psi(\tau)$ is given by

$$
\begin{aligned}
\psi(\tau) &= \frac{1}{\beta} \sum_{i\omega_n} e^{-i\omega_n \tau} \psi(\omega_n) \ , \\
\bar{\psi}(\tau) &= \frac{1}{\beta} \sum_{i\omega_n} e^{i\omega_n \tau} \bar{\psi}(\omega_n) \ .
\end{aligned} \tag{2.3.14}
$$

The Matsubara frequencies ω_n become $\omega_n = \pi k_B T(2n+1)$, and the Green function $\mathcal{G}(\tau) = -\langle T\psi(\tau)\psi^\dagger(0)\rangle$ is anti-periodic $\mathcal{G}(\tau+\beta) = -\mathcal{G}(\tau)$.

2.4 The Path Integral for the Gauge Field

Up to now, we have discussed the quantization of the bosons and fermions. Next, we will discuss the quantization of the gauge field with path integral methods.

For the case of a vanishing interaction, the action is quadratic, and the Green function is the inverse of the coefficient matrix of this quadratic form. Let us apply this fact to the electromagnetic field. In the imaginary time formalism, we set $x_\mu = (\tau, x, y, z)$ and $k_\mu = (\omega, k_x, k_y, k_z)$. Because in this formalism the space–time is Euclidian, we do not need to distinguish upper and lower indices. At the zero temperature, the action is given by

$$
\begin{aligned}
S &= \sum_{\mu,\nu} \frac{1}{16\pi} \int \mathrm{d}^4 x F_{\mu\nu}^2(x) \\
&= \sum_{\mu,\nu} \frac{1}{16\pi} \int \mathrm{d}^4 x (\partial_\mu A_\nu(x) - \partial_\nu A_\mu(x))^2 \\
&= \frac{1}{16\pi} \sum_{\mu,\nu,k} (k_\mu A_\nu(k) - k_\nu A_\mu(k))(k_\mu A_\nu(-k) - k_\nu A_\mu(-k)) \quad . \qquad (2.4.1)
\end{aligned}
$$

Splitting $A_\mu(k)$ into its longitudinal component $A_\mu^{\mathrm{L}}(k) = (k_\mu k_\nu / k^2) A_\nu(k)$ and its transversal component $A_\mu^{\mathrm{T}}(k) = A_\mu(k) - A_\mu^{\mathrm{L}}$, we can write (2.4.1) as

$$
\begin{aligned}
S &= \frac{1}{8\pi} \sum_{k,\mu,\nu} (k^2 \delta_{\mu,\nu} - k_\mu k_\nu) A_\mu(k) A_\nu(-k) \\
&= \frac{1}{8\pi} \sum_{k,\mu,\nu} (k^2 \delta_{\mu,\nu} - k_\mu k_\nu) A_\mu^{\mathrm{T}}(k) A_\nu^{\mathrm{T}}(-k) \quad . \qquad (2.4.2)
\end{aligned}
$$

This equation does not contain A_μ^{L}. Therefore, it is possible to define a Green function for the transversal component, but, curiously, not for the longitudinal component.

In Sect. 1.4, we performed the canonical quantization of the electromagnetic field using the commutation relations. So, what is the problem with the path integral description? The answer is that we fixed a gauge ($\mathrm{div}\, \boldsymbol{A} = 0$) in the previous case, and in (2.4.1) we did not say anything about the gauge. Therefore, when exponentiating (2.4.1) and performing the path integral $\int \mathcal{D}A_\mu$, paths that are in reality equal and differ only by a different choice of the gauge pile up in the calculation. Because there exist infinitely many choices for the gauge, there is nothing strange about it when the path integral diverges, and indeed because (2.4.2) does not contain A_μ^{L}, the functional integral in A_μ^{L} diverges.

Therefore, the question is: How do we implement the gauge fixing conditions in the path integral? The answer is given by the Faddeev–Popov technique. In what follows, we will explain this method.

Let us choose for A_μ one fixed function $\bar{A}_\mu(\boldsymbol{r},\tau)$. Performing a gauge transformation with $\Lambda(\boldsymbol{r},\tau)$, then $\bar{A}_\mu(\boldsymbol{r},\tau)$ is transformed to $A_\mu = \bar{A}_\mu(\boldsymbol{r},\tau) + \partial_\mu \Lambda$. Physically, this A_μ is identical to $\bar{A}_\mu$, and because the action is gauge invariant, $S(A_\mu) = S(\bar{A}_\mu)$. When performing the path integral $\int \mathcal{D}A_\mu$, for all possible functions Λ the physically identical field A_μ reappears again and again. We write

$$\begin{aligned} Z &= \int \mathcal{D}A_\mu \, \mathrm{e}^{-S(\{A_\mu\})} \\ &= \int \mathcal{D}\bar{A}_\nu \int \mathcal{D}\Lambda \, \mathrm{e}^{-S(\{A_\mu\})} \quad . \end{aligned} \tag{2.4.3}$$

Here, $\int \mathcal{D}\Lambda$ is responsible for the divergence.

In order to absorb this divergent integral, we introduce a functional $F(A_\mu)$ of A_μ and write instead of $\int \mathcal{D}\Lambda$

$$\begin{aligned} \int \mathcal{D}\Lambda &\to \int \mathcal{D}F(A_\mu) \exp\left[-\int \mathrm{d}\boldsymbol{r}\,\mathrm{d}\tau \frac{F^2}{2\alpha}\right] \\ &= \int \mathcal{D}\Lambda \det\left(\frac{\delta F}{\delta \Lambda}\right) \exp\left[-\int \mathrm{d}\boldsymbol{r}\,\mathrm{d}\tau \frac{F^2}{2\alpha}\right] \quad . \end{aligned} \tag{2.4.4}$$

This rewriting contains arbitrariness, because every function leading to a convergent result can be used. Because we want to recover the integral $\int \mathcal{D}\bar{A}_\mu \int \mathcal{D}\Lambda = \int \mathcal{D}A_\mu$ (this means that we want to perform the functional integration in A_μ without restrictions), we choose (2.4.4) in such a way that it is independent of $\bar{A}_\mu$ and contains a functional integral in Λ. Concerning F, from the requirement that $-F^2/2\alpha$ should be quadratic in A_μ; normally F is set to be

$$F = \partial_\mu A_\mu \quad . \tag{2.4.5}$$

$F = 0$ leads to the Lorentz gauge. In the above case we obtain $\delta F = F(\Lambda + \delta\Lambda) - F(\Lambda) = \partial_\mu^2 \delta\Lambda$ and therefore $\det[\delta F/\delta\Lambda] = \det[\partial_\mu^2]$. Because this is an A_μ-independent constant, we finally obtain

$$Z = \int \mathcal{D}A_\mu \exp\left[-S - \frac{1}{2\alpha}\int (\partial_\mu A_\mu)^2 \,\mathrm{d}\boldsymbol{r}\,\mathrm{d}\tau\right] \quad . \tag{2.4.6}$$

Here, instead of (2.4.2), in the exponent we obtain

$$-\frac{1}{8\pi}\sum_{k,\mu,\nu}(k^2\delta_{\mu,\nu} - k_\mu k_\nu)A_\mu^{\mathrm{T}}(k)A_\nu^{\mathrm{T}}(-k) - \frac{1}{2\alpha}\sum_{k,\mu,\nu} k_\mu k_\nu A_\mu^{\mathrm{L}}(k)A_\nu^{\mathrm{L}}(-k) \tag{2.4.7}$$

and a Green function for A_μ^{L} can be defined.

As demonstrated, for the case when the gauge is not totally fixed, the functional integral over the remaining degrees of freedom is made to converge by adding a new term to the action (in the above example this is the gauge fixing term $F^2/2\alpha$). This is the so-called the Faddeev–Popov technique.

2.5 The Path Integral for the Spin System

Quantization using path integral techniques is possible also for a spin system. For simplicity, we consider a system with only one spin $I = 1/2$. In this case, the space of states can be written as a two-vector with up-spin component $\uparrow$ and down-spin component $\downarrow$:

$$|\psi\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle = \begin{bmatrix}\alpha \\ \beta\end{bmatrix} \quad . \tag{2.5.1}$$

Here, α and β are complex numbers, and the normalization is $|\alpha|^2 + |\beta|^2 = 1$. The system has three real degrees of freedom. Using the variables b, θ and φ we can write

$$|\psi\rangle = |b, \theta, \varphi\rangle = \mathrm{e}^{\mathrm{i}b}\left(\mathrm{e}^{-\mathrm{i}\varphi/2}\cos\frac{\theta}{2}|\uparrow\rangle + \mathrm{e}^{\mathrm{i}\varphi/2}\sin\frac{\theta}{2}|\downarrow\rangle\right) \quad , \tag{2.5.2}$$

where $\mathrm{e}^{\mathrm{i}b}$ is an overall phase factor and therefore has no influence on the physics. More precisely, b corresponds to the degree of freedom of the gauge transformation. It can be proved as follows that $|b, \theta, \varphi\rangle$ is a complete set with b fixed and θ and φ variable:

$$\begin{aligned}\int_0^\pi \sin\theta\,\mathrm{d}\theta \int_0^{2\pi} \frac{\mathrm{d}\varphi}{2\pi}|b, \theta, \varphi\rangle\langle b, \theta, \varphi| &= |\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow| \\ &= \hat{1} \quad .\end{aligned} \tag{2.5.3}$$

Furthermore, the expectation value of the spin operator $\hat{\boldsymbol{I}} = \frac{1}{2}\boldsymbol{\sigma}$ is given by

$$\begin{aligned}\langle b, \theta, \varphi|\hat{\boldsymbol{I}}|b, \theta, \varphi\rangle &= \tfrac{1}{2}(\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta) \\ &= \tfrac{1}{2}\boldsymbol{n} \quad .\end{aligned} \tag{2.5.4}$$

$\boldsymbol{\sigma}$ are the so-called Pauli matrices

$$\sigma^x = \begin{bmatrix}0 & 1 \\ 1 & 0\end{bmatrix} \quad , \qquad \sigma^y = \begin{bmatrix}0 & -\mathrm{i} \\ \mathrm{i} & 0\end{bmatrix} \quad , \qquad \sigma^z = \begin{bmatrix}1 & 0 \\ 0 & -1\end{bmatrix} \quad , \tag{2.5.5}$$

written as a three-component vector.

As shown in (2.5.3), $|b, \theta, \varphi\rangle$ is a complete set; however, for different (θ, φ), the states $|b, \theta, \varphi\rangle$ are not orthogonal. However, when returning to the discussion of Sect. 2.1, it is clear that for the insertion of intermediate states into the path integral, (2.5.3) is sufficient. An important step for the calculation of the sum of states in $|\tau\rangle = |b(\tau), \theta(\tau), \varphi(\tau)\rangle$, is the following estimation of the time evolution during the infinitesimally small complex time $\Delta\tau$:

$$\begin{aligned}\langle\tau+\Delta\tau|\,\mathrm{e}^{-\Delta\tau H}|\tau\rangle &\cong \langle\tau+\Delta\tau|(1-\Delta\tau H)|\tau\rangle \\ &= \langle\tau+\Delta\tau|\tau\rangle - \Delta\tau\langle\tau+\Delta\tau|H|\tau\rangle \\ &\cong \left[\langle\tau| + \Delta\tau\left(\frac{\mathrm{d}\langle\tau|}{\mathrm{d}\tau}\right)\right]|\tau\rangle - \Delta\tau\langle\tau|H|\tau\rangle \\ &= 1+\Delta\tau[\langle\dot\tau|\tau\rangle - \langle\tau|H|\tau\rangle] \\ &\cong \mathrm{e}^{\Delta\tau[\langle\dot\tau|\tau\rangle-\langle\tau|H|\tau\rangle]} \quad . \end{aligned} \tag{2.5.6}$$

Because of

$$\begin{aligned} 0 = \frac{\mathrm{d}}{\mathrm{d}\tau}\langle\tau|\tau\rangle &= \langle\dot\tau|\tau\rangle + \langle\tau|\dot\tau\rangle \\ &= 2\,\mathrm{Re}\langle\tau|\dot\tau\rangle \end{aligned} \tag{2.5.7}$$

the first term in the exponential of (2.5.6) is imaginary and therefore leads to a phase factor. Because this phase was originally written as $\langle\tau+\Delta\tau \mid \tau\rangle$, in the time evolution of the system it has the meaning of the "overlap integral" of the wave functions at infinitesimally separated times, or in mathematical language is has the meaning of a "connection". For the single-particle path integral (Sect. 2.1), the corresponding factor is given by

$$\begin{aligned}\langle x(\tau+\Delta\tau)|x(\tau)\rangle &= \int \mathrm{d}p(\tau)\,\langle x(\tau+\Delta\tau)|p(\tau)\rangle\langle p(\tau)|x(\tau)\rangle \\ &= \int\frac{\mathrm{d}p(\tau)}{2\pi h}\,\mathrm{e}^{\mathrm{i}p(\tau)[x(\tau+\Delta\tau)-x(\tau)]} \\ &= \int\frac{\mathrm{d}p(\tau)}{2\pi h}\,\mathrm{e}^{\mathrm{i}\Delta\tau p(\tau)\dot x(\tau)} \quad . \end{aligned} \tag{2.5.8}$$

Notice that this is just the factor $\mathrm{i}p\dot{x}$.

Now, let us determine $\langle\dot\tau \mid \tau\rangle$ explicitely. With (2.5.2), we obtain

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\tau}|\tau\rangle = \mathrm{i}\dot b|\tau\rangle + \mathrm{e}^{\mathrm{i}b}\Big\{&\left(-\frac{\mathrm{i}\dot\varphi}{2}\cos\frac{\theta}{2} - \frac{\dot\theta}{2}\sin\frac{\theta}{2}\right)\mathrm{e}^{-\mathrm{i}\varphi/2}|\uparrow\rangle \\ &+\left(\frac{\mathrm{i}\dot\varphi}{2}\sin\frac{\theta}{2}+\frac{\dot\theta}{2}\cos\frac{\theta}{2}\right)\mathrm{e}^{\mathrm{i}\varphi/2}|\downarrow\rangle\Big\} \quad . \end{aligned} \tag{2.5.9}$$

Taking the inner product with $\langle\tau|$, we obtain

$$\begin{aligned}\langle\tau|\dot\tau\rangle &= -\langle\dot\tau|\tau\rangle \\ &= \mathrm{i}\dot b + \cos\frac{\theta}{2}\left(-\frac{\mathrm{i}\dot\varphi}{2}\cos\frac{\theta}{2}-\frac{\dot\theta}{2}\sin\frac{\theta}{2}\right) + \sin\frac{\theta}{2}\left(\frac{\mathrm{i}\dot\varphi}{2}\sin\frac{\theta}{2}+\frac{\dot\theta}{2}\cos\frac{\theta}{2}\right) \\ &= \mathrm{i}\left(\dot b - \frac{1}{2}\dot\varphi\cos\theta\right) \quad . \end{aligned} \tag{2.5.10}$$

Here, we will fix the gauge b with the following requirement. As is clear from equation (2.5.4), the physical meaning of θ and φ is the direction of the spin, and we require that $|\theta,\varphi\rangle$ should be unambiguously defined by the direction $\boldsymbol{n}$ of the spin. Then, the boundary condition $\boldsymbol{n}(\beta) = \boldsymbol{n}(0)$ in the path integral equals $|\theta(\beta),\varphi(\beta)\rangle = |\theta(0),\varphi(0)\rangle$, the periodicity of the wave function, which is convenient. In order to obtain an unambiguous expression, the factor $\mathrm{e}^{\pm\mathrm{i}\varphi/2}$ in (2.5.2) is problematic. This is due to the fact that when shifting $\varphi \to \varphi \pm 2\pi$, the direction of $\boldsymbol{n}$ is the same; however, $\mathrm{e}^{\pm\mathrm{i}\varphi/2}$ changes its sign. In order to resolve this problem, we could set $b = \pm\varphi/2$, so that $\mathrm{e}^{\pm\mathrm{i}\varphi/2}$ becomes either 1 or $\mathrm{e}^{\pm\mathrm{i}\varphi}$.

Now, let us choose $b = \varphi/2$. In order to calculate the sum of states, we have to perform the path integral in $\theta(\tau)$ and $\varphi(\tau)$ under the boundary condition $|\tau = \beta\rangle = |\tau = 0\rangle$. Every path corresponds to a closed path on the unit sphere, described by the vector $\boldsymbol{n}$ of (2.5.4). Then, the integrand of the integral in (2.5.6) becomes e^{-S}, and the action S for $I = 1/2$ becomes

$$
\begin{aligned}
S &= -\int_0^{\infty} \langle\dot{\tau}|\tau\rangle \,\mathrm{d}\tau + \int_0^{\beta} \langle\tau|\hat{H}|\tau\rangle \,\mathrm{d}\tau \\
&= \mathrm{i}I\int_0^{\beta} (1-\cos\theta)\dot{\varphi}\,\mathrm{d}\tau + \int_0^{\beta} H(I\boldsymbol{n}(\tau))\,\mathrm{d}\tau \quad . \qquad (2.5.11)
\end{aligned}
$$

The above equation also holds for general spin I.

The first term in (2.5.11) is called the Berry phase and has the following geometrical meaning, as shown in Fig. 2.5. Noting that $\Delta\tau\dot{\varphi}(1-\cos\theta)$ describes the solid angle between the z axis, $\boldsymbol{n}(\tau)$ and $\boldsymbol{n}(\tau+\Delta\tau)$, we may also express the Berry phase by the solid angle ω subtended by the closed path described by $\boldsymbol{n}$:

$$
\mathrm{i}I\omega \quad .
$$

The solid angle is determined moduli 4π, the surface of the unit ball. However, because $2I$ is an integer, $\mathrm{e}^{4\pi\mathrm{i}I} = 1$ and therefore this ambiguity does not affect physics. Saying it the other way round, we conclude that the spin I cannot reach any value, but is quantized in such a way that $2I$ is an integer.

Furthermore, the canonical conjugate relations of p and x in $\mathrm{i}p\dot{x}$ are also reflected in the commutation relations of the components of the spin. The

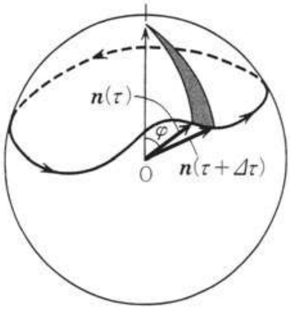

Fig. 2.5. The topological meaning of the Berry phase

term $\mathrm{i}I\cos\theta\dot{\varphi}$ signals that in the angle φ of the spin in the xy plane and $I^z = I\cos\theta$ are canonical conjugate. Indeed, from (2.5.4) for $I = 1/2$ we obtain

$$\hat{I}^{\pm} = \hat{I}^x \pm \mathrm{i}\hat{I}^y = I\,\mathrm{e}^{\pm\mathrm{i}\hat{\varphi}}\sin\hat{\theta} \quad , \tag{2.5.12}$$

the definition of the operators $\hat{\varphi}$ and $\hat{\theta}$. The commutation relation of the spin

$$[\hat{I}^z, \hat{I}^{\pm}] = \pm\hat{I}^{\pm} \tag{2.5.13}$$

equals

$$[\hat{I}^z, \mathrm{e}^{\pm\mathrm{i}\hat{\varphi}}] = \pm\mathrm{e}^{\pm\mathrm{i}\hat{\varphi}} \tag{2.5.14}$$

and this induces

$$[\hat{\varphi}, \hat{I}^z] = \mathrm{i} \quad . \tag{2.5.15}$$

The second term in (2.5.11) is the expectation value of the Hamiltonian $\hat{H} = H(\hat{\boldsymbol{I}})$ in the state $|\tau\rangle$ expressed with the spin variable $\boldsymbol{I} = I\boldsymbol{n}$. Let us ensure that the classical equations of motion can be obtained from the action (2.5.11). First, the variation with respect to the solid angle leads to

$$\begin{aligned}\delta\omega &= \int_0^\beta \mathrm{d}\tau\,[\dot{\varphi}\delta\theta\sin\theta - \delta\dot{\varphi}\cos\theta] \\ &= \int_0^\beta \mathrm{d}\tau\,[\dot{\varphi}\delta\theta - \dot{\theta}\delta\varphi]\sin\theta \\ &= \int_0^\beta \mathrm{d}\tau\,\delta\boldsymbol{n}(\tau)\cdot\left(\frac{\mathrm{d}\boldsymbol{n}(\tau)}{\mathrm{d}\tau}\times\boldsymbol{n}(\tau)\right) \quad .\end{aligned} \tag{2.5.16}$$

Therefore, $\delta S = 0$ leads to the equation

$$\mathrm{i}I\frac{\mathrm{d}\boldsymbol{n}(\tau)}{\mathrm{d}\tau}\times\boldsymbol{n}(\tau) = -\frac{\partial H(I\boldsymbol{n}(\tau))}{\partial\boldsymbol{n}(\tau)} \quad . \tag{2.5.17}$$

We now transform from $\tau = it$ to real time and take the cross product with $\boldsymbol{n}(\tau)$ on both sides:

$$I\frac{\mathrm{d}\boldsymbol{n}(t)}{\mathrm{d}t} = \boldsymbol{n}(t)\times\frac{\partial H(I\boldsymbol{n}(t))}{\partial\boldsymbol{n}(t)} \quad . \tag{2.5.18}$$

This equation equals the classical equation of motion of the spin. The torque acting on the spin is on the right-hand side.