Path Integrals in Quantum Mechanics

Joachim Ankerhold and Björn Kubala

WS 2014/15

Be aware: May still contain typos

December 11, 2014

I. Introduction

The conventional formulation of quantum mechanics as it is taught to students is based on the Schrödinger equation. This is in some contrast to the actual situation in theoretical physics, where all modern developments make extensive use of the path integral formalism, in particular in modern field theories in atomic, condensed matter, statistical, and polymer physics, in cosmology, elementary particle physics and even in econophysics.

The first who introduced 'a sum over paths' was N. Wiener who worked with Wiener measures to analyze problems in statistical physics and Brownian motion. This idea was extended by Paul Dirac in 1933/34 (Physical Journal of the Soviet Union **3**, 64 (1933) to quantum mechanics. However, it was R. Feynman who developed the full method in the 1940s and described it in detail in his seminal paper 'Space-Time Approach to Non-Relativistic Quantum Mechanics'. Rev. Mod. Phys. **20**, 367 (1948). Since then the path integral representation of quantum mechanics has been put forward, generalized, and laid on a firm mathematically basis.

It was clear from the very beginning that path integrals provide an alternative way of understanding quantum mechanics which allows for calculations, approximations, and formal manipulations that are very difficult, if not impossible, to achieve within the Schrödinger representation. In a way, the two framework are complementary: to obtain wave functions and eigenergies, the Schrödinger equation is the most convenient tool, for semiclassical approximations and many-body problems path integrals are the right tools.

In this lecture we will learn the basic ingredients of the formalism starting with the formulation as it was originally introduced by Feynman. This is not a math course in functional integration meaning that we have to skip all mathematical subtleties and instead follow a more 'pragmatic' approach. However, we will refer to the literature for those who are interested. There are many books which address the path integral formulation. Here is a selection:

- Feynman, R. P. and Hibbs, A. R. (1965). Quantum Mechanics and Path Integrals. New York: McGraw-Hill. ISBN 0-07-020650-3.
- Schulman, Larry S. (1981). Techniques & Applications of Path Integration. New York: John Wiley & Sons. ISBN 0486445283.

- Glimm, James, and Jaffe, Arthur (1981). Quantum Physics: A Functional Integral Point of View. New York: Springer-Verlag. ISBN 0-387-90562-6.
- Hagen Kleinert (2004). Path Integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets (4th ed.). Singapore: World Scientific. ISBN 981-238-107-4.
- About mathematical foundations: DeWitt-Morette, Ccile (1972). 'Feynman's path integral: Definition without limiting procedure'. Communication in Mathematical Physics **28** (1): 47; Albeverio, S. & Hoegh-Krohn. R. (1976). Mathematical Theory of Feynman Path Integral. Lecture Notes in Mathematics **523**. Springer-Verlag. ISBN 0-387-07785-5.

II. Schrödinger quantum mechanics

II.1. Time evolution and the propagator

The dynamics of a quantum system with Hamiltonian H follows from the Schr$\ddot{\text{d}}$inger equation

$$H|\psi(t)\rangle = i\hbar \frac{d}{dt}|\psi(t)\rangle \, . \tag{II.1}$$

For time-independent Hamiltonians one finds from $|\psi(t)\rangle = \mathrm{e}^{-\frac{i}{\hbar}E_n t}|\phi_n\rangle$ that the eigenstates are the stationary solutions to

$$H|\phi_n\rangle = E_n|\phi_n\rangle \tag{II.2}$$

and that they form a complete basis set of the Hilbert space with $\langle\phi_n|\phi_m\rangle = \delta_{n,m}$. A classical phase space with conjugate variables q and p with Poisson brackets $\{q,p\} = 1$, is quantized by imposing $[q,p] = i\hbar$.

A formal solution to the time-dependent Schrödinger equation is given for $t \geq 0$ by

$$|\psi(t)\rangle = G(t)\,|\psi(0)\rangle \quad , \quad G(t) = \mathrm{e}^{-iHt/\hbar} \, , \tag{II.3}$$

where the propagator has the spectral representation

$$G(t) = \sum_n \mathrm{e}^{-iE_n t/\hbar}\,|\phi_n\rangle\langle\phi_n| \quad , \quad t \geq 0 \tag{II.4}$$

and thus carries the same information as the solutions of the time-independent Schrödinger equation. Its formal Fourier transform

$$\tilde{G}(E) = \frac{1}{i}\sum_n \frac{|\phi_n\rangle\langle\phi_n|}{E_n - E - io^+} \tag{II.5}$$

gives direct access to the energy spectrum (here o^+ enures that the contour integration back to time-space has only contributions for $t \geq 0$).

The kernel can thus also be considered as the central object in quantum mechanics (instead of the wave functions). It has the following properties

1. It obeys a semi-group identity, i.e.,

$$G(t,0) = G(t,t')\, G(t',0) \quad \text{with } 0 \le t' \le t \tag{II.6}$$

2. In position representation, this identity reads

$$\begin{aligned} G(q_f, q_i, t) &\equiv \langle q_f | G(t) | q_i \rangle \\ &= \int dq G(q_f, q, t-t')\, G(q, q_i, t') \end{aligned} \tag{II.7}$$

   Remark: Note that the propagator depends on time differences only for time-independent Hamiltonians.

3. It easily follows that

$$i\hbar \frac{d}{dt} G(t,t') = H\, G(t,t') \quad \text{with } G(t',t') = 1 \tag{II.8}$$

4. The retarded propagator $G_r(t,t') = \theta(t-t')\, G(t,t')$ obeys in position space

$$\left[i\hbar \partial_{t_f} - H(q_f, -i\hbar \partial_{q_f}) \right] G(q_f, q_i, t_f, t_i) = i\hbar \delta(t_f - t_i)\, \delta(q_f - q_i)\,. \tag{II.9}$$

   and is thus the Greens-function of the Schrödinger equation.

Due to these properties, it was Feynman's idea to formulate quantum mechanics only based on a representation of the propagator. This then leads to the 'integral' form of the Schrödinger equation in terms of path integrals.

II.2. The free particle

As an example we consider the free particle with $H = p^2/2m$ for which the propagator can easily be calculated analytically. From

$$G(q_f, q_i, t) = \langle q_f | \mathrm{e}^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}} | q_i \rangle \tag{II.10}$$

we obtain by inserting a complete set of momentum eigenstates $1 = \int dp\, |p\rangle\langle p|$ with

$$\langle q | p \rangle = \frac{1}{\sqrt{2\pi\hbar}}\, \mathrm{e}^{\frac{i}{\hbar} pq} \tag{II.11}$$

the following integrals

$$
\begin{aligned}
G(q_f, q_i, t) &= \int_{-\infty}^{\infty} dp \ \langle q_f | p \rangle \ \mathrm{e}^{-\frac{i}{\hbar}\frac{p^2}{2m}} \ \langle p | q_i \rangle \\
&= \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dp \ \mathrm{e}^{-\frac{i}{\hbar}\frac{p^2}{2m}} \ \mathrm{e}^{\frac{i}{\hbar} p (q_f - q_i)} \\
&= \sqrt{\frac{m}{2\pi i \hbar t}} \ \mathrm{e}^{\frac{i}{\hbar}\frac{m}{2\,t}(q_f - q_i)^2} \, .
\end{aligned}
\tag{II.12}
$$

Remark: The exponent coincides with the classical action of a free particle running in time t from q_i to q_f, i.e.,

$$
S(q_f, q_i, t) = \int_0^t ds \frac{\dot{q}(s)^2}{2m} = \frac{m}{2\,t}(q_f - q_i)^2 \, . \tag{II.13}
$$

The corresponding path is

$$
q_{\mathrm{cl}}(s) = q_i + (q_f - q_i)\frac{s}{t} \tag{II.14}
$$

and the action is conveniently obtained from $S(q_f, q_i, t) = \frac{m}{2} q(s)\dot{q}(s)\big|_0^t$.

III. Path integral à la Feynman

III.1. Real-time propagator

We consider a system with Hamiltonian

$$\begin{aligned} H &= \frac{p^2}{2m} + V(q) \\ &= T + V \end{aligned} \qquad \text{(III.1)}$$

with conjugate operators $[p, q] = -i\hbar$.

Then, the whole path integral business starts with

$$\begin{aligned} G(t) &= \left(\mathrm{e}^{-i\epsilon H/\hbar}\right)^N \quad , \quad \epsilon = t/N \\ &= \left(\mathrm{e}^{-i\epsilon T/\hbar}\,\mathrm{e}^{-i\epsilon V/\hbar}\,\mathrm{e}^{-C/\hbar^2}\right)^N \quad , \end{aligned} \qquad \text{(III.2)}$$

where C is a 'correction' operator according to the Baker-Campbell-Hausdorff formula. The correction operator is a series in ϵ with its lowest order term being $C = \epsilon^2[T, V] + O(\epsilon^3)$. We thus think of dividing the time interval $[0, t]$ into $N - 1$ equidistant segments of length ϵ, where ϵ is assumed to be much smaller than any other relevant time scale. In the very end, we will consider limit, where $\epsilon \to 0$ but $\epsilon N = t = const.$. Mathematically, this 'factorization' is a special case of the Trotter formula

$$\mathrm{e}^{A+B} \equiv \left(\mathrm{e}^{A/N+B/N}\right)^N = \lim_{N\to\infty} \left(\mathrm{e}^{A/N}\ \mathrm{e}^{B/N}\right)^N \qquad \text{(III.3)}$$

which holds for bounded operators but can also be proven for unbounded operators under certain conditions. We do not discuss this subtle issue any further but proceed with its application for the propagator in position representation.

Accordingly,

$$\begin{aligned} G(q_f, q_i, t) &\equiv \langle q_f | G(t) | q_i \rangle \\ &= \langle q_f | \left(\mathrm{e}^{-i\epsilon H/\hbar} \right)^N | q_i \rangle \\ &= \langle q_f | \underbrace{\mathrm{e}^{-i\epsilon H/\hbar} \ldots \mathrm{e}^{-i\epsilon H/\hbar}}_{\text{N-times}} | q_i \rangle \\ &= \int \left(\prod_{k=1}^{N-1} dq_k \right) \prod_{k=1}^{N} \langle q_k | \mathrm{e}^{-i\epsilon H/\hbar} | q_{k-1} \rangle \,, \end{aligned} \tag{III.4}$$

where we inserted $N-1$ resolutions of the identity $\int dq_k \, |q_k\rangle\langle q_k| = 1; k = 1, \ldots, N-1$ and put $q_0 = q_i$ and $q_f = q_N$, see Fig. III.1. One may then write

$$\begin{aligned} \langle q_k | G(\epsilon) | q_{k-1} \rangle &= \langle q_k | \mathrm{e}^{-i\epsilon T/\hbar} \, \mathrm{e}^{-i\epsilon V/\hbar} \, \mathrm{e}^{-C/\hbar^2} | q_{k-1} \rangle \\ &\approx \langle q_k | \mathrm{e}^{-i\epsilon T/\hbar} | q_{k-1} \rangle \, \mathrm{e}^{-i\epsilon V(q_{k-1})/\hbar} \,, \end{aligned} \tag{III.5}$$

where the second line becomes a strict identity in the limit $N \to \infty$ with $N\epsilon = t = const.$

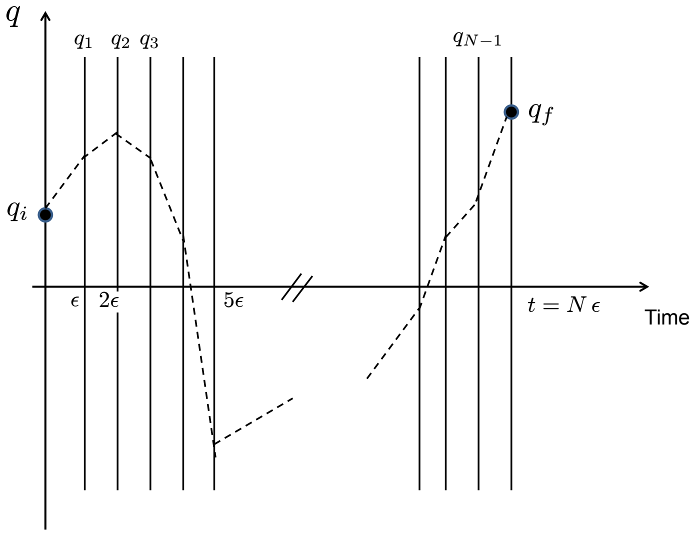

Figure III.1.: Trotter discretization for the real-time propagator according to (III.4).

What remains to do is, to plug in the expression for the propagator of a free particle in position space that we derived already in (II.12). For the above matrix element it reads

$$\langle q_k | \mathrm{e}^{-i\epsilon T/\hbar} | q_{k-1} \rangle = \sqrt{\frac{\sigma}{i\pi}} \, \mathrm{e}^{i\sigma(q_k - q_{k-1})^2} \tag{III.6}$$

with $\sigma = m/2\hbar\epsilon$. Accordingly,

$$G(q_f, q_i, t) = \int \left(\prod_{k=1}^{N-1} dq_k \sqrt{\frac{\sigma}{i\pi}} \right) \exp\left\{ \frac{i}{\hbar} \left[\sum_{k=1}^{N} \frac{m(q_k - q_{k-1})^2}{2\epsilon} - \epsilon V(q_{k-1}) \right] \right\} . \qquad \text{(III.7)}$$

The somewhat subtle part is now to perform the limit $N \to \infty$, $N\epsilon = t$. In the exponent we put $(q_k - q_{k-1})/\epsilon \to \dot{q}(s)$ and assume that in this limit the $\{q_k\}$ give rise to paths $q(s), 0 \leq s \leq t$ with boundary conditions $q(0) = q_0 \equiv q_i$ and $q(t) = q_N \equiv q_f$. Note that these paths are continuous but not necessarily differentiable. One then has

$$\begin{aligned} G(q_f, q_i, t) &= \mathcal{N} \lim_{N\to\infty, N\epsilon=t} \int \left(\prod_{k=1}^{N-1} dq_k \sqrt{\frac{\sigma}{i\pi}} \right) \mathrm{e}^{\frac{i}{\hbar} S[q]} \\ &= \mathcal{N} \int_{q(0)=q_i}^{q(t)=q_f} \mathcal{D}[q] \, \mathrm{e}^{\frac{i}{\hbar} S[q]} \end{aligned} \qquad \text{(III.8)}$$

with the action

$$S[q] = \int_0^t ds \left[\frac{m\dot{q}(s)^2}{2} - V(q) \right] \qquad \text{(III.9)}$$

and where the symbol $\mathcal{D}[q]$ abbreviates

$$\int \mathcal{D}[q] = \lim_{N\to\infty, N\epsilon=t} \int \left(\prod_{k=1}^{N-1} dq_k \sqrt{\frac{\sigma}{i\pi}} \right) . \qquad \text{(III.10)}$$

The factor $\mathcal{N}$, to be determined below, is included to make the limiting process in the integrations meaningful (to avoid any divergencies in the infinite product of $\sqrt{\frac{\sigma}{i\pi}}$, see below).

Remarks:

- The above integral is a formal object which must be understood as a result of the limiting procedure. As such it has properties different from ordinary integrals, e.g., with respect to the transformation of variables.

- The path integral is invariant against translations of the form $q(s) \to q_0(s) + y(s)$ as long as the boundary conditions are satisfied, e.g., via $q_0(0) = q_i, q(t) = q_f$ and $y(0) = y(t) = 0$, i.e.,

$$\int_{q(0)=q_i}^{q(t)=q_f} \mathcal{D}[q] \, \mathrm{e}^{\frac{i}{\hbar} S[q]} = \int_{q(0)=q_i}^{q(t)=q_f} \mathcal{D}[q] \, \mathrm{e}^{\frac{i}{\hbar} S[q+y]} . \qquad \text{(III.11)}$$

- Path integrals can be understood as sums over the functional space of all continuous paths connecting $q(0) = q_i$ with $q(t) = q_f$, where the contribution of each path is weighted by an action factor. Paths contributing to this sum are only determined by boundary conditions and not by initial conditions.

III.2. Canonical operator and partition function

The central object of the canonical ensemble of thermodynamics is the density operator

$$\rho_\beta = \frac{1}{Z}\,\mathrm{e}^{-\beta H} \tag{III.12}$$

with inverse temperature $\beta = 1/k_{\mathrm{B}}T$ and the partition function

$$Z = \mathrm{Tr}\{\mathrm{e}^{-\beta H}\}\,. \tag{III.13}$$

Apparently, there is a formal relation between the real-time propagator and the unnormalized canonical operator via a so-called Wick rotation, i.e., $t \to -i\hbar\beta$. A path integral in 'imaginary time' can thus be derived for the canonical operator from (III.8). One puts $\bar{q}(\tau) = q(-i\tau)$, $0 \le \tau \le \hbar\beta$ and introduces the so-called Euclidian action

$$S_E[\bar{q}] = \int_0^{\hbar\beta} d\tau \left[\frac{m\dot{\bar{q}}(\tau)^2}{2} + V(\bar{q})\right] \tag{III.14}$$

to arrive at

$$\tilde{\rho}_\beta \equiv \langle q_f|\mathrm{e}^{-\beta H}|q_i\rangle = \mathcal{N}' \int_{\bar{q}(0)=q_i}^{\bar{q}(\hbar\beta)=q_f} \mathcal{D}[\bar{q}]\ \mathrm{e}^{-S_E[\bar{q}]/\hbar} \tag{III.15}$$

This Euclidian dynamics is thus equivalent to a real-time motion in the inverted potential $-V(q)$. The partition function follows by summing over all closed paths

$$\begin{aligned} Z &= \mathcal{N}' \int dq_i \int_{\bar{q}(0)=q_i}^{\bar{q}(\hbar\beta)=q_i} \mathcal{D}[\bar{q}]\ \mathrm{e}^{-S_E[\bar{q}]/\hbar} \\ &= \oint_{\bar{q}(0)=q_i}^{\bar{q}(\hbar\beta)=q_i} \mathcal{D}[\bar{q}]\ \mathrm{e}^{-S_E[\bar{q}]/\hbar}\,. \end{aligned} \tag{III.16}$$

III.3. Ehrenfest's theorem and functional derivatives

Let us consider paths contributing to (III.8) which are shifted according to $q(s)+\delta q(s)$, where $\delta q(s)$ is assumed to be infinitesimal small with $\delta q(0) = \delta q(t) = 0$. This then means

$$S[q(s)+\delta q(s)] = S[q(s)] + \delta S[q(s)]\,, \tag{III.17}$$

where the variation reads according to what we know from classical mechanics

$$\delta S[q] = \int_0^t ds \left(\frac{\partial L}{\partial q} - \frac{\partial}{\partial t} \frac{\partial L}{\partial \dot{q}} \right) \delta q(s) \tag{III.18}$$

with the Lagrange functional $L[q, \dot{q}] = \dot{q}^2/2m - V(q)$. The invariance of the path integral against translations (III.11) then implies

$$\int_{q(0)=q_i}^{q(t)=q_f} \mathcal{D}[q]\, \delta S[q]\, \mathrm{e}^{\frac{i}{\hbar} S[q]} = 0 \tag{III.19}$$

meaning that quantum mechanics obeys the classical equations of motion (Ehrenfest's theorem) when averaged over all possible paths connecting q_i with q_f in time t.

At this point, we will spend a few words on functional derivatives. Further details are found in the respective literature. Consider a functional $F[\rho] : \mathbf{M} \to \mathbf{R}$ as a mapping of a function space $\mathbf{M}$ onto c-numbers and an infinitesimal variation $y \in \mathbf{M}$. The differential of the functional $F[\rho]$ is then defined as

$$\delta F = \int dx \frac{\delta F[\rho]}{\delta \rho(x)}\, y(x)\,. \tag{III.20}$$

This can be seen as the functional form of the total derivative $df = \sum_{k=1}^{N} [\partial f / \partial x_k]\, dx_k$ of a function $f = f(x_1, \ldots, x_N)$ on a N-dimensional space of variables.

The functional derivative has the following properties

$$\begin{aligned} \frac{\delta(\lambda F + \mu G)}{\delta \rho} &= \lambda \frac{\delta F}{\delta \rho} + \mu \frac{\delta G}{\delta \rho} \\ \frac{\delta F[f[\rho]]}{\delta \rho} &= \frac{\delta F[f]}{\delta f} \frac{\delta f[\rho]}{\delta \rho} \\ \frac{\delta \rho(x)}{\delta \rho(s)} &= \delta(x - s) \end{aligned} \tag{III.21}$$

and the functional Taylor expansion around a reference function ϕ reads

$$F[\rho = \phi + y] = F[\phi] + \sum_{k=1}^{\infty} \frac{1}{k!} \delta^k F[\phi, y] \tag{III.22}$$

with

$$\delta^k F[\phi, y] = \int dx_1 \ldots dx_k \; \left. \frac{\delta F[\rho]}{\delta \rho(x_1) \cdots \delta \rho(x_k)} \right|_{\rho=\phi} \; y(x_1) \cdots y(x_k)\,. \tag{III.23}$$

Example:

$$F[q] = \int_0^t dsq(s)^2 \tag{III.24}$$

so that

$$\begin{aligned}\frac{\delta^2 F[q]}{\delta q(u)\delta q(v)} &= \int_0^t ds\ 2\delta(s-v)\delta(s-u) \\ &= 2\delta(v-u)\end{aligned} \tag{III.25}$$

which leads to

$$\begin{aligned}\delta^2 F &= \int_0^t dudv \frac{\delta^2 F[q]}{\delta q(u)\delta q(v)} y(v)y(u) \\ &= 2\int_0^t duy(u)^2 .\end{aligned} \tag{III.26}$$

III.4. Correlation functions

We now turn to expectation values and more generally to correlation functions of Heisenberg operators of the position $\hat{q}(t_0)$ at time $0 \le t_0 \le t_f$. Let us start with

$$\begin{aligned}\langle q_f, t_f|\hat{q}(t_0)|q_i, 0\rangle &= \int dq_0 \langle q_f, t_f|\hat{q}(t_0)|q_0, t_0\rangle\langle q_0, t_0|q_i, 0\rangle \\ &= \int dq_0 \langle q_f, t_f|q_0, t_0\rangle\langle q_0, t_0|q_i, 0\rangle\, q_0 \\ &= \mathcal{N} \int_{q(0)=q_i}^{q(t)=q_f} \mathcal{D}[q]\, q(t_0)\, \mathrm{e}^{\frac{i}{\hbar}S[q]} ,\end{aligned} \tag{III.27}$$

where we used $q(t_0) \equiv q_0$ and further exploited the semi-group property (II.7) of the propagator. See also (III.4), where in the fourth line the additional $\hat{q}(t_0)$ acts on the respective position eigenfunction, thus producing the c-number q_0.

Now, when it comes to products $\hat{q}(t_1)\hat{q}(t_2)$, the semi-group property of the propagator can only be applied when a time-ordering is performed. If $t_1 > t_2$ we simply follow the above procedure to end up with

$$\langle q_f, t_f|\hat{q}(t_1)\hat{q}(t_2)|q_i, 0\rangle = \mathcal{N} \int_{q(0)=q_i}^{q(t)=q_f} \mathcal{D}[q]\, q(t_1)q(t_2)\, \mathrm{e}^{\frac{i}{\hbar}S[q]} . \tag{III.28}$$

Note that in the integrand of the path integral we work with c-number valued functions so that $q(t_1)q(t_2) = q(t_2)q(t_1)$, while on the operator level this is not the case. Hence, in case of $t_2 > t_1$ the semi-group property can only be applied to $\hat{q}(t_2)\hat{q}(t_1)$. In essence,

$$\mathcal{N} \int_{q(0)=q_i}^{q(t)=q_f} \mathcal{D}[q]\, q(t_1) \cdots q(t_k)\, \mathrm{e}^{\frac{i}{\hbar} S[q]} = \langle q_f, t_f | \mathcal{T} \hat{q}(t_1) \cdots \hat{q}(t_k) | q_i, 0 \rangle \tag{III.29}$$

with the time ordering operator $\mathcal{T}$ which implies the prescription to arrange operators from left to right in descending time order starting with the latest time.

IV. Gaussian path integrals and harmonic oscillator

In the previous section we have learned in (III.22) how to perform a Taylor expansion of a functional around a fixed element in function space. Obviously, for functional which are at most quadratic, this expansion terminates after the second term, thus leading in the path integral to Gaussian integrals which can be done exactly. Here, we discuss in detail how to solve the corresponding functional integrals. This is not just a nice exercise but will also elucidate the normalization issue. Further, it turns out that all exactly solvable models (hydrogen atom, Morse potential etc.) can be mapped onto Gaussian integrals. Third, Gaussian integrals are the starting point to treat nonlinear problems perturbatively around linear ones. One very convenient way to do so, is to apply an expansion in $\hbar$, i.e. a so-called semiclassical expansion (we will discuss this approach in another section).

In general, quadratic action functionals are of the form

$$S[q] = \int_0^t ds \left[\frac{m\dot{q}(s)^2}{2} - \frac{m\omega(s)^2}{2} q(s)^2 + j(s)\, q(s)\right] \tag{IV.1}$$

with the function $j(s)$ often referred to as a source term, since

$$\frac{\delta}{\delta j(u)} \mathrm{e}^{\frac{i}{\hbar}S[q]} = \frac{i}{\hbar}\, q(u)\, \mathrm{e}^{\frac{i}{\hbar}S[q]} \quad ,0 \leq u \leq t \tag{IV.2}$$

generates moments of q, see Sec. III.4.

IV.1. Harmonic oscillator and normalization

To start with, let us consider a simple harmonic problem with $\omega(t) \equiv \omega_0$ and $j(s) = 0$. Now, to calculate

$$G(q_f, q_i, t) = \mathcal{N} \int_{q(0)=q_i}^{q(t)=q_f} \mathcal{D}[q]\, \exp\left\{\frac{i}{\hbar}\int_0^t ds \left[\frac{m\dot{q}(s)^2}{2} - \frac{m\omega_0^2}{2} q(s)^2\right]\right\} \tag{IV.3}$$

a good strategy is to expand the action around the classical path $q_{\rm cl}$ (stationary path): Then, the first derivative vanishes and we can rely on what we have learned in classical mechanics. Hence

$$q(s) = q_{\rm cl}(s) + y(s) \quad , \quad q_{\rm cl}(0) = q_i, \quad q_{\rm cl}(t) = q_f \quad , \quad y(0) = y(t) = 0 \tag{IV.4}$$

so that one has the exact expansion

$$\begin{aligned} S[q] &= S[q_{\rm cl}] + \frac{1}{2}\int_0^t ds \int_0^t du \left.\frac{\delta^2 S[q]}{\delta q(s)\delta q(u)}\right|_{q=q_{\rm cl}} y(s)y(u) \\ &= S[q_{\rm cl}] + \frac{m}{2}\int_0^t ds y(s)\left[-\frac{d^2}{ds^2} - \omega_0^2\right] y(s) \\ &= S[q_{\rm cl}] + \frac{1}{2}\int_0^t ds \left[m\dot{y}(s)^2 - m\omega_0^2 y(s)^2\right] . \end{aligned} \tag{IV.5}$$

Exercise: show how to get from the first to the third line

The classical path follows from

$$\ddot{q}_{\rm cl}(s) + \omega_0^2 q_{\rm cl}(s) = 0 \tag{IV.6}$$

with the above boundary conditions. We already note here that boundary value problems may have multiple solutions in contrast to initial value problems. In path integration one carefully has to sum over contributions of all classical paths (see below). The solution to (IV.6) is simple and reads

$$q_{\rm cl}(s) = q_i \, \cos(\omega_0 s) + \frac{q_f - q_i \cos(\omega_0 t)}{\sin(\omega_0 t)} \sin(\omega_0 s) \tag{IV.7}$$

so that

$$\begin{aligned} S[q_{\rm cl}] &= \frac{m}{2} q_{\rm cl}(s)\dot{q}_{\rm cl}(s)\Big|_0^t \\ &= \frac{m\omega_0}{2\sin(\omega_0 t)}\left[(q_i^2 + q_f^2)\cos(\omega_0 t) - 2q_i q_f\right] \end{aligned} \tag{IV.8}$$

which leads to

$$G(q_f, q_i, t) = \mathrm{e}^{\frac{i}{\hbar}S[q_{\rm cl}]}\, \mathcal{N}\int_{y(0)=0}^{y(t)=0} \mathcal{D}[y]\mathrm{e}^{\frac{i}{\hbar}S[y]} . \tag{IV.9}$$

Here we used that for this problem the second derivative of the action has the same form as the full one with q replaced by y.

To solve the path integral over the fluctuations, we realize [see (IV.5)] that $S[y] \sim$

$\int_0^t dsy(s)\, L(s)\, y(s)$ with the operator

$$L(s) = -\partial_s^2 - \omega_0^2 \,. \tag{IV.10}$$

The strategy is then to represent the fluctuations in the eigenbasis of L and to solve the Gaussian integrals over the expansion coefficients. We will first follow this strategy and later discuss this issue on more general grounds. Accordingly, we write

$$y(s) = \sum_{k=1}^{\infty} a_k\, \phi_k(s) \quad \text{with} \quad L(s)\phi_k(s) = \lambda_k\, \phi_k(s) \ , \ \phi_k(0) = \phi_k(t) = 0 \ , k = 1, 2, 3, \ldots \,. \tag{IV.11}$$

Since L is a hermitian operator on the interval $[0, t]$ (regular Sturm-Liouville problem), it has a complete set of orthonormal eigenfunctions

$$\phi_k(s) = \sqrt{\frac{2}{t}}\, \sin(k\pi\, s/t) \quad , \quad \lambda_k = \frac{k^2\pi^2}{t^2} - \omega_0^2 \,, \tag{IV.12}$$

where the normalization follows from

$$\int_0^t ds\phi_k(s)\, \phi_n(s) = \delta_{k,n} \,. \tag{IV.13}$$

Thus,

$$S[y] = \frac{m}{2} \sum_k \lambda_k\, a_k^2 \tag{IV.14}$$

and

$$\begin{aligned} \int \mathcal{D}[y]\, \mathrm{e}^{\frac{im}{2\hbar}\int_0^t dsy(s)L(s)y(s)} &\sim \prod_k \int da_k\, \mathrm{e}^{\frac{im}{2\hbar}\lambda_k a_k^2} \\ &= \left(\prod_k \frac{m}{2\pi i\hbar}\lambda_k\right)^{-\frac{1}{2}} \,. \end{aligned} \tag{IV.15}$$

The Jacobian for the transformation from the y to the coefficients $\{a_k\}$ is absorbed in the normalization prefactor that we fix at the very end.

The infinite product

$$\prod_k \frac{m}{2\pi i\hbar}\lambda_k \tag{IV.16}$$

diverges, a fact that reveals the necessity of the normalization $\mathcal{N}$ introduced above. We thus write

$$\begin{aligned}
\prod_k \frac{m}{2\pi i\hbar}\lambda_k &= \prod_k \frac{m}{2\pi i\hbar}\frac{k^2\pi^2}{t^2}\left(1-\frac{\omega_0^2 t^2}{\pi^2 k^2}\right) \\
&= \left(\prod_k \frac{m}{2\pi i\hbar}\frac{k^2\pi^2}{t^2}\right)\left[\prod_k \left(1-\frac{\omega_0^2 t^2}{\pi^2 k^2}\right)\right] \\
&= \mathcal{M}\,\frac{\sin(\omega_0 t)}{\omega_0 t}\,, \qquad \text{(IV.17)}
\end{aligned}$$

where we used

$$\prod_{k=1}^{\infty}\left(1-\frac{x^2}{k^2\pi^2}\right) = \frac{\sin(x)}{x}\,. \qquad \text{(IV.18)}$$

For the full fluctuation path integral, we then have

$$\begin{aligned}
G(0,0,t) &= \mathcal{N}\prod_k \int da_k \; \mathrm{e}^{\frac{im}{2\hbar}\lambda_k a_k^2} \\
&= \frac{\mathcal{N}}{\sqrt{\mathcal{M}}}\sqrt{\frac{\omega_0 t}{\sin(\omega_0 t)}}\,. \qquad \text{(IV.19)}
\end{aligned}$$

Apparently, the singular factor $\mathcal{M}$ does not depend on ω_0 and thus appears also in case of a free particle. We thus use the expression of a free particle (II.12) to define the normalization such as to compensate for the singularity and regain the correct result for $\omega_0 \to 0$. Hence,

$$\mathcal{N} = \sqrt{\frac{m}{2\pi i\hbar t}}\;\sqrt{\mathcal{M}}\,. \qquad \text{(IV.20)}$$

Finally, this provides us with the real-time propagator of a harmonic oscillator

$$G(q_f,q_i,t) = \sqrt{\frac{m\omega_0}{2\pi i\hbar\sin(\omega_0 t)}}\;\exp\left[i\frac{m\omega_0}{2\hbar}\frac{(q_f^2+q_i^2)\cos(\omega_0 t)-2q_i q_f}{\sin(\omega_0 t)}\right]\,. \qquad \text{(IV.21)}$$

There is still a little problem though, namely, this expression diverges for all times $t_\nu = \nu\pi/\omega_0, \nu = 1,2,3,\ldots$! In fact, a careful analysis close to these times shows that

$$\lim_{t\to t_\nu} G(q_f,q_i,t) = \delta[q_f-(-1)^\nu q_i]\,\mathrm{e}^{-i\nu\pi/2}\,. \qquad \text{(IV.22)}$$

At times t_ν all paths starting from q_i coalesce at $-q_f$ (odd number of half periods) or $+q_f$ (even number of half periods). This phenomenon, called caustic, is characteristic for a harmonic potential, where the period is independent of the energy, i.e. initial momentum for fixed initial position. At a caustic the sin-function in the prefactor changes its sign and the root approaches a new Riemann surface. To avoid any ambiguities, one writes

$$G(q_f, q_i, t) = \sqrt{\frac{m\omega_0}{2\pi i\hbar|\sin(\omega_0 t)|}}\ \exp\left[i\frac{m\omega_0}{2\hbar}\frac{(q_f^2+q_i^2)\cos(\omega_0 t) - 2q_i q_f}{\sin(\omega_0 t)}\right]\ \mathrm{e}^{-i\nu\pi/2}\,. \quad \text{(IV.23)}$$

where $\omega_0 t = \nu\pi + \delta\phi, 0 \leq \delta\phi < \pi$.

Remark:

- In differential geometry one speaks about classical paths as geodetics and denotes pairs of points which are connected by at least two geodetics as conjugate points. The phase factor counting the number of caustics is also known as Maslov phase.
- The Euclidian version of the above expression yields the canonical density operator (III.2), the unnormalized form of which reads

$$\begin{aligned}\tilde{\rho}_\beta(q,q') &= \langle q|\mathrm{e}^{-\beta H}|q'\rangle \\ &= \sqrt{\frac{m\omega_0}{2\pi\hbar\sinh(\omega_0\hbar\beta)}}\ \exp\left[-\frac{m\omega_0}{2\hbar}\frac{(q^2+q'^2)\cosh(\omega_0\hbar\beta) - 2qq'}{\sinh(\omega_0\hbar\beta)}\right]\end{aligned} \quad \text{(IV.24)}$$

IV.2. Gaussian path integrals and determinants

Here, we will take a closer look onto gaussian path integrals of the type (IV.15), i.e.,

$$G(0,0,t) = \mathcal{N}\int \mathcal{D}[y]\ \mathrm{e}^{\frac{im}{2\hbar}\int_0^t ds y(s)L(s)y(s)}\,. \quad \text{(IV.25)}$$

Interpreting the operator $L(s)$ as a matrix of infinite dimension (think, for example, on the representation in terms of eigenfunctions), the calculation of the above path integral can be seen as the generalization of

$$\begin{aligned}\int dx^D\ \mathrm{e}^{\frac{i}{2}\vec{x}^t\mathbf{A}\vec{x}} &= \frac{1}{\sqrt{\mathrm{Det}[\mathbf{A}/2\pi i]}} \\ &= \left(\prod_{k=1}^{D}\frac{\lambda_k}{2\pi i}\right)^{-1/2}\,,\end{aligned} \quad \text{(IV.26)}$$

where the $\{\lambda_k\}$ are the eigenvalues of the hermitian $D \times D$-matrix $\mathbf{A}$. Hence, we may formally write

$$\begin{aligned} G(0,0,t) &\sim 1/\sqrt{\frac{m}{2\pi i\hbar}\,\mathrm{Det}[L(s)]} \\ &\sim \left(\frac{m}{2\pi i\hbar}[-\partial_s^2 - \omega_0^2]\right)^{-1/2} . \end{aligned} \tag{IV.27}$$

The normalization is then choosen such as to obtain the correct free particle propagator for $\omega_0 \to 0$, i.e.,

$$G(0,0,t) = \sqrt{\frac{m}{2\pi i\hbar t}}\left(\frac{\mathrm{Det}[-\partial_s^2]}{\mathrm{Det}[-\partial_s^2 - \omega_0^2]}\right)^{1/2} . \tag{IV.28}$$

Apparently, for the ratio of determinants one finds from (IV.17)

$$\begin{aligned} \frac{\mathrm{Det}[-\partial_s^2]}{\mathrm{Det}[-\partial_s^2 - \omega_0^2]} &= \prod_k \frac{\lambda_k(0)}{\lambda_k(\omega_0)} \\ &= \frac{\omega_0 t}{\sin(\omega_0 t)} , \end{aligned} \tag{IV.29}$$

where the $\lambda_k(x) = k^2\pi^2/t^2 - x^2$ are the corresponding eigenvalues.

In the literature, two approaches have been developed to relate the ratio of two determinants to simple entities of classical mechanics. The first one is the so-called van Vleck Pauli Morette formula

$$\sqrt{\frac{m}{2\pi i\hbar t}}\left(\frac{\mathrm{Det}[-\partial_s^2]}{\mathrm{Det}[-\partial_s^2 - \omega(s)^2]}\right)^{1/2} = \sqrt{\frac{1}{2\pi i\hbar t}}\sqrt{-\frac{\partial^2 S[q_{\mathrm{cl}}]}{\partial q_f \partial q_i}} \tag{IV.30}$$

which contains the action evaluated along the classical path. Obviously, by inserting (IV.8) into this expression, one indeed regains the prefactor of the result (IV.21).

An alternative formula goes back to Gelfand-Yaglom and reads

$$\frac{\mathrm{Det}[-\partial_s^2 - \omega(s)^2]}{\mathrm{Det}[-\partial_s^2]} = \frac{F_\omega(t)}{F_0(t)} \;,\; 0 \le s \le t , \tag{IV.31}$$

where

$$[\partial_s^2 + \omega(s)^2]F_\omega(s) = 0 \;\;, F_\omega(0) = 0 \;,\; \dot{F}_\omega(0) = 1 . \tag{IV.32}$$

Accordingly, with $F_0(s) = s$

$$\sqrt{\frac{m}{2\pi i\hbar t}}\left(\frac{\mathrm{Det}[-\partial_s^2]}{\mathrm{Det}[-\partial_s^2 - \omega(s)^2]}\right)^{1/2} = \sqrt{\frac{m}{2\pi i\hbar F_\omega(t)}} . \tag{IV.33}$$

Given the above boundary conditions, one has in case of a simple harmonic oscillator

$$F_\omega(t) = \sin(\omega_0 t)/\omega_0 \,. \tag{IV.34}$$

Remarks:

- If $f(s)$ is a solution of the harmonic oscillator with $f(0) = 0$, the Gelfand-Yaglom solution reads $F_\omega(t) = f(t)/\dot{f}(0)$. Further, if $f(s)$ is a harmonic solution with $f(0) \neq 0$, the Gelfand-Yaglom solution can be constructed from

$$F_\omega(s) = f(0)f(s)\int_0^s du \frac{1}{f(u)^2} \,. \tag{IV.35}$$

- The Gelfand-Yaglom formula can proven in two ways:
  (i) one uses the discretized version of the path integral (IV.25) for N time steps and then derives a recursion relation between the corresponding determinants in N and in $N+1$ dimension. For $N \to \infty$, one obtains (IV.31).

  (ii) One considers operators $L_\lambda(\omega) = -\partial_s^2 - \omega(s)^2 - \lambda$ and functions $F_{\lambda,\omega}$ with $L_\lambda(\omega)F_{\lambda,\omega} = 0$ which obey Gelfand-Yaglom boundary conditions. The claim is now that

$$\frac{\mathrm{Det}[L_\lambda(\omega)]}{\mathrm{Det}[L_\lambda(0)]} = \frac{F_{\lambda,\omega}(t)}{F_{\lambda,0}(t)} \tag{IV.36}$$

  which reduces to (IV.31) for $\lambda = 0$. To establish this claim, one considers the left and right hand sides as functions of the complex variable λ. The left hand side is a meromorphic function of λ with a simple zero at each eigenvalue λ_n of $L_0(\omega)$ and a simple pole at each eigenvalue λ_n^0 of $L_0(0)$. Exactly the same is true for the right hand side (because then the eigenfunction satisfies $F_{\lambda,\omega}(t) = 0$). In particular, the ratio of the left and the right hand sides has no poles and is therefore an analytic function of λ_n. Moreover, provided that $\omega(t)$ is a bounded function of s, for $|\lambda| \to \infty$, both sides approach 1. Hence, the ratio of the two sides is an analytic function which is 1 for $|\lambda| \to \infty$ and is thus 1 everywhere.

- To prove the van-Vleck expression, one exploits the Jacobian formulation of classical mechanics to relate it to the Gelfand-Yaglom formula.

- As we have discussed above, Gaussian integrals (determinants) of non-normalized path integrals (those without the prefactor $\mathcal{N}$) are ill-defined. This is why we considered ratios of determinants above. However, there is another and more formal way to define the meaning of a not-normalized path integral. This treatment exploits the ζ function of the eigenvalues λ_k of an operator L

$$\zeta_L(s) = \sum_k \frac{1}{\lambda_k^s} \quad \rightarrow \quad \left.\frac{d\zeta_L}{ds}\right|_{s=0} = \sum_k \ln \lambda_k = \ln \prod_k \lambda_k \, . \tag{IV.37}$$

Apparently, the last expression provides a representation of the determinant of L. However, since the ζ function as it stands above is only defined for $s > 1$, one must employ an analytical continuation of the ζ-function to the complex s-plane (similar to what has been done for the Weierstrass ζ-function). Based on this continuation, one is able to give a meaningful result for $\zeta'(0)$ and thus define the determinant of an operator without resorting to normalization. Practically, this does not make any difference though.