Chapter 14
Path Integrals in Quantum Mechanics

Path integrals provide in many instances an elegant complementary description of quantum mechanics and also for the quantization of fields, which we will study from a canonical point of view in Chapter 17 and following chapters. Path integrals are particularly popular in scattering theory, because the techniques of path integration were originally developed in the study of time evolution operators. Other areas where path integrals are used include statistical physics and the description of dissipative systems.

Path integration is based on a beautiful intuitive description of the quantum mechanical time evolution of particles or wave functions from initial to final states. The prize for the intuitive elegance in the description of time evolution is that the description of bound systems and the identification of the corresponding states is often cumbersome with path integral methods. On the other hand, path integration and canonical quantization complement each other particularly well in relativistic scattering theory, where canonical methods are needed for unitarity of the scattering matrix, for the normalization of the scattering states, and also for the correct choice of propagators in perturbation theory, while the path integral formulation provides an elegant tool for the development of rules for covariant perturbation theory.

Path integrals had been developed by Richard Feynman as a tool for understanding the role of the classical action in quantum mechanics, and had then evolved into a basis for covariant perturbation theory in relativistic field theories[1]. Our introductory exposition will focus on the use of path integrals in scattering theory. The first authoritative textbook on path integrals was co-authored by Feynman himself [10]. Extensive discussions and many applications of path integrals can be found in [13] and [23]. The use of path integrals in perturbative relativistic quantum field theory from a particle physics perspective is discussed e.g. in [18, 31, 41].

[1]R.P. Feynman, Ph.D. thesis, Princeton University 1942; Rev. Mod. Phys. 20, 367 (1948).

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14.1 Correlation and Green's functions for free particles

Before we enter the discussion of free particle motion and potential scattering in terms of path integrals, it is useful to discuss Green's functions for the Newton equation and canonical correlation functions for free particles.

The equation of motion of a classical non-relativistic particle under the influence of a force $\boldsymbol{F}(t)$ is directly integrable,

$$\boldsymbol{x}(t) = \boldsymbol{x}_i + \boldsymbol{v}_i(t-t_i) + \frac{1}{m}\int_{t_i}^{t} dt' \int_{t_i}^{t'} dt''\, \boldsymbol{F}(t''). \tag{14.1}$$

Partial integration of the acceleration term yields a Green's function representation

$$\begin{aligned}\boldsymbol{x}(t) &= \boldsymbol{x}_i + \boldsymbol{v}_i(t-t_i) + \frac{1}{m}\int_{t_i}^{t} dt'\,(t-t')\boldsymbol{F}(t') \\ &= \boldsymbol{x}_i + \boldsymbol{v}_i(t-t_i) + \frac{1}{m}\int_{-\infty}^{\infty} dt'\, G_i(t,t')\boldsymbol{F}(t'),\end{aligned} \tag{14.2}$$

with a Green's function which satisfies homogeneous initial conditions,

$$\begin{aligned}G_i(t,t') &= (t-t')\left[\Theta(t-t') - \Theta(t_i-t')\right] \\ &= (t-t')\left[\Theta(t'-t_i) - \Theta(t'-t)\right],\end{aligned} \tag{14.3}$$

$$\frac{\partial^2}{\partial t^2}G_i(t,t') = \delta(t-t'), \quad \left.\frac{\partial}{\partial t}G_i(t,t')\right|_{t=t_i} = 0, \quad G_i(t_i,t') = 0.$$

If we determine the velocity $\boldsymbol{v}_i$ such that $\boldsymbol{x}(t_f) = \boldsymbol{x}_f$, we find another Green's function representation

$$\begin{aligned}\boldsymbol{x}(t) &= \boldsymbol{x}_i\frac{t-t_f}{t_i-t_f} + \boldsymbol{x}_f\frac{t-t_i}{t_f-t_i} + \int_{t_f}^{t} dt'\,\frac{tt_f + t't_i}{t_f-t_i}\frac{\boldsymbol{F}(t')}{m} \\ &\quad + \int_{t_i}^{t} dt'\,\frac{tt_i + t't_f}{t_i-t_f}\frac{\boldsymbol{F}(t')}{m} + \int_{t_i}^{t_f} dt'\,\frac{tt' + t_it_f}{t_f-t_i}\frac{\boldsymbol{F}(t')}{m} \\ &= \boldsymbol{x}_i\frac{t-t_f}{t_i-t_f} + \boldsymbol{x}_f\frac{t-t_i}{t_f-t_i} + \frac{1}{m}\int_{-\infty}^{\infty} dt'\, G_{fi}(t,t')\boldsymbol{F}(t'),\end{aligned} \tag{14.4}$$

with a Green's function which satisfies homogeneous boundary conditions,

$$\begin{aligned}G_{fi}(t,t') = {} & \frac{tt_f + t't_i}{t_f-t_i}\left[\Theta(t-t') - \Theta(t_f-t')\right] \\ & + \frac{tt_i + t't_f}{t_i-t_f}\left[\Theta(t-t') - \Theta(t_i-t')\right]\end{aligned}$$

$$
\begin{aligned}
&+\frac{tt' + t_i t_f}{t_f - t_i}\left[\Theta(t_f - t') - \Theta(t_i - t')\right] \\
&= \Theta(t_f - t')\frac{(t - t_i)(t' - t_f)}{t_f - t_i} + \Theta(t_i - t')\frac{(t - t_f)(t_i - t')}{t_f - t_i} \\
&+ (t - t')\Theta(t - t'), \qquad (14.5)
\end{aligned}
$$

$$
\frac{\partial^2}{\partial t^2} G_{fi}(t,t') = \delta(t - t'), \quad G_{fi}(t_f,t') = 0, \quad G_{fi}(t_i,t') = 0.
$$

The most general form of the Green's function for the Newton equation is

$$
G(t,t') = \frac{|t - t'|}{2} + \alpha(t')t + \beta(t'). \tag{14.6}
$$

A particular of these Green's functions appears also in canonical quantum mechanics in the time ordered two-point correlation function of the Heisenberg position operator

$$
\mathbf{x}(t) = \exp\left(\frac{\mathrm{i}t}{2m\hbar}\mathbf{p}^2\right)\mathbf{x}\exp\left(-\frac{\mathrm{i}t}{2m\hbar}\mathbf{p}^2\right) = \mathbf{x} + \frac{t}{m}\mathbf{p}.
$$

In general we can define N-point correlation functions without or with time-ordering,

$$
\boldsymbol{g}_{fi}^{(N)}(t_N, t_{N-1}, \ldots, t_1) = \langle \boldsymbol{x}_f, t_f|\mathbf{x}(t_N) \otimes \mathbf{x}(t_{N-1}) \otimes \ldots \otimes \mathbf{x}(t_1)|\boldsymbol{x}_i, t_i\rangle, \tag{14.7}
$$

$$
\boldsymbol{G}_{fi}^{(N)}(t_N, t_{N-1}, \ldots, t_1) = \langle \boldsymbol{x}_f, t_f|\mathrm{T}_+\mathbf{x}(t_1) \otimes \mathbf{x}(t_2) \otimes \ldots \otimes \mathbf{x}(t_N)|\boldsymbol{x}_i, t_i\rangle. \tag{14.8}
$$

Here the time ordering operator T_+ arranges the Heisenberg operators from right to left by increasing time, but does not affect the times t_i and t_f, e.g.

$$
\boldsymbol{G}_{fi}^{(2)}(t,t') = \Theta(t - t')\boldsymbol{g}_{fi}^{(2)}(t,t') + \Theta(t' - t)\boldsymbol{g}_{fi}^{(2)}(t',t).
$$

The states $|\boldsymbol{x}, t\rangle$ are the position eigenkets in the Heisenberg picture,

$$
|\boldsymbol{x}, t\rangle = \exp\left(\frac{\mathrm{i}t}{2m\hbar}\mathbf{p}^2\right)|\boldsymbol{x}\rangle, \quad \mathbf{x}(t)|\boldsymbol{x}, t\rangle = \boldsymbol{x}|\boldsymbol{x}, t\rangle,
$$

and their products coincide with the position representation of the free non-relativistic particle propagator which we have encountered on several occasions before, see e.g. (3.33) and (4.45),

$$\begin{aligned}
g_{fi}^{(0)} &= \langle \boldsymbol{x}_f, t_f | \boldsymbol{x}_i, t_i \rangle = \langle \boldsymbol{x}_f | \exp\!\left(-\mathrm{i}\frac{t_f - t_i}{2m\hbar}\mathbf{p}^2\right) |\boldsymbol{x}_i\rangle = \langle \boldsymbol{x}_f | U_0(t_f, t_i | \boldsymbol{x}_i\rangle \\
&= \sqrt{\frac{m}{2\pi \mathrm{i}\hbar(t_f - t_i)}}^{\,3} \exp\!\left[-\frac{m\left(\boldsymbol{x}_f - \boldsymbol{x}_i\right)^2}{2\mathrm{i}\hbar(t_f - t_i)}\right].
\end{aligned} \tag{14.9}$$

A small imaginary shift $t_f - t_i \to t_f - t_i - \mathrm{i}\epsilon$ is implied for convergence properties of Gaussian integrals which appear in the evaluation of $\langle \boldsymbol{x}_f, t_f | \boldsymbol{x}_i, t_i \rangle$.

Note that $\ddot{\mathbf{x}}(t) = -[H_0, [H_0, \mathbf{x}(t)]]/\hbar^2 = 0$ and therefore the second order time derivatives of $g_{fi}^{(N)}(t_N, t_{N-1}, \ldots, t_1)$ with respect to the time arguments t_I of the Heisenberg operators vanish. However, this implies that the time ordered two-point function contains a Green's function of the Newton equation on the diagonal (no summation over the index pair aa),

$$\begin{aligned}
\frac{\partial^2}{\partial t^2} G^{(2)}_{fi,aa}(t, t') &= \delta(t - t')\frac{1}{m}\langle \boldsymbol{x}_f, t_f | [p_a, x_a(t')] | \boldsymbol{x}_i, t_i \rangle \\
&= \delta(t - t')\frac{\hbar}{\mathrm{i}m}\langle \boldsymbol{x}_f, t_f | \boldsymbol{x}_i, t_i \rangle.
\end{aligned} \tag{14.10}$$

The functions $g_{fi}^{(N)}(t_N, t_{N-1}, \ldots, t_1)$ will generically not be symmetric in their time arguments. They are easily evaluated by observing that the relation

$$\exp\!\left(-\frac{\mathrm{i}t_f}{2m\hbar}\mathbf{p}^2\right)\mathbf{x}(t)\exp\!\left(\frac{\mathrm{i}t_f}{2m\hbar}\mathbf{p}^2\right) = \mathbf{x} + \frac{t - t_f}{m}\mathbf{p} = \mathbf{x}(t - t_f)$$

implies the recursion relation

$$g_{fi}^{(N)}(t_N, t_{N-1}, \ldots, t_1) = \left(\boldsymbol{x}_f - \frac{\mathrm{i}\hbar}{m}(t_N - t_f)\frac{\partial}{\partial \boldsymbol{x}_f}\right) g_{fi}^{(N-1)}(t_{N-1}, \ldots, t_1).$$

The one-point function is in particular

$$\begin{aligned}
g_{fi}^{(1)}(t) \equiv G_{fi}^{(1)}(t) &= \langle \boldsymbol{x}_f, t_f | \mathbf{x}(t) | \boldsymbol{x}_i, t_i \rangle \\
&= \langle \boldsymbol{x}_f | \left(\mathbf{x} + \frac{t - t_f}{m}\mathbf{p}\right) \exp\!\left(-\mathrm{i}\frac{t_f - t_i}{2m\hbar}\mathbf{p}^2\right) |\boldsymbol{x}_i\rangle \\
&= \left(\boldsymbol{x}_f - \frac{\mathrm{i}\hbar}{m}(t - t_f)\frac{\partial}{\partial \boldsymbol{x}_f}\right) \langle \boldsymbol{x}_f | U_0(t_f, t_i) | \boldsymbol{x}_i \rangle \\
&= \left(\boldsymbol{x}_f + \left(\boldsymbol{x}_f - \boldsymbol{x}_i\right)\frac{t - t_f}{t_f - t_i}\right) \langle \boldsymbol{x}_f | U_0(t_f, t_i) | \boldsymbol{x}_i \rangle,
\end{aligned} \tag{14.11}$$

i.e. the ratio between the one-point function and the zero-point function is the free classical path which passes through $\boldsymbol{x}_i$ and $\boldsymbol{x}_f$,

$$\frac{g_{fi}^{(1)}(t)}{g_{fi}^{(0)}} = \boldsymbol{x}_f\frac{t - t_i}{t_f - t_i} + \boldsymbol{x}_i\frac{t_f - t}{t_f - t_i}.$$

The canonical two-point function is

$$\begin{aligned}
\boldsymbol{g}_{fi}^{(2)}(t,t') &= \langle \boldsymbol{x}_f, t_f|\mathbf{x}(t)\otimes\mathbf{x}(t')|\boldsymbol{x}_i, t_i\rangle \\
&= \left(\boldsymbol{x}_f - \frac{\mathrm{i}\hbar}{m}(t-t_f)\frac{\partial}{\partial\boldsymbol{x}_f}\right)\otimes\left(\boldsymbol{x}_f - \frac{\mathrm{i}\hbar}{m}(t'-t_f)\frac{\partial}{\partial\boldsymbol{x}_f}\right)\langle\boldsymbol{x}_f|U_0(t_f,t_i)|\boldsymbol{x}_i\rangle \\
&= \left(\boldsymbol{x}_f\frac{t-t_i}{t_f-t_i} + \boldsymbol{x}_i\frac{t_f-t}{t_f-t_i}\right)\otimes\left(\boldsymbol{x}_f\frac{t'-t_i}{t_f-t_i} + \boldsymbol{x}_i\frac{t_f-t'}{t_f-t_i}\right)\langle\boldsymbol{x}_f|U_0(t_f,t_i)|\boldsymbol{x}_i\rangle \\
&\quad + \frac{\mathrm{i}\hbar}{m}\frac{(t_f-t)(t'-t_i)}{t_f-t_i}\underline{1}\langle\boldsymbol{x}_f|U_0(t_f,t_i)|\boldsymbol{x}_i\rangle. \qquad (14.12)
\end{aligned}$$

The relation (14.10) for the diagonal entries of the time-ordered two-point function is easily confirmed.

The primary use of N-point functions in quantum mechanics concerns the perturbative evaluation of scattering amplitudes in analytic scattering potentials. We will see this in Section 14.3.

14.2 Time evolution in the path integral formulation

The standard formulation of path integrals derives from the time evolution of states in the $\boldsymbol{x}$ representation,

$$\langle\boldsymbol{x}|\psi(t)\rangle = \langle\boldsymbol{x}|U(t,t_0)|\psi(t_0)\rangle,$$

We can also write this as

$$\langle\boldsymbol{x}|\psi(t)\rangle = \langle\boldsymbol{x},t,t_0|\psi(t_0)\rangle$$

if we define the time-dependent states

$$|\boldsymbol{x},t,t_0\rangle = U^+(t,t_0)|\boldsymbol{x}\rangle = \mathrm{T}\exp\!\left(-\frac{\mathrm{i}}{\hbar}\int_t^{t_0}d\tau\, H(\tau)\right)|\boldsymbol{x}\rangle. \qquad (14.13)$$

Recall the definition of the time ordering operator T which was given following equation (13.2).

The parameter t_0 is usually suppressed in the notation of states, $|\boldsymbol{x},t,t_0\rangle \equiv |\boldsymbol{x},t\rangle$, $|\psi(t_0)\rangle \equiv |\psi\rangle$. The time-dependent basis states (14.13) are just the eigenstates of the Heisenberg picture operator

$$\mathbf{x}(t) = U^+(t,t_0)\mathbf{x}U(t,t_0), \quad \mathbf{x}(t)|\boldsymbol{x},t\rangle = \boldsymbol{x}|\boldsymbol{x},t\rangle, \qquad (14.14)$$

and the time parameter t_0 is the time parameter where the Schrödinger picture and the Heisenberg picture coincide.

The Heisenberg picture eigenstates satisfy the completeness relation

$$\int d^3\boldsymbol{x}\,|\boldsymbol{x},t\rangle\langle\boldsymbol{x},t| = 1 \tag{14.15}$$

as a consequence of the completeness relation of the **x** eigenstates $|\boldsymbol{x}\rangle$ and the unitarity of the time evolution operators. Furthermore, the composition property (13.7) of time evolution operators implies that the products of the Heisenberg picture eigenstates yield the $\boldsymbol{x}$ representation of the time evolution operator,

$$\langle\boldsymbol{x},t|\boldsymbol{x}',t'\rangle = \langle\boldsymbol{x}|U(t,t')|\boldsymbol{x}'\rangle. \tag{14.16}$$

The properties (14.15) and (14.16) imply the following representation of the time evolution of a state,

$$\begin{aligned}\langle\boldsymbol{x},t|\psi\rangle &= \langle\boldsymbol{x},t|\left(\prod_{n=1}^{N}\int d^3\boldsymbol{x}_n\,|\boldsymbol{x}_n,t_n\rangle\langle\boldsymbol{x}_n,t_n|\right)|\psi\rangle\\ &= \int d^3\boldsymbol{x}_N\ldots\int d^3\boldsymbol{x}_1\langle\boldsymbol{x}|U(t,t_N)|\boldsymbol{x}_N\rangle\langle\boldsymbol{x}_N|U(t_N,t_{N-1})|\boldsymbol{x}_{N-1}\rangle\ldots\\ &\quad\times\langle\boldsymbol{x}_2|U(t_2,t_1)|\boldsymbol{x}_1\rangle\langle\boldsymbol{x}_1|U(t_1,t_0)|\psi\rangle.\end{aligned} \tag{14.17}$$

Equivalently, we could also have arrived at this equation directly from the composition property (13.7) of the time evolution operator and the completeness of the Schrödinger picture eigenkets $|\boldsymbol{x}\rangle$.

Equation (14.17) implies in particular for the initial state $|\psi(t_0)\rangle = |\boldsymbol{x}_0\rangle \equiv |\boldsymbol{x}_0,t_0\rangle$ the evolution equation

$$\begin{aligned}\langle\boldsymbol{x},t|\boldsymbol{x}_0\rangle &= \langle\boldsymbol{x}|U(t,t_0)|\boldsymbol{x}_0\rangle\\ &= \int d^3\boldsymbol{x}_N\ldots\int d^3\boldsymbol{x}_1\langle\boldsymbol{x}|U(t,t_N)|\boldsymbol{x}_N\rangle\langle\boldsymbol{x}_N|U(t_N,t_{N-1})|\boldsymbol{x}_{N-1}\rangle\ldots\\ &\quad\times\langle\boldsymbol{x}_2|U(t_2,t_1)|\boldsymbol{x}_1\rangle\langle\boldsymbol{x}_1|U(t_1,t_0)|\boldsymbol{x}_0\rangle.\end{aligned} \tag{14.18}$$

Intuitively the formula (14.18) can be considered as an integration over the set of all paths that a particle can take from an initial location $\boldsymbol{x}_0$ at time t_0 to the location $\boldsymbol{x}$ at time t. In particular, if we use

$$\begin{aligned}\langle\boldsymbol{x}|U(t,t_0)|\boldsymbol{x}_0\rangle &= \langle\boldsymbol{x}|\exp\!\left[-\mathrm{i}\frac{t-t_0}{\hbar}\left(\frac{\mathbf{p}^2}{2m}+V(\mathbf{x})\right)\right]|\boldsymbol{x}_0\rangle\\ &= \langle\boldsymbol{x}|\lim_{N\to\infty}\left[1-\mathrm{i}\frac{t-t_0}{N\hbar}\left(\frac{\mathbf{p}^2}{2m}+V(\mathbf{x})\right)\right]^N|\boldsymbol{x}_0\rangle\end{aligned} \tag{14.19}$$

and substitute the following peculiar decomposition of unity,

$$\begin{aligned} 1 &= \int d^3\boldsymbol{x} \int d^3\boldsymbol{p}\, |\boldsymbol{x}\rangle\langle\boldsymbol{x}|\boldsymbol{p}\rangle\langle\boldsymbol{p}| \\ &= \int d^3\boldsymbol{x} \int \frac{d^3\boldsymbol{p}}{\sqrt{2\pi\hbar}^3}\, |\boldsymbol{x}\rangle \exp\!\left(\frac{\mathrm{i}}{\hbar}\boldsymbol{p}\cdot\boldsymbol{x}\right) \langle\boldsymbol{p}| \end{aligned} \tag{14.20}$$

between any two factors in the product (14.19), we find

$$\begin{aligned} \langle\boldsymbol{x}, t|\boldsymbol{x}_0\rangle &= \langle\boldsymbol{x}|U(t,t_0)|\boldsymbol{x}_0\rangle \\ &= \lim_{N\to\infty}\left(\prod_{I=1}^{N}\int\frac{d^3\boldsymbol{x}_I d^3\boldsymbol{p}_I}{\sqrt{2\pi\hbar}^3}\right)\exp\!\left(\frac{\mathrm{i}}{\hbar}\sum_{J=1}^{N}\boldsymbol{p}_J\cdot\boldsymbol{x}_J\right)\langle\boldsymbol{x}|\boldsymbol{x}_N\rangle\langle\boldsymbol{p}_N| \\ &\quad\times\left[1-\mathrm{i}\frac{t-t_0}{N\hbar}\left(\frac{\mathbf{p}^2}{2m}+V(\mathbf{x})\right)\right]|\boldsymbol{x}_{N-1}\rangle\langle\boldsymbol{p}_{N-1}|\ldots \\ &\quad\times|\boldsymbol{x}_2\rangle\langle\boldsymbol{p}_2|\left[1-\mathrm{i}\frac{t-t_0}{N\hbar}\left(\frac{\mathbf{p}^2}{2m}+V(\mathbf{x})\right)\right]|\boldsymbol{x}_1\rangle\langle\boldsymbol{p}_1| \\ &\quad\times\left[1-\mathrm{i}\frac{t-t_0}{N\hbar}\left(\frac{\mathbf{p}^2}{2m}+V(\mathbf{x})\right)\right]|\boldsymbol{x}_0\rangle. \end{aligned} \tag{14.21}$$

The momentum integrals are

$$\begin{aligned} &\int\frac{d^3\boldsymbol{p}_I}{\sqrt{2\pi\hbar}^3}\exp\!\left(\frac{\mathrm{i}}{\hbar}\boldsymbol{p}_I\cdot\boldsymbol{x}_I\right)\langle\boldsymbol{p}_N|\left[1-\mathrm{i}\frac{t-t_0}{N\hbar}\left(\frac{\mathbf{p}^2}{2m}+V(\mathbf{x})\right)\right]|\boldsymbol{x}_{I-1}\rangle \\ &=\int\frac{d^3\boldsymbol{p}_I}{(2\pi\hbar)^3}\left[1-\mathrm{i}\frac{t-t_0}{N\hbar}\left(V(\boldsymbol{x}_{I-1})-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\boldsymbol{x}_{I-1}^2}\right)\right] \\ &\quad\times\exp\!\left(\frac{\mathrm{i}}{\hbar}\boldsymbol{p}_I\cdot(\boldsymbol{x}_I-\boldsymbol{x}_{I-1})\right) \\ &=\left[1-\mathrm{i}\frac{t-t_0}{N\hbar}\left(V(\boldsymbol{x}_{I-1})-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\boldsymbol{x}_{I-1}^2}\right)\right]\delta\left(\boldsymbol{x}_I-\boldsymbol{x}_{I-1}\right), \end{aligned} \tag{14.22}$$

and this exactly returns equation (14.19) if we would have substituted N copies of

$$1 = \int d^3\boldsymbol{x}\, |\boldsymbol{x}\rangle\langle\boldsymbol{x}|$$

instead of (14.20). This is exactly as it should be. However, if we substitute instead

$$\left[1-\mathrm{i}\frac{t-t_0}{N\hbar}\left(\frac{\boldsymbol{p}_I^2}{2m}+V(\boldsymbol{x}_{I-1})\right)\right]\simeq\exp\!\left[-\mathrm{i}\frac{t-t_0}{N\hbar}\left(\frac{\boldsymbol{p}_I^2}{2m}+V(\boldsymbol{x}_{I-1})\right)\right]$$

in (14.22), we find that the momentum integrals are

$$\int\frac{d^3\boldsymbol{p}_I}{(2\pi\hbar)^3}\exp\left[-\mathrm{i}\frac{t-t_0-\mathrm{i}\epsilon}{2m\hbar N}\left(\boldsymbol{p}_I-mN\frac{\boldsymbol{x}_I-\boldsymbol{x}_{I-1}}{t-t_0-\mathrm{i}\epsilon}\right)^2+\mathrm{i}N\frac{m}{2\hbar}\frac{(\boldsymbol{x}_I-\boldsymbol{x}_{I-1})^2}{t-t_0}\right]$$
$$=\sqrt{\frac{mN}{2\pi\mathrm{i}\hbar(t-t_0-\mathrm{i}\epsilon)}}^{3}\exp\left[\frac{\mathrm{i}}{\hbar}\frac{m}{2}\left(N\frac{\boldsymbol{x}_I-\boldsymbol{x}_{I-1}}{t-t_0}\right)^2\frac{t-t_0}{N}\right].$$

This motivates the following formula for the matrix elements of the time evolution operator,

$$\begin{aligned}\langle\boldsymbol{x},t|\boldsymbol{x}_0\rangle &= \langle\boldsymbol{x}|U(t,t_0)|\boldsymbol{x}_0\rangle\\ &\simeq \lim_{N\to\infty}\exp\left(\frac{\mathrm{i}}{\hbar}\sum_{J=1}^{N}\left[\frac{m}{2}\left(N\frac{\boldsymbol{x}_J-\boldsymbol{x}_{J-1}}{t-t_0}\right)^2-V(\boldsymbol{x}_{J-1})\right]\frac{t-t_0}{N}\right)\\ &\quad\times\sqrt{\frac{mN}{2\pi\mathrm{i}\hbar(t-t_0)}}^{3N}\left(\prod_{I=1}^{N}\int d^3\boldsymbol{x}_I\right)\delta(\boldsymbol{x}-\boldsymbol{x}_N).\end{aligned}\tag{14.23}$$

The exponent is a discretized version of the action integral of a non-relativistic particle, and this motivates the further short hand notation

$$\begin{aligned}\langle\boldsymbol{x}|U(t,t_0)|\boldsymbol{x}_0\rangle &= \int_{\boldsymbol{x}(t_0)=\boldsymbol{x}_0}^{\boldsymbol{x}(t)=\boldsymbol{x}}D^3\boldsymbol{x}(t')\,\exp\left[\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}dt'\,\left(\frac{m}{2}\dot{\boldsymbol{x}}^2(t')-V(\boldsymbol{x}(t'))\right)\right]\\ &= \int_{\boldsymbol{x}(t_0)=\boldsymbol{x}_0}^{\boldsymbol{x}(t)=\boldsymbol{x}}D^3\boldsymbol{x}(t')\,\exp\left(\frac{\mathrm{i}}{\hbar}S[\boldsymbol{x}(t')]\right),\end{aligned}\tag{14.24}$$

where $S[\boldsymbol{x}(t')]$ is the action functional of the particle (see Appendix A). Please note that this standard notation for path integrals is misleading with regard to the length dimension or units of the path integral. The $\boldsymbol{x}$ matrix elements of the time evolution operator have dimension length^{-3} in agreement with the dimension length$^{-3/2}$ of $\mathbf{x}$ eigenstates in three dimensions, see Section 5.3. This of course agrees with the discretized version on the right hand side of equation (14.23). The three-dimensional path integral therefore has dimension length^{-3}, but the notation $\int D^3\boldsymbol{x}\exp(\mathrm{i}S[\boldsymbol{x}]/\hbar)$ suggests length dimension length^3. A dimensionally correct, but also more awkward notation would be

$$\begin{aligned}\langle\boldsymbol{x}|U(t,t_0)|\boldsymbol{x}_0\rangle &= \delta\big(\boldsymbol{x}(t_0)-\boldsymbol{x}_0\big)\delta\big(\boldsymbol{x}(t)-\boldsymbol{x}\big)\\ &\quad\times\int D^3\boldsymbol{x}(t')\,\exp\left(\frac{\mathrm{i}}{\hbar}S[\boldsymbol{x}(t')]\right),\end{aligned}\tag{14.25}$$

where the end point integration of the path would implement the boundary point constraints. We will continue to use the standard notation (14.24), but keep the fact in mind that this notation is not dimensionally correct.

Equation (14.24) defines the path integral representation of the propagator in configuration ($\boldsymbol{x}$) space. Note that nothing in the derivation required forward evolution $t > t_0$ in time. Of course, the same results apply for backward evolution. However, the discretization into time steps $(t - t_0)/N$ imply that consecutive steps are either always later or always earlier depending on $t > t_0$ or $t < t_0$, respectively. Therefore path integrals with factors like $\boldsymbol{x}(t_1)\boldsymbol{x}(t_2)$ in the integrand correspond to time ordered matrix elements in canonical quantization, but whether time ordering refers to later times or earlier times depends on whether we are studying forward or backward evolution in time. Usually we are interested in forward evolution, i.e. we assume $t > t_0$ in the following.

A virtue of the path integral is that it explains the principle of stationary action of classical paths as a consequence of dominant contributions from those trajectories where small fluctuations of the path do not yield cancellation of the integral from phase fluctuations.

As a relatively simple exercise, let us see how this reproduces the $\boldsymbol{x}$ representation (4.45) of the free propagator.

The integrations in (14.23) for $V(\boldsymbol{x}) = 0$ include a set of $N-1$ Gaussian integrals. The first integral over $d^3\boldsymbol{x}_1$ yields

$$\sqrt{\frac{mN}{2\pi i\hbar(t-t_0-i\epsilon)}}^{\,3}\exp\left[-\frac{mN}{2i\hbar(t-t_0-i\epsilon)}\frac{1}{2}(\boldsymbol{x}_2-\boldsymbol{x}_0)^2\right]$$
$$\times\int d^3\boldsymbol{x}_1\,\exp\left[-\frac{mN}{2i\hbar(t-t_0-i\epsilon)}2\left(\boldsymbol{x}_1-\frac{\boldsymbol{x}_2+\boldsymbol{x}_0}{2}\right)^2\right]$$
$$=\frac{1}{\sqrt{2}^3}\exp\left[-\frac{mN}{2i\hbar(t-t_0-i\epsilon)}\frac{1}{2}(\boldsymbol{x}_2-\boldsymbol{x}_0)^2\right].$$

Next we evaluate the $\boldsymbol{x}_2$ integral and then work consecutively through all the integrals. This reproduces always a similar result with minor variations. One can show by induction with respect to I that the $\boldsymbol{x}_I$ integral yields

$$\sqrt{\frac{mN}{2\pi i\hbar(t-t_0-i\epsilon)I}}^{\,3}\exp\left[-\frac{mN}{2i\hbar(t-t_0-i\epsilon)}\frac{1}{I+1}(\boldsymbol{x}_{I+1}-\boldsymbol{x}_0)^2\right]$$
$$\times\int d^3\boldsymbol{x}_I\,\exp\left[-\frac{mN}{2i\hbar(t-t_0-i\epsilon)}\frac{I+1}{I}\left(\boldsymbol{x}_I-\frac{I}{I+1}\left(\boldsymbol{x}_{I+1}+\frac{\boldsymbol{x}_0}{I}\right)\right)^2\right]$$
$$=\frac{1}{\sqrt{I+1}^3}\exp\left[-\frac{mN}{2i\hbar(t-t_0-i\epsilon)}\frac{1}{I+1}(\boldsymbol{x}_{I+1}-\boldsymbol{x}_0)^2\right].$$

After the final integrations over $\boldsymbol{x}_{N-1}$ and $\boldsymbol{x}_N$ (which is trivial due to the δ function in (14.23)), we are left with

$$\begin{aligned}\langle \boldsymbol{x}, t|\boldsymbol{x}_0\rangle &= \langle \boldsymbol{x}|U(t,t_0)|\boldsymbol{x}_0\rangle \\ &= \sqrt{\frac{m}{2\pi i\hbar(t-t_0-i\epsilon)}}^{\,3} \exp\left[-\frac{m\,(\boldsymbol{x}-\boldsymbol{x}_0)^2}{2i\hbar(t-t_0-i\epsilon)}\right],\end{aligned}$$

which is indeed the $\boldsymbol{x}$ representation (4.45) of the free propagator.

Note that the classical trajectory of the particle from the location $\boldsymbol{x}_0$ at time t_0 to the location $\boldsymbol{x}$ at time t is given by

$$\boldsymbol{x}_{cl}(t') = \boldsymbol{x}_0 + \frac{\boldsymbol{x}-\boldsymbol{x}_0}{t-t_0}(t'-t_0) = \boldsymbol{x}\frac{t'-t_0}{t-t_0} + \boldsymbol{x}_0\frac{t'-t}{t_0-t},$$

and therefore the factor in the exponent of the free propagator is just the action functional evaluated on the classical trajectory,

$$\frac{m}{2}\frac{(\boldsymbol{x}-\boldsymbol{x}_0)^2}{t-t_0} = S[\boldsymbol{x}_{cl}(t')].$$

This holds in general for propagators where the Lagrange function contains at most second order terms in particle velocities and locations, and the path integral formulation is particularly well suited to prove this. If the Lagrange function contains at most second order terms in $\dot{\boldsymbol{x}}$ and $\boldsymbol{x}$, then due to fixed initial and final points $\boldsymbol{x}(t_0) \equiv \boldsymbol{x}_0$ and $\boldsymbol{x}(t) \equiv \boldsymbol{x}$, the action functional for all admissible paths $\boldsymbol{x}(t')$ is exactly

$$\begin{aligned}S[\boldsymbol{x}(t')] = S[\boldsymbol{x}_{cl}(t')] &+ \frac{1}{2}\int_{t_0}^{t} dt'' \int_{t_0}^{t} dt' \left(\boldsymbol{x}(t'') - \boldsymbol{x}_{cl}(t'')\right) \\ &\times \frac{\delta^2 S}{\delta\boldsymbol{x}(t'')\delta\boldsymbol{x}(t')} \cdot \left(\boldsymbol{x}(t') - \boldsymbol{x}_{cl}(t')\right),\end{aligned} \tag{14.26}$$

see Problem 14.1. Functional integration over $\exp(iS[\boldsymbol{x}(t')]/\hbar)$ then yields a constant from the Gaussian integral over the fluctuations $\boldsymbol{x}(t') - \boldsymbol{x}_{cl}(t')$, and a remnant exponential factor,

$$\langle \boldsymbol{x}|U(t,t_0)|\boldsymbol{x}_0\rangle \sim \exp\left(\frac{i}{\hbar}S[\boldsymbol{x}_{cl}(t')]\right).$$

However, note that this requires vanishing fluctuations at the boundaries, $\boldsymbol{x}(t_{(0)}) - \boldsymbol{x}_{cl}(t_{(0)}) = \boldsymbol{0}$. Otherwise boundary terms involving $\boldsymbol{x}(t_{(0)}) - \boldsymbol{x}_{cl}(t_{(0)})$ will appear in the exponent. This is important e.g. in scattering theory in the following section, when we are really concerned with fixed initial and final momenta rather than locations.

14.3 Path integrals in scattering theory

We have seen in Chapter 13 that the calculation of transition probabilities or scattering cross section from an initial state $|\psi_i(t')\rangle$ to a final state $|\psi_f(t)\rangle$ requires the calculation of the scattering matrix element

$$S_{fi}(t,t') = \langle\psi_f(t)|U(t,t')|\psi_i(t')\rangle = \langle\psi_f|U_D(t,t')|\psi_i\rangle,$$

where

$$U_D(t,t') = \exp\left(\frac{\mathrm{i}}{\hbar}H_0 t\right)\mathrm{T}\exp\left(-\frac{\mathrm{i}}{\hbar}\int_{t'}^{t} d\tau\, H(\tau)\right)\exp\left(-\frac{\mathrm{i}}{\hbar}H_0 t'\right)$$

is the time evolution operator on the states in the interaction picture. We also recall that the usual default definition of the scattering matrix involves $t\to\infty$, $t'\to-\infty$, $S_{fi}\equiv S_{fi}(\infty,-\infty)$. For the following discussion it is convenient to relabel initial and final times as $t'\to t_i$, $t\to t_f$. Equation (14.24) then implies a connection between scattering matrix elements and path integrals,

$$S_{fi} = \lim_{t_i\to-\infty,t_f\to\infty}\int d^3\boldsymbol{x}_f\int d^3\boldsymbol{x}_i\,\langle\psi_f|\exp\left(\frac{\mathrm{i}}{\hbar}H_0 t_f\right)|\boldsymbol{x}_f\rangle$$
$$\times\int_{\boldsymbol{x}(t_i)=\boldsymbol{x}_i}^{\boldsymbol{x}(t_f)=\boldsymbol{x}_f} D^3\boldsymbol{x}(t)\,\exp\left(\frac{\mathrm{i}}{\hbar}S[\boldsymbol{x}(t)]\right)\langle\boldsymbol{x}_i|\exp\left(-\frac{\mathrm{i}}{\hbar}H_0 t_i\right)|\psi_i\rangle. \quad (14.27)$$

This is still a mixed formula involving both canonical operators and a path integral. We now assume that our initial and final states are momentum eigenstates $|\psi_i\rangle = |\boldsymbol{p}_i\rangle$ and $|\psi_f\rangle = |\boldsymbol{p}_f\rangle$, and we also assume that the scattering potential $V(\boldsymbol{x},t)$ is analytic with finite range. The free Hamiltonian for the free-free scattering problem is $H_0 = \mathbf{p}^2/2m$. The resulting scattering matrix element is then

$$S_{fi} = \lim_{t_i\to-\infty,t_f\to\infty}\int d^3\boldsymbol{x}_f\int d^3\boldsymbol{x}_i\int_{\boldsymbol{x}(t_i)=\boldsymbol{x}_i}^{\boldsymbol{x}(t_f)=\boldsymbol{x}_f} D^3\boldsymbol{x}(t)\,\exp\left(\frac{\mathrm{i}}{\hbar}S[\boldsymbol{x}(t)]\right)$$
$$\times\frac{1}{(2\pi\hbar)^3}\exp\left[\frac{\mathrm{i}}{\hbar}\left(\frac{\boldsymbol{p}_f^2 t_f - \boldsymbol{p}_i^2 t_i}{2m} + \boldsymbol{p}_i\cdot\boldsymbol{x}_i - \boldsymbol{p}_f\cdot\boldsymbol{x}_f\right)\right]. \quad (14.28)$$

For the perturbative evaluation of (14.28) we introduce an auxiliary external force $\boldsymbol{F}(t)$, such that the Lagrange function including the scattering potential $V(\boldsymbol{x},t)$ takes the form

$$L = \frac{m}{2}\dot{\boldsymbol{x}}^2(t) - V(\boldsymbol{x}(t),t) + \boldsymbol{F}(t)\cdot\boldsymbol{x}(t).$$

The path integral in (14.28) then takes the form

$$\begin{aligned}
\int D^3\boldsymbol{x}(t)\,\exp\!\left(\frac{\mathrm{i}}{\hbar}S[\boldsymbol{x}(t)]\right) &= \int D^3\boldsymbol{x}(t)\,\sum_{n=0}^{\infty}\frac{1}{(\mathrm{i}\hbar)^n n!}\int_{t_i}^{t_f}dt_1\ldots\int_{t_i}^{t_f}dt_n \\
&\quad\times V(\boldsymbol{x}(t_1),t_1)\ldots V(\boldsymbol{x}(t_n),t_n)\exp\!\left[\frac{\mathrm{i}}{\hbar}\int_{t_i}^{t_f}dt\left(\frac{m}{2}\dot{\boldsymbol{x}}^2(t)+\boldsymbol{F}(t)\cdot\boldsymbol{x}(t)\right)\right] \\
&= \int D^3\boldsymbol{x}(t)\,\sum_{n=0}^{\infty}\frac{1}{(\mathrm{i}\hbar)^n n!}\int_{t_i}^{t_f}dt_1\ldots\int_{t_i}^{t_f}dt_n\,V\!\left(\frac{\hbar}{\mathrm{i}}\frac{\delta}{\delta\boldsymbol{F}(t_1)},t_1\right)\ldots \\
&\quad\times V\!\left(\frac{\hbar}{\mathrm{i}}\frac{\delta}{\delta\boldsymbol{F}(t_n)},t_n\right)\exp\!\left[\frac{\mathrm{i}}{\hbar}\int_{t_i}^{t_f}dt\left(\frac{m}{2}\dot{\boldsymbol{x}}^2(t)+\boldsymbol{F}(t)\cdot\boldsymbol{x}(t)\right)\right] \\
&= \int D^3\boldsymbol{x}(t)\,\exp\!\left[-\frac{\mathrm{i}}{\hbar}\int_{t_i}^{t_f}dt'\,V\!\left(\frac{\hbar}{\mathrm{i}}\frac{\delta}{\delta\boldsymbol{F}(t')},t'\right)\right] \\
&\quad\times\exp\!\left[\frac{\mathrm{i}}{\hbar}\int_{t_i}^{t_f}dt\left(\frac{m}{2}\dot{\boldsymbol{x}}^2(t)+\boldsymbol{F}(t)\cdot\boldsymbol{x}(t)\right)\right].
\end{aligned}\tag{14.29}$$

Evaluation of the Gaussian integrals as in equation (14.23) for $V(\boldsymbol{x}) = 0$ reproduces the canonical perturbation series (13.18). However, a different representation is gotten if we pull the variational derivative operators $V(-\mathrm{i}\hbar\delta/\delta\boldsymbol{F}(t),t)$ out of the path integral,

$$\int D^3\boldsymbol{x}(t)\,\exp\!\left(\frac{\mathrm{i}}{\hbar}S[\boldsymbol{x}(t)]\right) = \exp\!\left[-\frac{\mathrm{i}}{\hbar}\int_{t_i}^{t_f}dt'\,V\!\left(\frac{\hbar}{\mathrm{i}}\frac{\delta}{\delta\boldsymbol{F}(t')},t'\right)\right]Z[\boldsymbol{F}],$$

$$Z[\boldsymbol{F}] = \int D^3\boldsymbol{x}(t)\,\exp\!\left[\frac{\mathrm{i}}{\hbar}\int_{t_i}^{t_f}dt\left(\frac{m}{2}\dot{\boldsymbol{x}}^2(t)+\boldsymbol{F}(t)\cdot\boldsymbol{x}(t)\right)\right].\tag{14.30}$$

It is useful to have a convolution notation for the following calculations. We define

$$(G\circ\boldsymbol{F})(t) \equiv \int_{-\infty}^{\infty}dt'\,G(t,t')\boldsymbol{F}(t')$$

and

$$(\dot{G}\circ\boldsymbol{F})(t) \equiv \int_{-\infty}^{\infty}dt'\,\frac{\partial}{\partial t}G(t,t')\boldsymbol{F}(t').$$

Partial integration yields the following representation of the action of a particle under the influence of a force $\boldsymbol{F}(t)$ for every Green's function (14.6),

$$
\begin{aligned}
S[\boldsymbol{x},\boldsymbol{F}] &= \int_{t_i}^{t_f} dt\left(\frac{m}{2}\dot{\boldsymbol{x}}^2(t)+\boldsymbol{F}(t)\cdot\boldsymbol{x}(t)\right)\\
&= \frac{m}{2}\int_{t_i}^{t_f} dt\left(\dot{\boldsymbol{x}}(t)-\frac{(\dot{G}\circ\boldsymbol{F})(t)}{m}\right)^2+\frac{1}{2m}\int_{t_i}^{t_f} dt\,\boldsymbol{F}(t)\cdot(G\circ\boldsymbol{F})(t)\\
&\quad+\left(\boldsymbol{x}(t_f)-\frac{(G\circ\boldsymbol{F})(t_f)}{2m}\right)\cdot(\dot{G}\circ\boldsymbol{F})(t_f)\\
&\quad-\left(\boldsymbol{x}(t_i)-\frac{(G\circ\boldsymbol{F})(t_i)}{2m}\right)\cdot(\dot{G}\circ\boldsymbol{F})(t_i).
\end{aligned}
\tag{14.31}
$$

The trajectory $\boldsymbol{x}(t)$ between $\boldsymbol{x}_i$ and $\boldsymbol{x}_f$ appears only in the free particle action for the trajectory

$$
\boldsymbol{X}(t)=\boldsymbol{x}(t)-\frac{1}{m}(G\circ\boldsymbol{F})(t),
\tag{14.32}
$$

which classically satisfies $\ddot{\boldsymbol{X}}(t) = \boldsymbol{0}$. Therefore the path integral (14.30) can be evaluated in terms of the result for the free particle,

$$
\begin{aligned}
Z[\boldsymbol{F}] &= \sqrt{\frac{m}{2\pi\mathrm{i}\hbar(t_f-t_i)}}^{\,3}\exp\left[\frac{\mathrm{i}}{\hbar}\left(\boldsymbol{X}_f\cdot(\dot{G}\circ\boldsymbol{F})(t_f)-\boldsymbol{X}_i\cdot(\dot{G}\circ\boldsymbol{F})(t_i)\right)\right]\\
&\quad\times\exp\left(\frac{\mathrm{i}}{2m\hbar}\left[(G\circ\boldsymbol{F})(t_f)\cdot(\dot{G}\circ\boldsymbol{F})(t_f)-(G\circ\boldsymbol{F})(t_i)\cdot(\dot{G}\circ\boldsymbol{F})(t_i)\right]\right)\\
&\quad\times\exp\left(\mathrm{i}m\frac{\left(\boldsymbol{X}_f-\boldsymbol{X}_i\right)^2}{2\hbar(t_f-t_i)}+\frac{\mathrm{i}}{2m\hbar}\int_{t_i}^{t_f} dt\,\boldsymbol{F}(t)\cdot(G\circ\boldsymbol{F})(t)\right)\\
&= \langle\boldsymbol{X}_f|U_0(t_f,t_i)|\boldsymbol{X}_i\rangle\exp\left(\frac{\mathrm{i}}{2m\hbar}\int_{t_i}^{t_f} dt\,\boldsymbol{F}(t)\cdot(G\circ\boldsymbol{F})(t)\right)\\
&\quad\times\exp\left(\frac{\mathrm{i}}{2m\hbar}\left[(G\circ\boldsymbol{F})(t_f)\cdot(\dot{G}\circ\boldsymbol{F})(t_f)-(G\circ\boldsymbol{F})(t_i)\cdot(\dot{G}\circ\boldsymbol{F})(t_i)\right]\right)\\
&\quad\times\exp\left[\frac{\mathrm{i}}{\hbar}\left(\boldsymbol{X}_f\cdot(\dot{G}\circ\boldsymbol{F})(t_f)-\boldsymbol{X}_i\cdot(\dot{G}\circ\boldsymbol{F})(t_i)\right)\right].
\end{aligned}
\tag{14.33}
$$

We can summarize our results in the equations

$$
S_{fi}=\lim_{t_i\to-\infty,t_f\to\infty}\exp\left[-\frac{\mathrm{i}}{\hbar}\int_{t_i}^{t_f} dt\,V\left(\frac{\hbar}{\mathrm{i}}\frac{\delta}{\delta\boldsymbol{F}(t)},t\right)\right]S_{fi}[\boldsymbol{F}]\bigg|_{\boldsymbol{F}=\boldsymbol{0}},
\tag{14.34}
$$

$$
\begin{aligned}
S_{fi}[\boldsymbol{F}] =& \frac{1}{(2\pi\hbar)^3}\int d^3\boldsymbol{X}_f \int d^3\boldsymbol{X}_i\, Z[\boldsymbol{F}](\boldsymbol{X}_f,t_f;\boldsymbol{X}_i,t_i)\\
&\times \exp\left(\mathrm{i}\frac{\boldsymbol{p}_f^2 t_f - \boldsymbol{p}_i^2 t_i}{2m\hbar}\right)\exp\left[\frac{\mathrm{i}}{\hbar}\boldsymbol{p}_i\cdot\left(\boldsymbol{X}_i + \frac{1}{m}(G\circ\boldsymbol{F})(t_i)\right)\right] \qquad (14.35)\\
&\times \exp\left[-\frac{\mathrm{i}}{\hbar}\boldsymbol{p}_f\cdot\left(\boldsymbol{X}_f + \frac{1}{m}(G\circ\boldsymbol{F})(t_f)\right)\right].
\end{aligned}
$$

The integrals over $\boldsymbol{X}_f$ and $\boldsymbol{X}_i$ amount to a Gaussian integral involving $\boldsymbol{X}_f - \boldsymbol{X}_i$ and an integral over a Fourier monomial involving $\boldsymbol{X}_i$. Evaluation of the integrals yields

$$
\begin{aligned}
S_{fi}[\boldsymbol{F}] =& \exp\left(\frac{\mathrm{i}}{2m\hbar}\int_{t_i}^{t_f} dt\, \boldsymbol{F}(t)\cdot(G\circ\boldsymbol{F})(t)\right)\\
&\times \exp\left(\frac{\mathrm{i}}{2m\hbar}\left[2\boldsymbol{p}_f - (\dot{G}\circ\boldsymbol{F})(t_f)\right]\cdot\left[t_f(\dot{G}\circ\boldsymbol{F})(t_f) - (G\circ\boldsymbol{F})(t_f)\right]\right)\\
&\times \exp\left(-\frac{\mathrm{i}}{2m\hbar}\left[2\boldsymbol{p}_i - (\dot{G}\circ\boldsymbol{F})(t_i)\right]\cdot\left[t_i(\dot{G}\circ\boldsymbol{F})(t_i) - (G\circ\boldsymbol{F})(t_i)\right]\right)\\
&\times \delta\big(\boldsymbol{p}_f - (\dot{G}\circ\boldsymbol{F})(t_f) - \boldsymbol{p}_i + (\dot{G}\circ\boldsymbol{F})(t_i)\big)\,. \qquad (14.36)
\end{aligned}
$$

For consistency we note that this reproduces the correct result $S_{fi} = \delta\big(\boldsymbol{p}_f - \boldsymbol{p}_i\big)$ for the free particle. The δ function implies conservation of the free momentum $\boldsymbol{P} = \boldsymbol{p}(t) - (\dot{G}\circ\boldsymbol{F})(t)$, or equivalently matching of the external momenta under evolution with the force $\boldsymbol{F}(t)$,

$$
\boldsymbol{p}_f = \boldsymbol{p}_i + \int_{t_i}^{t_f} dt\, \boldsymbol{F}(t). \qquad (14.37)
$$

Please note that it is not possible to impose simultaneous boundary conditions

$$
t_f\,\frac{\partial}{\partial t}G(t,t')\bigg|_{t=t_f} = G(t_f,t')
$$

and

$$
t_i\,\frac{\partial}{\partial t}G(t,t')\bigg|_{t=t_i} = G(t_i,t'),
$$

because such a Green's function does not exist. As a consequence it is not possible to eliminate the initial and final state dependent exponentials in the scattering matrix through a clever choice of the Green's function. This is of course as it should be, because the scattering amplitude $\mathcal{M}_{fi} = \mathrm{i}(S_{fi} - \delta_{fi})/\delta(\boldsymbol{P}_f - \boldsymbol{P}_i)$ generically must depend on the initial and final states.

The functionals $S[\boldsymbol{x},\boldsymbol{F}]$ (14.31), $Z[\boldsymbol{F}]$ (14.33) and $S_{fi}[\boldsymbol{F}]$ (14.36) are all independent of the boundary functions $\alpha(t')$ and $\beta(t')$ in the general Green's function (14.6). The easiest way to show this is by observing that the functionals are invariant under shifts

$$(G\circ\boldsymbol{F})(t)\to(G\circ\boldsymbol{F})(t)+\boldsymbol{A}t+\boldsymbol{B}$$

with constant vectors $\boldsymbol{A}$ and $\boldsymbol{B}$. For $Z[\boldsymbol{F}]$ the demonstration has to take into account that $\boldsymbol{X}_f$ and $\boldsymbol{X}_i$ contain $(G\circ\boldsymbol{F})(t_f)$ or $(G\circ\boldsymbol{F})(t_i)$ according to (14.32).

We are therefore free to use e.g. the Green's functions $G_i(t,t')$ (14.3) or $G_{fi}(t,t')$ (14.5), or the retarded Green's function $G_{ret}(t,t')=(t-t')\Theta(t-t')$ or a Stückelberg-Feynman type Green's function with equal contributions from retarded and advanced components, $G_{SF}(t,t')=|t-t'|/2$, or any other Green's function of the form (14.6).

The limit $t_i\to-\infty$, $t_f\to\infty$ in equation (14.36) yields the following representation of the S-matrix element for scattering due to the external force $\boldsymbol{F}(t)$,

$$\begin{aligned}S_{fi}[\boldsymbol{F}]={}&\delta\left(\boldsymbol{p}_f-\boldsymbol{p}_i-\int_{-\infty}^{\infty}dt\,\boldsymbol{F}(t)\right)\exp\left(\mathrm{i}\frac{\boldsymbol{p}_f+\boldsymbol{p}_i}{2m\hbar}\cdot\int_{-\infty}^{\infty}dt\,t\boldsymbol{F}(t)\right)\\&\times\exp\left(\frac{\mathrm{i}}{4m\hbar}\int_{-\infty}^{\infty}dt\int_{-\infty}^{\infty}dt'\,|t-t'|\boldsymbol{F}(t)\cdot\boldsymbol{F}(t')\right).\end{aligned}\tag{14.38}$$

In the next steps we will compare the correlation functions between the canonical and the path integral formalism.

The calculation of the one-point function from the path integral (14.33) has to take into account that the generic Green's function (14.6) shifts $\boldsymbol{x}_{f/i}$ to $\boldsymbol{X}_{f/i}$ according to equation (14.32). This implies for the one-point function in the path integral formalism

$$\begin{aligned}\langle\boldsymbol{x}_f,t_f|\boldsymbol{x}(t)|\boldsymbol{x}_i,t_i\rangle={}&-\mathrm{i}\hbar\,\frac{\delta}{\delta\boldsymbol{F}(t)}Z[\boldsymbol{F}]\bigg|_{\boldsymbol{F}=\boldsymbol{0}}=\langle\boldsymbol{x}_f|U_0(t_f,t_i)|\boldsymbol{x}_i\rangle\\&\times\left(\frac{\boldsymbol{x}_f+\boldsymbol{x}_i}{2}+\alpha(t)\left(\boldsymbol{x}_f-\boldsymbol{x}_i\right)+m\frac{\delta}{\delta\boldsymbol{F}(t)}\left(\boldsymbol{X}_f-\boldsymbol{X}_i\right)\cdot\frac{\boldsymbol{x}_f-\boldsymbol{x}_i}{t_f-t_i}\right).\end{aligned}$$

However, we have

$$m\frac{\delta}{\delta\boldsymbol{F}(t)}\left(\boldsymbol{X}_f-\boldsymbol{X}_i\right)=\alpha(t)(t_i-t_f)+t-\frac{t_f+t_i}{2},$$

and therefore the path integral result for the one-point function is indeed independent on the gauge functions $\alpha(t')$ and $\beta(t')$, as was already clear from the cancellation of those terms in $Z[\boldsymbol{F}]$,

$$\langle \boldsymbol{x}_f, t_f|\boldsymbol{x}(t)|\boldsymbol{x}_i, t_i\rangle = -\mathrm{i}\hbar \left.\frac{\delta}{\delta \boldsymbol{F}(t)} Z[\boldsymbol{F}]\right|_{\boldsymbol{F}=\boldsymbol{0}} = \langle \boldsymbol{x}_f|U_0(t_f, t_i)|\boldsymbol{x}_i\rangle \\ \times \left(\boldsymbol{x}_f \frac{t - t_i}{t_f - t_i} + \boldsymbol{x}_i \frac{t_f - t}{t_f - t_i}\right), \tag{14.39}$$

i.e. we do find the same result (14.11) as in the canonical formalism.

For the calculation of the two-point functions in the functional formalism

$$\langle \boldsymbol{x}_f, t_f|\boldsymbol{x}(t_2) \otimes \boldsymbol{x}(t_1)|\boldsymbol{x}_i, t_i\rangle = -\hbar^2 \left.\frac{\delta^2 Z[\boldsymbol{F}]}{\delta \boldsymbol{F}(t_2) \otimes \delta \boldsymbol{F}(t_1)}\right|_{\boldsymbol{F}=\boldsymbol{0}}$$

it is useful to observe that

$$\frac{1}{Z[\boldsymbol{F}]} \frac{\delta^2 Z[\boldsymbol{F}]}{\delta \boldsymbol{F}(t_2) \otimes \delta \boldsymbol{F}(t_1)} = \frac{\delta^2 \ln Z[\boldsymbol{F}]}{\delta \boldsymbol{F}(t_2) \otimes \delta \boldsymbol{F}(t_1)} + \frac{\delta \ln Z[\boldsymbol{F}]}{\delta \boldsymbol{F}(t_2)} \otimes \frac{\delta \ln Z[\boldsymbol{F}]}{\delta \boldsymbol{F}(t_1)}.$$

The factors in the last term were evaluated at $\boldsymbol{F} = \boldsymbol{0}$ in (14.39) and reproduce the tensor product of one-point functions in (14.12). The second order variational derivative of $\ln Z[\boldsymbol{F}]$ yields for $t_i \leq t_1 \leq t_2 \leq t_f$ (but *only* in that case)

$$-\hbar^2 \frac{\delta^2 \ln Z[\boldsymbol{F}]}{\delta \boldsymbol{F}(t_2) \otimes \delta \boldsymbol{F}(t_1)} = \frac{\mathrm{i}\hbar}{m} \frac{(t_f - t_2)(t_1 - t_i)}{t_f - t_i} \underline{1}.$$

The general result for $t_i < t_f$ is

$$-\hbar^2 \frac{\delta^2 \ln Z[\boldsymbol{F}]}{\delta \boldsymbol{F}(t_2) \otimes \delta \boldsymbol{F}(t_1)} = \frac{\mathrm{i}\hbar}{m(t_f - t_i)} \Big[\Theta(t_f - t_2)\Theta(t_2 - t_1)\Theta(t_1 - t_i) \\ \times (t_f - t_2)(t_1 - t_i) + \Theta(t_f - t_1)\Theta(t_1 - t_2)\Theta(t_2 - t_i)(t_f - t_1)(t_2 - t_i)\Big]\underline{1}.$$

Therefore we cannot in general simply identify $-\hbar^2 \delta^2 Z[\boldsymbol{F}]/(\delta \boldsymbol{F}(t_2) \otimes \delta \boldsymbol{F}(t_1))$ at $\boldsymbol{F} = \boldsymbol{0}$ with either $\boldsymbol{g}^{(2)}_{fi}(t_2, t_1)$ or $\boldsymbol{G}^{(2)}_{fi}(t_2, t_1)$, but we have

$$-\hbar^2 \left.\frac{\delta^2 Z[\boldsymbol{F}]}{\delta \boldsymbol{F}(t_2) \otimes \delta \boldsymbol{F}(t_1)}\right|_{\boldsymbol{F}=\boldsymbol{0}} = \boldsymbol{g}^{(2)}_{fi}(t_2, t_1) = \boldsymbol{G}^{(2)}_{fi}(t_2, t_1)$$

if $t_i \leq t_1 \leq t_2 \leq t_f$.

It seems surprising that substitution of (14.38) into equation (14.34) and setting $\boldsymbol{F} = \boldsymbol{0}$ after evaluation of the functional derivatives yields scattering from the potential V. However, equations (14.34, 14.38) compare to the practically useful relation (13.18) (or the equivalent relation (14.29)) for the scattering matrix elements like the representation

$$\langle \boldsymbol{x}|U_0(t-t')|\boldsymbol{x}'\rangle = \exp\left(\mathrm{i}\hbar\frac{t-t'-\mathrm{i}\epsilon}{2m}\frac{\partial^2}{\partial \boldsymbol{x}^2}\right)\delta(\boldsymbol{x}-\boldsymbol{x}')$$

for the $\boldsymbol{x}$ matrix elements of the free time evolution operator compares to the practically more useful representation (4.45).

Recasting the perturbation series in terms of the operator $V(-\mathrm{i}\hbar\delta/\delta\boldsymbol{F}(t), t)$ instead of $V(\boldsymbol{x}, t)$ does not yield a more efficient or practical representation for potential scattering theory. However, recasting interactions in terms of functional derivatives is useful when interactions are expressed in terms of higher order products of wave functions instead of potentials. Therefore we used the transcription of potential scattering theory in terms of functional derivatives with respect to auxiliary forces as an illustration for functional methods in perturbation theory.

14.4 Problems

14.1. Verify equation (14.26) for the general second order particle action

$$S[\boldsymbol{x}(t')] = \int_{t_0}^{t} dt' \left(\frac{1}{2}\dot{\boldsymbol{x}}(t')\cdot\underline{M}\cdot\dot{\boldsymbol{x}}(t') + \frac{1}{2}\boldsymbol{x}(t')\cdot\underline{F}\cdot\dot{\boldsymbol{x}}(t')\right.$$
$$\left. -\frac{1}{2}\boldsymbol{x}(t')\cdot\underline{\Omega^2}\cdot\boldsymbol{x}(t') + \boldsymbol{F}\cdot\boldsymbol{x}(t')\right),$$
$$\underline{F}^T = -\underline{F}, \quad \boldsymbol{x}(t_0) = \boldsymbol{x}_{cl}(t_0) = \boldsymbol{x}_0, \quad \boldsymbol{x}(t) = \boldsymbol{x}_{cl}(t) = \boldsymbol{x}.$$

14.2. Which exponential factor in the propagator $\langle \boldsymbol{x}|U(t,t_0)|\boldsymbol{x}_0\rangle$ do you find for a harmonic oscillator?

14.3. Derive the particular Green's functions (14.3) and (14.5) from the general form (14.6).

14.4. Show that the terms

$$\mathcal{A}[\boldsymbol{F}] = \frac{1}{2m}\left[(G\circ\boldsymbol{F})(t_f)\cdot(\dot{G}\circ\boldsymbol{F})(t_f) - (G\circ\boldsymbol{F})(t_i)\cdot(\dot{G}\circ\boldsymbol{F})(t_i)\right]$$
$$+\frac{1}{2m}\int_{t_i}^{t_f} dt\,\boldsymbol{F}(t)\cdot(G\circ\boldsymbol{F})(t)$$

in the exponent in (14.33) are actually the action $S[\boldsymbol{x},\boldsymbol{F}]$ for the classical trajectory $\boldsymbol{x}(t) = (G\circ\boldsymbol{F})(t)/m$.

Why is $Z[\boldsymbol{F}]$ not just given by $\langle\mathbf{0}|U_0(t_f,t_i)|\mathbf{0}\rangle\exp(\mathrm{i}\mathcal{A}[\boldsymbol{F}]/\hbar)$, in spite of what you might have expected from (14.26)?

14.5. Calculate the time ordered three-point function

$$\langle \boldsymbol{x}_f, t_f | \mathbf{x}(t_3) \otimes \mathbf{x}(t_2) \otimes \mathbf{x}(t_1) | \boldsymbol{x}_i, t_i \rangle, \quad t_i < t_1 < t_2 < t_3 < t_f,$$

both in the canonical formalism and in the path integral formalism.

14.6. The functional $S_{fi}[\boldsymbol{F}] \equiv S(\boldsymbol{p}_f, \boldsymbol{p}_i)[\boldsymbol{F}]$ (14.38) is a scattering matrix element between momentum eigenstates. The functional $Z[\boldsymbol{F}]$ (14.33) on the other hand is *not* a scattering matrix element in position space because it does *not* correspond to a position space matrix element of an *interaction picture time evolution operator*. Instead it corresponds to the path integral result for the position matrix element of the *full time evolution operator* of a free particle under the influence of a spatially homogeneous force $\boldsymbol{F}(t)$. However, we can derive a position space scattering matrix element through Fourier transformation of $S(\boldsymbol{p}_f, \boldsymbol{p}_i)[\boldsymbol{F}]$. Show that

$$\begin{aligned} S(\boldsymbol{x}_f, \boldsymbol{x}_i)[\boldsymbol{F}] &= \int d^3\boldsymbol{p}_f \int d^3\boldsymbol{p}_i \, \exp\!\left(\frac{\mathrm{i}}{\hbar}\left(\boldsymbol{p}_f \cdot \boldsymbol{x}_f - \boldsymbol{p}_i \cdot \boldsymbol{x}_i\right)\right) \frac{S(\boldsymbol{p}_f, \boldsymbol{p}_i)[\boldsymbol{F}]}{(2\pi\hbar)^3} \\ &= \delta\!\left(\boldsymbol{x}_f - \boldsymbol{x}_i + \frac{1}{m}\int_{-\infty}^{\infty} dt\, t\boldsymbol{F}(t)\right) \exp\!\left(\mathrm{i}\frac{\boldsymbol{x}_f + \boldsymbol{x}_i}{2\hbar} \cdot \int_{-\infty}^{\infty} dt\, \boldsymbol{F}(t)\right) \\ &\times \exp\!\left(\frac{\mathrm{i}}{4m\hbar}\int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dt'\, |t - t'| \boldsymbol{F}(t) \cdot \boldsymbol{F}(t')\right). \end{aligned} \tag{14.40}$$

Show also that with the conditions

$$\lim_{t\to\pm\infty} t \int_{-\infty}^{t} dt'\, \boldsymbol{F}(t') = \boldsymbol{0} \tag{14.41}$$

the δ function implies

$$\boldsymbol{x}_f = \boldsymbol{x}_i + \frac{1}{m}\int_{-\infty}^{\infty} dt \int_{-\infty}^{t} dt'\, \boldsymbol{F}(t'), \tag{14.42}$$

while the conditions

$$\lim_{t\to\pm\infty} t \int_{t}^{\infty} dt'\, \boldsymbol{F}(t') = \boldsymbol{0} \tag{14.43}$$

yield with the δ function the relation

$$\boldsymbol{x}_i = \boldsymbol{x}_f + \frac{1}{m}\int_{\infty}^{-\infty} dt \int_{\infty}^{t} dt'\, \boldsymbol{F}(t'). \tag{14.44}$$

Equation (14.42) describes the asymptotic solution of a classical trajectory of a non-relativistic particle which started out at rest in $\boldsymbol{x}_i$ at $t \to -\infty$, while (14.44) reconstructs the initial location for $t \to -\infty$ of a particle which comes to rest in $\boldsymbol{x}_f$ in the limit $t \to \infty$. The conditions (14.41) or (14.43) do not generate extra restrictions on the physical motion of the particle, but are mathematical conditions for convergence of the time integrals in (14.42) or (14.44), respectively, i.e. they are necessary for existence of solutions of the Newton equation for $t \to \pm\infty$.