8 Introduction to path integrals

Whereas classical mechanics can be formulated in a Lagrange as well as a Hamilton formalism, one may wonder how a Lagrange formalism for quantum mechanics looks like. So far, the Hamiltonian formulation was essential, as quantization proceeds via demanding a non-commutative structure in <u>phase</u> space

$$[q, p] = i\hbar \qquad (8.1)$$

In fact, path integrals can be viewed as the Lagrange formulation of quantum mechanics. But path integrals differ from canonical quantization in several further respects:

- no operator valued quantities are needed
- time evolution is described <u>globally</u> (instead of evolving a state locally (or incrementally) in time)
- the notion of states is lost (or at least, doesn't

occur naturally in path integrals)

8.1 Propagator of a free particle in position space

Consider the Hamiltonian of a free particle

$$\hat{H} = \frac{\hat{\vec{P}}^2}{2m} \qquad (8.2)$$

(Here and in the following, we will use hats "^" to characterize operators.)

$\hat{H}$ is diagonal in momentum space

$$\hat{H} \, |\vec{p}\rangle = \frac{\vec{P}^2}{2m} \, |\vec{p}\rangle \qquad (8.3)$$

As $\hat{H}$ is time independent, the time evolution operator is simply given by

$$\hat{U}(t_b, t_a) = e^{-\frac{i}{\hbar}\frac{\hat{\vec{P}}^2}{2m}(t_b - t_a)} \qquad (8.4)$$

Let us determine the time-evolution operator in position space:

$$\langle \vec{x}_b, t_b | \vec{x}_a, t_a \rangle = \langle \vec{x}_b | \, e^{-\frac{i}{\hbar}\frac{\hat{\vec{P}}^2}{2m}(t_b - t_a)} \, | \vec{x}_a \rangle$$

$$= \langle \vec{x}_b | \, e^{-\frac{i}{\hbar}\frac{\hat{\vec{P}}^2}{2m}(t_b - t_a)} \underbrace{\int d^D\vec{p} \, |\vec{p}\rangle\langle\vec{p}|}_{= \mathbb{1}} \vec{x}_a \rangle$$

$$\Rightarrow \langle \vec{x}_b t_b | \vec{x}_a t_a \rangle = \int d^D p \, \langle \vec{x}_b | \vec{p} \rangle \langle \vec{p} | \vec{x}_a \rangle \, e^{-\frac{i}{\hbar} \frac{\vec{p}^2}{2m} (t_b - t_a)}$$

$$= \int \frac{d^D p}{(2\pi\hbar)^D} \, e^{\frac{i}{\hbar} \vec{p} \cdot (\vec{x}_b - \vec{x}_a)} \, e^{-\frac{i}{\hbar} \frac{\vec{p}^2}{2m} (t_b - t_a)}$$

$$\vec{p}\,' = \vec{p} - m \frac{(\vec{x}_b - \vec{x}_a)}{(t_b - t_a)}$$

$$= e^{\frac{i}{\hbar} \frac{m}{2} \frac{(\vec{x}_b - \vec{x}_a)^2}{(t_b - t_a)}} \cdot \int \frac{d^D p'}{(2\pi\hbar)^D} \, e^{-\frac{i\hbar}{2m} (t_b - t_a) \vec{p}\,'^2}$$

$$\overset{(t_b > t_a)}{=} \frac{1}{\left(\frac{2\pi i \hbar}{m} (t_b - t_a) \right)^{D/2}} \cdot e^{\frac{i}{\hbar} \frac{m}{2} \frac{(\vec{x}_b - \vec{x}_a)^2}{(t_b - t_a)}} \qquad (8.5)$$

In the last step, we have assumed $t_b > t_a$ and used the Fresnel integral

$$\int_{-\infty}^{\infty} \frac{dp}{(2\pi)^{1/2}} \, e^{i \frac{a}{2} p^2} = \pm \frac{e^{i \frac{\pi}{4}}}{\sqrt{|a|}} \quad \text{for } a \gtrless 0 \qquad (8.6)$$

(obtained from an analytic continuation of the Gauß integral).

As a check, we observe that (8.5) is a representation of a δ function in the limit $t_b \to t_a$

$$\lim_{t_b \to t_a} \langle \vec{x}_b t_b | \vec{x}_a t_a \rangle = \delta^{(D)} (\vec{x}_b - \vec{x}_a) \qquad (8.7)$$

as it should.

The interesting observation at this point is that the exponent in (8.5) is related to the classical action.

The classical path of a free particle obeys

$$\vec{x}_0(t) = \vec{x}_a + \frac{t - t_a}{t_b - t_a} (\vec{x}_b - \vec{x}_a) \qquad t \in [t_b, t_a]$$

which satisfies $\vec{x}_0(t_a) = \vec{x}_a$ and $\vec{x}_0(t_b) = \vec{x}_b$.

From this, we can directly compute the classical action,

$$S_{cl} = S[x_0(t)] = \frac{m}{2} \int_{t_a}^{t_b} dt \ \dot{x}_0^2 = \frac{m}{2} \int_{t_a}^{t_b} dt \ \frac{(\vec{x}_b - \vec{x}_a)^2}{(t_b - t_a)^2}$$

$$= \frac{m}{2} \frac{(\vec{x}_b - \vec{x}_a)^2}{(t_b - t_a)} . \qquad (8.8)$$

Hence, we found

$$\langle \vec{x}_b t_b | \vec{x}_a t_a \rangle \sim e^{\frac{i}{\hbar} S_{cl}} \qquad (8.9)$$

A relation of this type was already anticipated by Dirac and properly constructed and derived by Feynman in his PhD thesis in terms of path integrals.

8.2 Path integral representation of the time-evolution operator

Let us for simplicity consider a time evolution in $D=1$ dimension. Using the multiplication property of the time evolution operator, we write

$$\langle x_b t_b | x_a t_a \rangle = \langle x_b | \hat{U}(t_b, t_a) | x_a \rangle \quad , t_b > t_a$$

$$= \langle x_b | \hat{U}(t_b, t_N) \hat{U}(t_N, t_{N-1}) \dots \hat{U}(t_2, t_1) U(t_1, t_a) | x_a \rangle , \tag{8.10}$$

where we have introduced time "slices" of "thickness"

$$\varepsilon := t_n - t_{n-1} = \frac{t_b - t_a}{N+1} > 0 \tag{8.11}$$

Each $\hat{U}$ in (8.10) describes the time evolution during one time slice. Inserting

$$\mathbb{1} = \int_{-\infty}^{\infty} dx_n |x_n\rangle\langle x_n| \quad , \quad n = 1, \dots, N \tag{8.12}$$

for each time slice, the multiplicative property of $\hat{U}$ translates into a similar one for $\langle x_b t_b | x_a t_a \rangle$,

$$\langle x_b t_b | x_a t_a \rangle = \prod_{n=1}^{N} \int_{-\infty}^{\infty} dx_n \prod_{n=1}^{N+1} \langle x_n t_n | x_{n-1} t_{n-1} \rangle \tag{8.13}$$

where we have defined $x_b = x_{N+1}$, $x_a = x_0$, $t_b = t_{N+1}$, $t_a = t_0$.

In the following, we consider Hamiltonians which can be decomposed into kinetic and potential terms of the form

$$\hat{H}(\hat{p},\hat{x},t) = \hat{T}(\hat{p},t) + \hat{V}(\hat{p},t) \,. \tag{8.14}$$

In case of explicit time dependencies, we assume that $\hat{H}$ is slowly varying within each time slice

$$\begin{aligned} \hat{U}(t_n,t_{n-1}) &= \mathcal{T}\, e^{-\frac{i}{\hbar}\int_{t_{n-1}}^{t_n} dt\, \hat{H}(t)} \\ &\simeq e^{-\frac{i}{\hbar}\varepsilon \hat{H}(t_n)} \,, \quad \varepsilon = t_n - t_{n-1} \end{aligned} \tag{8.15}$$

(which becomes exact in the limit $\varepsilon \to 0$).

Hamiltonians of the form (8.14) can be factorized by means of the Baker-Campbell-Hausdorff formula

$$e^{-\frac{i}{\hbar}\varepsilon(\hat{T}+\hat{V})} = e^{-\frac{i}{\hbar}\varepsilon\hat{V}}\, e^{-\frac{i}{\hbar}\varepsilon\hat{T}}\, e^{-\frac{i}{\hbar^2}\varepsilon^2\hat{X}} \tag{8.16}$$

where $\hat{X} = \frac{i}{2}[\hat{V},\hat{T}] - \frac{\varepsilon}{\hbar}\left(\frac{1}{6}[\hat{V},[\hat{V},\hat{T}]] - \frac{1}{3}[[\hat{V},\hat{T}],\hat{T}]\right)$

$$+\underbrace{\mathcal{O}(\varepsilon^2)}_{\text{fully known}} \tag{8.17}$$

In the following, we will assume that the $\hat{X}$-terms are irrelevant in the limit $\varepsilon \to 0$. This actually imposes conditions on $\hat{T}$ and $\hat{V}$ which will be discussed below.

With this assumption, the time evolution operator in each time slice is

$$\langle x_n t_n | x_{n-1} t_{n-1} \rangle \simeq \langle x_n | e^{-\frac{i}{\hbar}\varepsilon \hat{H}(t_n)} | x_{n-1} \rangle$$

$$\overset{(8.16)}{\simeq} \int_{-\infty}^{\infty} dx' \langle x_n | e^{-\frac{i}{\hbar}\varepsilon \hat{V}(\hat{x}, t_n)} | x' \rangle \langle x' | \underset{\mathbb{1} = \int dp_n |p_n\rangle\langle p_n|}{\wedge} e^{-\frac{i}{\hbar}\varepsilon \hat{T}(\hat{p}, t_n)} | x_{n-1} \rangle$$

$$= \int_{-\infty}^{\infty} dx' \, e^{-\frac{i}{\hbar}\varepsilon V(x_n, t_n)} \, \delta(x_n - x') \int \frac{dp_n}{2\pi\hbar} \, e^{\frac{i}{\hbar} p_n (x' - x_{n-1})} \cdot e^{-\frac{i}{\hbar}\varepsilon T(p_n, t_n)}$$

$$= \int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar} \, e^{\frac{i}{\hbar} p_n (x_n - x_{n-1}) - \frac{i}{\hbar}\varepsilon \left(T(p_n, t_n) + V(x_n, t_n) \right)} \qquad (8.18)$$

Insertion into (8.13) yields the (preliminary) path integral formula

$$\langle x_b t_b | x_a t_a \rangle \simeq \left(\prod_{n=1}^{N} \int_{-\infty}^{\infty} dx_n \right) \left(\prod_{n=1}^{N+1} \int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar} \right) e^{\frac{i}{\hbar} S_N} \qquad (8.19)$$

where

$$S_N = \sum_{n=1}^{N+1} \left[p_n(x_n - x_{n-1}) - \varepsilon H(x_n, p_n, t_n) \right] \quad (8.20)$$

What are the conditions for a convergence of the continuum limit of the RHS of (8.19) towards the left-hand side?

There are at least some partial answers:

- for $\hat{T} = \frac{\hat{p}^2}{2m}$ and smooth potentials $V(\hat{x})$, the quantity $\hat{X}$ consists of products of momentum operators $\hat{p}$ and well-defined derivatives of $V(\hat{x})$. Then the expansion of

  $e^{-\frac{i}{\hbar^2}\varepsilon^2 \hat{X}} = 1 - \frac{i}{\hbar^2}\varepsilon^2 \hat{X} + \dots$ can be evaluated at each order yielding finite answers. In the limit $\varepsilon \to 0$ only $e^{-\frac{i}{\hbar}\varepsilon^2\hat{X}} \to 1$ remains.

- For time-independent Hamiltonians $\hat{H} = H(\hat{x}, \hat{p})$ and for Potentials bounded from below, the Trotter product formula holds

$$e^{-\frac{i}{\hbar}(t_b - t_a)\hat{H}} = \lim_{N\to\infty} \left(e^{-\frac{i}{\hbar}\varepsilon\hat{V}} e^{-\frac{i}{\hbar}\varepsilon\hat{T}} \right)^{N+1} \quad (8.21)$$

(The proof requires tedious functional analysis, see E Nelson, J M P 5, 322 ('64))

This formula controls the $\varepsilon \to 0$ limit in the desired manner.

- for potential unbounded from below, e.g. the Coulomb potential, the BCH expansion of $\hat{X}$ becomes more and more singular and generally does not converge. In such a case (8.15) cannot straightforwardly be applied

In the following, we assume that $\hat{H}$ is of the appropriate type such that the limit $\varepsilon \to 0$ can be performed. Then we find

$$\langle x_b t_b | x_a t_a \rangle = \int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}x \int \frac{\mathcal{D}p}{2\pi\hbar} \, e^{\frac{i}{\hbar} S[x,p]} , \quad (8.22)$$

where

$$\int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}x \int \frac{\mathcal{D}p}{2\pi\hbar} = \left(\prod_{n=1}^{N} \int_{-\infty}^{\infty} dx_n \right) \left(\prod_{n=1}^{N+1} \int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar} \right) \Bigg|_{N\to\infty}$$

and

$$S[x,p] = \int_{t_a}^{t_b} dt \left[p(t)\, \dot{x}(t) - H(p, x, t) \right] . \quad (8.23)$$

Let us specialize to the case

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x},t) \tag{8.24}$$

and go back to the discrete form (8.20):

$$S_N = \sum_{n=1}^{N+1} \left[p_n (x_n - x_{n-1}) - \varepsilon \frac{p_n^2}{2m} - \varepsilon V(x_n, t_n) \right]$$

$$= \sum_{n=1}^{N+1} \left[-\frac{\varepsilon}{2m} \left(p_n - \frac{x_n - x_{n-1}}{\varepsilon} m \right)^2 + \frac{m}{2} \varepsilon \left(\frac{x_n - x_{n-1}}{\varepsilon} \right)^2 - \varepsilon V(x_n, t_n) \right] \tag{8.25}$$

In this case, all $N+1$ momentum integrals in (8.19) are of Fresnel-type

$$\int_{-\infty}^{\infty} \frac{dp_n}{2\pi\hbar} \left[e^{-\frac{i}{\hbar} \frac{\varepsilon}{2m} \left(p_n - \frac{x_n - x_{n-1}}{\varepsilon} m \right)^2} \right] = \frac{1}{\sqrt{\frac{2\pi i \hbar \varepsilon}{m}}},$$

$$\Rightarrow \langle x_b t_b | x_a t_a \rangle \approx \frac{1}{\sqrt{\frac{2\pi i \hbar \varepsilon}{m}}} \prod_{n=1}^{N} \int_{-\infty}^{\infty} \frac{dx_n}{\sqrt{\frac{2\pi i \hbar \varepsilon}{m}}} \, e^{\frac{i}{\hbar} S_N[x]} \tag{8.26}$$

where

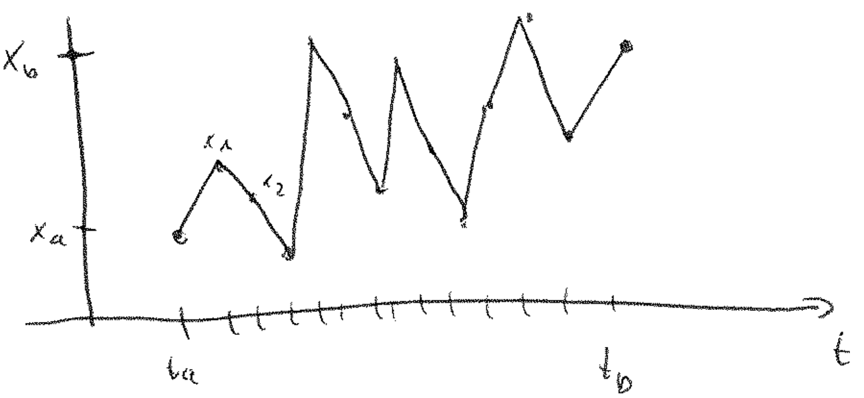
$$S_N[x] = \varepsilon \sum_{n=1}^{N+1} \left[\frac{m}{2} \left(\frac{(x_n - x_{n-1})}{\varepsilon} \right)^2 - V(x_n, t_n) \right] \quad (8.27)$$

In the continuum limit, we write

$$\langle x_b t_b | x_a t_a \rangle = \int_{x(t_a)=x_a}^{x(t_b)=x_b} \mathcal{D}x \; e^{\frac{i}{\hbar} S[x]}$$

where
$$S[x] = \int_{t_a}^{t_b} dt \left(\frac{m}{2} \dot{x}^2 - V(x,t) \right) \quad (8.28)$$

So the path integral is an integral over all paths obeying the boundary conditions $x(t_{a/b}) = x_{a/b}$ weighed by the exponential $e^{\frac{i}{\hbar} S[x]}$ (which is reminiscent to a thermodynamical/statistical partition function with Boltzmann weight $e^{-\frac{E}{kT}}$).
Picking one representative value x out of each of the N x integrals, we get one representative path:



As the first example, let us come back to the free particle

$$\langle x_b t_b | x_a t_a \rangle = \int_{x_a}^{x_b} \mathcal{D}x \; e^{\frac{i}{\hbar}\int_{t_a}^{t_b} dt \, \frac{m}{2} \dot{x}^2}$$

$$= \lim_{N\to\infty} \frac{1}{\sqrt{\frac{2\pi i\hbar\varepsilon}{m}}} \prod_{n=1}^{N} \int_{-\infty}^{\infty} \frac{dx_n}{\sqrt{\frac{2\pi i\hbar\varepsilon}{m}}} \; e^{\frac{i}{\hbar}\varepsilon \sum_{n=1}^{N+1} \frac{m}{2} \frac{(x_n - x_{n-1})^2}{\varepsilon^2}} \qquad (8.29)$$

Consider the x_n integral,

$$\frac{1}{\sqrt{\frac{2\pi i\hbar\varepsilon}{m}}} \int_{-\infty}^{\infty} \frac{dx_n}{\sqrt{\frac{2\pi i\hbar\varepsilon}{m}}} \; e^{\frac{i}{\hbar}\frac{m}{2\varepsilon}(x_{n+1}-x_n)^2 + \frac{i}{\hbar}\frac{m}{2\varepsilon}(x_n - x_{n-1})^2}$$

$$= \frac{1}{\sqrt{\frac{2\pi i\hbar\varepsilon}{m}\cdot 2}} \; e^{\frac{i}{\hbar}\frac{m}{2}\frac{(x_{n+1}-x_{n-1})^2}{2\varepsilon}} \qquad (8.30)$$

It's N-fold application yields

$$\langle x_b t_b | x_a t_a \rangle = \frac{1}{\sqrt{\frac{2\pi i\hbar\varepsilon}{m}(N+1)}} \; e^{\frac{i}{\hbar}\frac{m}{2}\frac{(x_b - x_a)^2}{(N+1)\varepsilon}}$$

$$\overset{\varepsilon(N+1) = t_b - t_a}{=} \frac{1}{\sqrt{\frac{2\pi i\hbar}{m}(t_b - t_a)}} \; e^{\frac{i}{\hbar}\frac{m}{2}\frac{(x_b - x_a)^2}{t_b - t_a}} \qquad (8.31)$$

which agrees with (8.5) (for $D=1$), as it should.

8.3 Correspondence limit

The path integral formalism is remarkably close to the classical formalism (in some sense at least). In fact, at least heuristically the "semi classical" limit can be studied rather straight forwardly.

Starting with the propagator

$$\langle x_b t_b | x_a t_a \rangle = \int_{x_a}^{x_b} \mathcal{D}x \; e^{\frac{i}{\hbar} S[x]} , \tag{8.32}$$

We are interested in the limit $\hbar \to 0$. As an analogous example, we consider an ordinary integral of the form

$$F(\lambda) = \int_{-\infty}^{\infty} dx \; e^{i\lambda f(x)} \tag{8.33}$$

in the limit $\lambda \to \infty$. For large λ, the integrand oscillates rapidly for varying f, except for those points, where $f(x)$ is stationary, $f'(x_0) = 0$.

We expect that the largest contribution to the integral for $\lambda \to \infty$ arises from the vicinity of the stationary points x_0.

An expansion about x_0 yields

$$F(\lambda) = \sum_{\{x_0\}} \int dx \; e^{i\lambda f(x_0) + \frac{\lambda}{2} i (x-x_0)^2 f''(x_0) + \dots}$$

$$= \sum_{\{x_0\}} \sqrt{\frac{2\pi i}{\lambda f''(x_0)}} \; e^{i\lambda f(x_0)} \left(1 + \mathcal{O}(1/\lambda)\right) \qquad (8.35)$$

where we have assumed $f''(x_0) \neq 0$ and extended the integration ranges at each point x_0 from $x \to -\infty$ to $x \to \infty$ (which is only an exponentially small error).

Applying the same strategy to (8.32) leads to the dictionary

$$\begin{array}{ccc}
\lambda \to \infty & \leftrightarrow & \hbar = \frac{1}{\lambda} \to 0 \\
\int dx & \leftrightarrow & \int \mathcal{D}x \\
\text{stationary points} & \leftrightarrow & \text{stationary paths} \\
x_0 & \leftrightarrow & x_0(t) \\
f'(x_0) = 0 & \leftrightarrow & \frac{\delta S[x(t) = x_0(t)]}{\delta x(t)} = 0
\end{array} \qquad (8.36)$$

Hence, we expect that the classical limit $\hbar \to 0$ implies a domination of the classical paths that satisfy the action principle $\delta S = 0$.

The limit $\hbar \to 0$ may sound rather formal but has a physical correspondence. We expect the stationary-path approximation to be reasonable,

if

$$\frac{S[x_0(t)]}{\hbar} \gg 1 . \qquad (8.37)$$

For instance, a particle of mass 1g which moves at velocity $v = 1\frac{m}{s}$ during 1 s has an action

$$S = \frac{1g}{2} \int_0^{1s} dt \, (1 \tfrac{m}{s})^2 = 5 \; 10^{-4} \, \frac{kg \, m^2}{s} \simeq \underline{\underline{5 \cdot 10^{30} \hbar}} \qquad (8.38)$$

Still, these considerations go beyond just the classical limit. Consider a system allowing for 2 (or more) stationary paths $x_{0,1}(t) \neq x_{0,2}(t)$

with

$$S_1 = S[x_{0,1}] \; , \; S_2 = S[x_{0,2}] \text{ and}$$

$$\left. \frac{\delta S}{\delta x} \right|_{x = x_{0,1/2}} = 0 \qquad (8.39)$$

Then, in the limit $\hbar \to 0$ the propagator acquires the form

$$\langle x_b t_b | x_a t_a \rangle = c_1 \, e^{\frac{i}{\hbar} S_1} + c_2 \, e^{\frac{i}{\hbar} S_2} \qquad (8.40)$$

where c_1 and c_2 are the analogues the $\sqrt{\%}$ term in (8.35).

Now (8.40) determines a transition amplitude with the corresponding probability given by

$$|\langle x_b t_b | x_a t_a \rangle|^2 = \left(c_1 \, e^{\frac{i}{\hbar} S_1} + c_2 \, e^{\frac{i}{\hbar} S_2} \right) \left(c_1^* \, e^{-\frac{i}{\hbar} S_1} + c_2^* \, e^{-\frac{i}{\hbar} S_2} \right)$$

$$= \underbrace{|c_1|^2 + |c_2|^2}_{\text{classical contribution}} + \underbrace{2 \, \mathrm{Re} \, c_2^* c_1 \, e^{\frac{i}{\hbar}(S_1 - S_2)}}_{\text{interference term}} \qquad (8.41)$$

So, even in the correspondence limit $\hbar \to 0$, i.e. $\frac{S_1}{\hbar}, \frac{S_2}{\hbar} \gg 1$, a quantum mechanical interference term can arise, im $\frac{S_1 - S_2}{\hbar}$ is sufficiently small ("Schrödinger-cat states").

8.4 Schrödinger equation

To demonstrate the one-to-one correspondence between the canonical formalism and the path integral formalism, it is instructive to rederive Schrödinger's equation from the path integral.
As we need only local infinitesimal information, we may assume that x_a, t_a and $x_b t_b$ are infinitesimally close to each other and introduce only one intermediate time slice:

$$\langle x_b t_b | x_a t_a \rangle = \int_{-\infty}^{\infty} \frac{dx'}{\sqrt{\frac{2\pi i \hbar \varepsilon}{m}}} \exp\left(\frac{im}{2\hbar} \varepsilon \frac{(x_b - x')^2}{\varepsilon^2} - \frac{i}{\hbar} V(x) \varepsilon \right) \cdot \langle x' t_b - \varepsilon | x_a t_a \rangle \qquad (8.42)$$

Set

$$t_b = t + \varepsilon \quad , \quad x_b = x \quad , \qquad (8.43)$$
$$\text{and} \quad x' = x - \xi$$

$$\Rightarrow \langle x, t+\varepsilon | x_a t_a \rangle = \int_{-\infty}^{\infty} \frac{d\xi}{\sqrt{\frac{2\pi i \hbar \varepsilon}{m}}} \exp\left(\frac{im}{2\hbar} \varepsilon \frac{\xi^2}{\varepsilon^2} - \frac{i}{\hbar} V(x) \varepsilon \right) \cdot \langle x - \xi \; t | x_a t_a \rangle \qquad (8.44)$$

In the limit $\varepsilon \to 0$, we expect the ξ integral to be dominated by the $\xi \simeq 0$ region. Hence we may expand $\langle x-\xi\, t | x_a t_a \rangle$ in powers of ξ. We also expand the left-hand side as well as $e^{-\frac{i}{\hbar} V \varepsilon}$ in powers of ε,

$$\langle x t | x_a t_a \rangle + \varepsilon \frac{\partial}{\partial t} \langle x t | x_a t_a \rangle$$

$$= \frac{1}{\sqrt{\frac{2\pi i \hbar \varepsilon}{m}}} \int_{-\infty}^{\infty} d\xi \; e^{\frac{im}{2\hbar}\frac{\xi^2}{\varepsilon}} \left(1 - \frac{iV}{\hbar}\varepsilon + \dots\right) \tag{8.45}$$

$$\cdot \left[\langle x t | x_a t_a \rangle + \left(\frac{\xi^2}{2}\right) \frac{\partial^2}{\partial x^2} \langle x t | x_a t_a \rangle + \dots \right]$$

where the term linear in ξ vanishes due to the symmetry $\xi \to -\xi$ of the ξ integral.

The leading terms in ε on both sides match (after having performed one Fresnel integral).

To first order in ε, we find

$$\varepsilon \frac{\partial}{\partial t} \langle x t | x_a t_a \rangle = \frac{1}{\sqrt{\frac{2\pi i \hbar \varepsilon}{m}}} \int_{-\infty}^{\infty} d\xi \; \xi^2 e^{\frac{im}{2\hbar}\frac{\xi^2}{\varepsilon}} \; \frac{1}{2}\frac{\partial^2}{\partial x^2} \langle x t | x_a t_a \rangle$$

$$- \frac{i}{\hbar} \varepsilon V \langle x t | x_a t_a \rangle \tag{8.46}$$

The ξ integral can be done by differentiating the Fresnel integral twice with respect to the prefactor in the exponent, yielding

$$\int_{-\infty}^{\infty} d\xi \, \xi^2 \, e^{\frac{im}{2\hbar}\frac{\xi^2}{\varepsilon}} = \sqrt{2\pi} \left(\frac{i\hbar\varepsilon}{m} \right)^{3/2} \qquad (8.47)$$

and thus

$$i\hbar \frac{\partial}{\partial t} \langle xt | x_a t_a \rangle = -\left(\frac{\hbar^2}{2m} \right) \frac{\partial^2}{\partial x^2} \langle xt | x_a t_a \rangle + V \langle xt | x_a t_a \rangle \qquad (8.48)$$

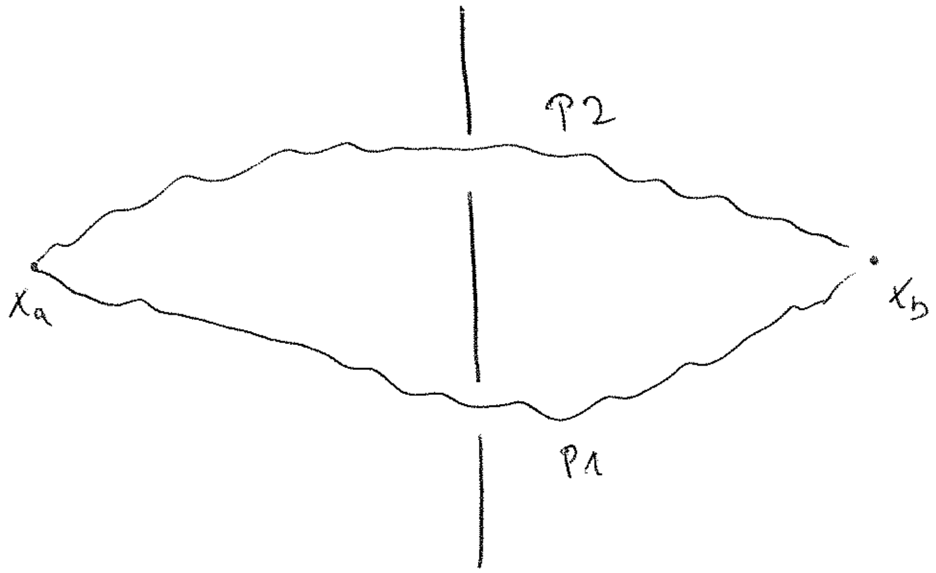
which is the standard Schrödinger equation. In this derivation, we haven't actually used that $x_a t_a$ and xt are infinitesimally close to each other. If they are at a finite separation the whole derivation also holds if the x' integral in (8.42) is taken as the integral x_N at the last time slice at t_N. Hence (8.48) also holds for a wave function at x and t evolved out of a wave function at x_a and t_a by

$$\begin{aligned} \psi(x,t) &= \int dx_a \, \langle x\, t \,|\, x_a\, t_a \rangle \langle x_a\, t_a \,|\, \psi \rangle \\ &= \int dx_a \, \langle x\, t \,|\, x_a\, t_a \rangle \, \psi(x_a, t_a) \, . \end{aligned} \tag{8.49}$$

8.5 Path integrals and double-slit type experiments with potentials

As path integrals constitute a global approach to time evolution and propagation, they are very valuable for efficiently computing interference phenomena of the double slit type involving different paths in the presence of potentials.

Imagine a quantum mechanical particle can propagate from x_a to x_b via two different paths (or classes of paths):



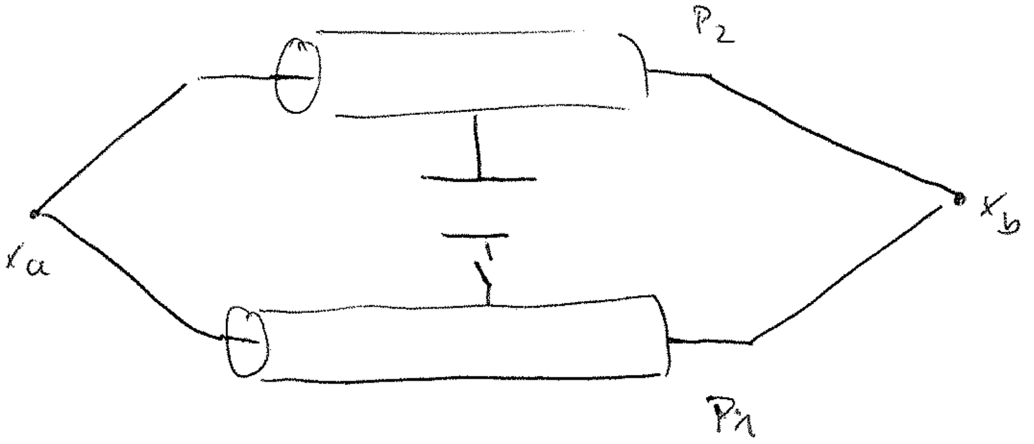
From the path integral approach, it is immediately obvious that an interference effect arises if the actions S_{P_1} and S_{P_2} differ. Even for a free propagation this is usually the case; by varying x_b (on the screen), the free propagations along P_1 and P_2 acquire different x_b dependent actions resulting in an interference pattern on the screen. The action diffence can be computed from

$$\int_{P_1} dt\, L - \int_{P_2} dt\, L = \oint_{P_1 \cup P_2} L \quad = \text{phase diffence} \tag{8.50}$$

where $\oint_{P_1 \cup P_2}$ symbolically denotes a "round trip" (from x_a to x_b along P_1 and then back to x_a along P_2).

Now, let us modify this situation a bit. Let us choose x_b such that the free actions along P_1 and P_2 are identical.

Next, we switch on a potential difference (e.g. electrostatic or gravitational potential difference) between the two diffent paths



Then the phase difference arises only from the potential term in the action:

$$\Delta\varphi = \frac{1}{\hbar} \int_{t_a}^{t_b} \left[V_2(t) - V_1(t)\right] \qquad (8.51)$$

Note that (8.51) also gives a contribution if $V_{1/2}$ is constant,

$$\Delta\varphi = \frac{1}{\hbar} (V_2 - V_1)(t_b - t_a), \qquad (8.52)$$

Implying that an interference effect can be detected even if classically no force is exerted onto the particle. This is a purely quantum mechanical effect.
(NB: Still no absolute potential heights can be measured, as (8.52) only involves the potential difference between the two paths).

This effect can be used to detect even gravitational potential differences between different paths of neutrons bouncing above a surface in the earth's gravitational field. ($\Rightarrow$ PERKEO experiment, Heidelberg - Grenoble)

As another example, let us consider a particle moving in a magnetic field.
From classical mechanics, we recall that the action is obtained from that of the free-field case by replacing

$$L_0 \rightarrow L_0 + \frac{e}{c} \frac{d\vec{x}}{dt} \cdot \vec{A} \qquad (8.53)$$

where $\vec{A}$ is the gauge vector potential. (This term gives rise to the Lorentz force if inserted into the Euler-Lagrange equations.)

In this example, the round-trip integral in (8.50) can further be simplified:

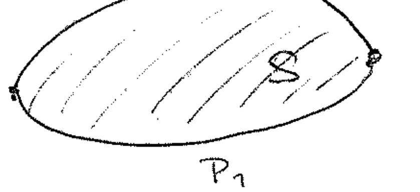
$$\frac{e}{c}\int_{P_1} dt\,\frac{d\vec{x}}{dt}\cdot\vec{A} - \frac{e}{c}\int_{P_2} dt\,\frac{d\vec{x}}{dt}\cdot\vec{A}$$

$$= \frac{e}{c}\oint_{P_1\cup P_2} d\vec{x}\cdot\vec{A}$$

$$= \frac{e}{c}\int_S d\vec{\sigma}\cdot\vec{B}\,, \qquad (8.54)$$

$$= \frac{e}{c}\,\Phi_B$$

where we have used Stokes theorem to rewrite the line integral in terms of a surface integral

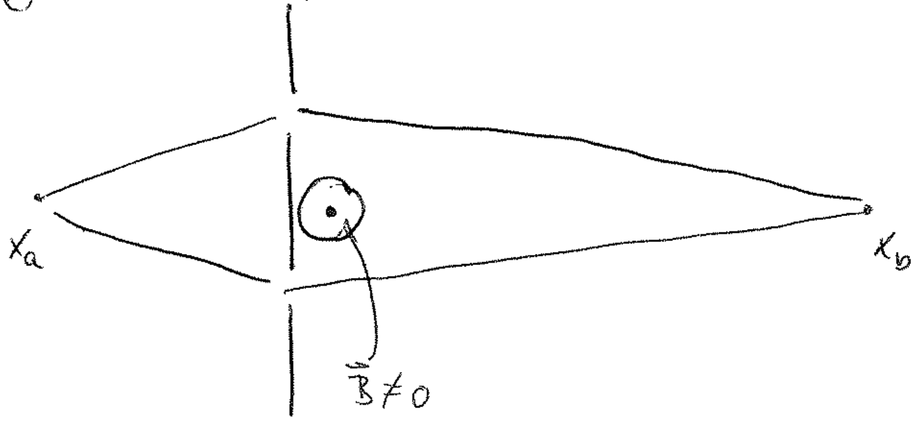


$$P_1 \cup P_2 = \partial S$$

The phase difference hence is proportional to the magnetic flux Φ_B trough the surface S.

This gives rise to a very peculiar effect, the so-called Aharonov-Bohm effect.

Consider a magnetic field which is confined to a finite region of space (e.g. an infinitely long solenoid):



At x_b, we expect to see an interference pattern that depends on the flux Φ_B.

The phase difference is

$$\Delta\varphi = \frac{1}{\hbar}\,\frac{e}{c}\oint_{P_1+P_2} d\vec{x}\cdot\vec{A} = \frac{e}{c\hbar}\,\Phi_B \qquad (8.55)$$

By tuning the flux, we expect to see a variation of the interference pattern even if the wave functions propagate only through space where $\vec{B} = 0$!

But even if $\vec{B} = 0$, this does not imply that $\vec{A} = 0$ (in fact, we can't set $\vec{A} = 0$ everywhere in the "outer space" to sustain a finite $\vec{B}$ field inside).

Note that the interference pattern depends on the phase difference mod 2π. I.e. it changes periodically with a period given by the fundamental unit of magnetic flux

$$\Phi_q = \frac{2\pi\hbar c}{e} = 4.135 \cdot 10^{-7} \frac{\text{Gauss}}{\text{cm}^2} \qquad (8.56)$$

(flux quantum)

8.6 Path integral for the harmonic oscillator (HO)

The classical action for the HO is

$$S = \int dt \left(\frac{1}{2} m \dot{x}^2 - \frac{1}{2} m \omega^2 x^2 \right) \qquad (8.57)$$

Let us try to compute the propagator via the path integral

$$\langle x_b t_b | x_a t_a \rangle = \int_{x_a(t_a)}^{x_b(t_b)} \mathcal{D}x \; e^{\frac{i}{\hbar} S} \qquad (8.58)$$

We assume that we already have the classical solution at our disposal

$$\delta S[x_0] = 0 \quad \Rightarrow \quad m \ddot{x}_0 + m\omega^2 x_0 = 0 \qquad (8.59)$$

where

$$x_0(t_a) = x_a$$

$$x_0(t_b) = x_b$$

Let us introduce a new integration variable $y(t)$

$$x(t) = x_0(t) + y(t) \qquad \Rightarrow y(t) = x(t) - x_0(t)$$

$$(8.60)$$

which parametrizes the fluctuations about the classical solution.

The Jacobi determinant of this transformation is $=1$,

$$\mathcal{D}x \sim \prod_n dx_n = \prod_n d(x_n - \underset{\substack{\| \\ \text{const}}}{x_{0n}}) = \prod_n dy_n \sim \mathcal{D}y \qquad (8.61)$$

A functional Taylor expansion of the action yields

$$S[x(t)] = S[y(t) + x_0(t)]$$

$$= S[x_0(t)] + \int dt \left.\frac{\delta S}{\delta x}\right|_{x_0(t)} y(t)$$

$$+ \frac{1}{2}\int dt\, dt'\, y(t) \left.\frac{\delta^2 S}{\delta x^2}\right|_{x_0(t)}^{(t,t')} y(t'). \qquad (8.62)$$

As the action is quadratic in $x(t)$, the expansion terminates at this order; hence (8.62) is exact. As the classical solution satisfies $\left.\frac{\delta S}{\delta x}\right|_{x_0(t)} = 0$,

we have

$$S^{(2)}[x_0] := \left.\frac{\delta^2 S}{\delta x^2}\right|_{x_0} \qquad (8.63)$$

$$S^{(2)}[x_0](t,t') \quad \left.\frac{\delta^2 S}{\delta x(t)\, \delta x(t')}\right|_{x}$$

$$\Rightarrow \quad S[x(t)] = S[x_0(t)] + \frac{1}{2}\int dt\,dt'\, y(t)\, S^{(2)}_{[x_0]}(t,t')\, y(t') \tag{8.64}$$

where $S^{(2)}$ is the "quadratic fluctuation matrix". Using $\dfrac{\delta x(t)}{\delta x(t')} = \delta(t-t')$, we find

$$\frac{\delta S}{\delta x(t)} = \frac{\delta}{\delta x(t)} \int dt'' \left(\frac{1}{2} m \dot{x}^2(t) - \frac{1}{2} m\omega^2 x(t)^2 \right)$$

$$= -\left[m \ddot{x}(t) + m\omega^2 x(t) \right]$$

$$\Rightarrow \frac{\delta^2 S}{\delta x(t)\,\delta x(t')} = \left(-m \frac{d^2}{dt^2} - m\omega^2 \right) \delta(t-t') \tag{8.65}$$

or symbolically $\quad S^{(2)} = -m \dfrac{d^2}{dt^2} - m\omega^2$

Insertion of (8.62) into (8.58) yields

$$\langle x_b t_b | x_a t_a \rangle = e^{\frac{i}{\hbar} S[x_0; x_b, x_a]} \langle 0, t_b | 0\, t_a \rangle \tag{8.66}$$

where

$$\langle 0\, t_b | 0\, t_a \rangle = \int_{y(t_a)=0}^{y(t_b)=0} \mathcal{D}y \;\; e^{\frac{i}{\hbar} \frac{1}{2} \iint y\, S^{(2)} y} \tag{8.67}$$

Without explicit computation, we recall the classical action of the HO for the present boundary conditions

$$S[x_0; x_b, x_a] = \frac{m\omega}{2\sin\omega(t_b - t_a)}\left[(x_a^2 + x_b^2)\cos\omega(t_b - t_a) - 2x_a x_b\right]$$

(8.68)

Finally, we need to compute the path integral (8.67).

This can indeed straightforwardly be done in the discretized form, as all $\int dy_n$ integrals are of Fresnel type. The limit of $N \to \infty$, $\varepsilon \to 0$ of the final expression exists an can be taken.

Instead we will use a continuum formulation here, assuming that the limit $N \to \infty$, $\varepsilon \to 0$ exists. For this, we replace the "absolute" measure

$$\int \mathcal{D}y = \frac{1}{\sqrt{\frac{2\pi i\hbar\varepsilon}{m}}} \prod_n \int_{-\infty}^{\infty} \frac{dy_n}{\sqrt{\frac{2\pi i\hbar\varepsilon}{m}}} \qquad (8.69)$$

by a "relative" measure with some unknown normalization $\mathcal{N}$

$$\langle 0 t_b | 0 t_a \rangle = \mathcal{N} \int_{y(t_a)=0}^{y(t_b)=0} \widetilde{\mathcal{D}y} \; e^{\frac{i}{\hbar}\frac{1}{2}\iint y\, S^{(2)}\, y} \qquad (8.67)$$

As the measure is independent of the integrand, $\mathcal{N}$ is the same for all systems. So, we can fix $\mathcal{N}$, for instance, using the free particle:

$$\langle 0 t_b | 0 t_a \rangle \overset{(8.31)}{=} \frac{1}{\sqrt{\frac{2\pi i \hbar (t_b - t_a)}{m}}}$$

$$\overset{(8.67)}{=} \mathcal{N} \int_{y(t_a)=0}^{y(t_b)=0} \widetilde{\mathcal{D}y} \; e^{\frac{i}{\hbar}\frac{1}{2}\iint y\, S^{(2)}_{\text{free}}\, y}$$

$$\rightarrow \quad \mathcal{N} = \sqrt{\frac{m}{2\pi i \hbar (t_b - t_a)}} \left\{ \int_{y(t_a)=0}^{y(t_b)=0} \widetilde{\mathcal{D}y} \; e^{\frac{i}{\hbar}\frac{1}{2}\iint y\, S^{(2)}_{\text{free}}\, y} \right\}^{-1} \qquad (8.68)$$

(NB: With the same argument, the normalization for the more general amplitude $\langle x_b t_b | x_a t_a \rangle$ can be worked out:

$$\mathcal{N} = \sqrt{\frac{m}{2\pi i \hbar (t_b - t_a)}} \; e^{\frac{i}{\hbar} S_{\text{free}}[x_0]} \left\{ \int_{x(t_a)=x_a}^{x(t_b)=x_b} \widetilde{\mathcal{D}x} \; e^{\frac{i}{\hbar}\frac{1}{2}\iint y\, S^{(2)}_{\text{free}}\, y} \right\}^{-1} \qquad (8.69)$$
)

Splitting the action into

$$S = S_{free} + S_{int} \tag{8.69}$$

where S_{int} is the interaction term, we can write the amplitude (8.67) as

$$\langle 0 t_b | 0 t_a \rangle = \sqrt{\frac{m}{2\pi i \hbar (t_b - t_a)}} \left\langle e^{\frac{i}{\hbar} S_{int}} \right\rangle_{free} \tag{8.70}$$

where $\langle \ldots \rangle$ is an expectation value with respect to the free theory:

$$\langle \mathcal{O} \rangle_{free} = \frac{\int \tilde{\mathcal{D}}y \, \mathcal{O}[y] \, e^{\frac{i}{\hbar} S_{free}}}{\int \tilde{\mathcal{D}}y \, e^{\frac{i}{\hbar} S_{free}}}, \tag{8.71}$$

normalized such that $\langle 1 \rangle_{free} = 1$.

Let us return now to the HO problem, where

$$\frac{i}{\hbar} S_{int} = \frac{i}{\hbar} \frac{1}{2} \iint y \, S^{(2)}_{int} \, y$$

$$\left.\begin{aligned} S^{(2)} &= -m \frac{d^2}{dt^2} - m\omega^2 \\ &= \underbrace{-m \frac{d^2}{dt}}_{S^{(2)}_{free}} + S^{(2)}_{int} \end{aligned}\right\} \quad S^{(2)}_{int} = -m\omega^2 \tag{8.72}$$

Now, imagine we could parameterize all paths in terms of eigenfunctions of $S^{(2)}$ (as $S^{(2)}$ is hermitean, this is indeed possible):

$$y(t) = \sum_n a_n f_n(t) \tag{8.73}$$

with coefficients a_n and

$$S^{(2)} f_n(t) = \lambda f_n(t) \tag{8.74}$$

Then the integral over all paths $y(t)$ can be written as an integral over all values of the coefficients a_n:

$$\prod_n dy_n = \prod_n da_n \cdot J \tag{8.75}$$

where J is a Jacobi determinant of this variable substitution. However, as J occurs in (8.71) in the numerator as well as in the denominator, and as (8.73) is a linear base change, J cancels out.

The eigenfunctions can be worked out straightforwardly,

$$\begin{aligned} (S^{(2)} - \lambda_n) f_n(t) &= 0 \\ \left(-\frac{d^2}{dt^2} - \left(\omega^2 + \frac{\lambda_n}{m}\right)\right) f_n(t) &= 0 \end{aligned} \tag{8.76}$$

The solution to (8.76) satisfying the boundary conditions $y(t_a)=0$, $y(t_b)=0$ are

$$f_n(t) = \sqrt{2}\,\sin\left[\left(\omega^2 + \frac{\lambda_n}{m}\right)^{1/2}(t-t_a)\right] \qquad (8.77)$$

with the condition

$$f_n(t_b)=0 \qquad \Rightarrow \left(\omega^2 + \frac{\lambda_n}{m}\right)^{1/2}(t_b - t_a) = n\pi$$

$$\Rightarrow \lambda_n = m\left[\left(\frac{n\pi}{t_b-t_a}\right)^2 - \omega^2\right] \qquad (8.78)$$

Now the path integral yields

$$\frac{\int \hat{\mathcal{D}}y\; e^{\frac{i}{\hbar}\frac{1}{2}\int y\, S^{(2)}_{HO}\, y}}{\int \hat{\mathcal{D}}y\; e^{\frac{i}{\hbar}\frac{1}{2}\int y\, S^{(2)}_{free}\, y}} = \frac{\int \prod_n da_n\; e^{\frac{i}{\hbar}\frac{1}{2}\sum_n \lambda_n a_n^2}}{\int \prod_n da_n\; e^{\frac{i}{\hbar}\frac{1}{2}\sum_n \lambda_n^{free} a_n^2}}$$

$$\overset{\text{Fresnel}}{=} \frac{\sqrt{\prod_n \lambda_n^{free}}}{\sqrt{\prod_n \lambda_n}} = \frac{\sqrt{\det S^{(2)}_{free}}}{\sqrt{\det S^{(2)}_{HO}}} \qquad (8.79)$$

where λ_n^{free} is simply $\lambda_n^{free} = \lambda_n\big|_{\omega=0}$

The products can straightforwardly be computed:

$$(8.79) = \sqrt{\prod_n \frac{\cancel{m}\left(\frac{n\pi}{t_b-t_a}\right)^2}{\cancel{m}\left[\left(\frac{n\pi}{t_b-t_a}\right)^2 - \omega^2\right]}} = \sqrt{\prod_n \left(1-\left(\frac{\omega(t_b-t_a)}{\pi n}\right)^2\right)^{-1}}$$

$$= \sqrt{\frac{\omega(t_b-t_a)}{\sin\omega(t_b-t_a)}} \qquad (8.80)$$

Upon insertion into (8.70), we get

$$\langle 0\, t_b | 0\, t_a\rangle = \sqrt{\frac{m\omega}{2\pi i\hbar \sin\omega(t_b-t_a)}} \qquad (8.81)$$

The final result for the propagator of the harmonic oscillator is (see (8.66) + (8.68))

$$\langle x_b t_b | x_a t_a\rangle = \sqrt{\frac{m\omega}{2\pi i\hbar \sin\omega(t_b-t_a)}}\; e^{\frac{i}{\hbar}\frac{m\omega}{2\sin\omega(t_b-t_a)}\left[(x_a^2+x_b^2)\cos\omega(t_b-t_a) - 2x_b x_a\right]} \qquad (8.82)$$

Let us try to squeeze a simple piece of information out of this result: what is the ground state energy of the HO?

For this, we use the Feynman-Kac formula,

$$E_0 = -\lim_{\tau\to\infty}\frac{1}{\tau}\log \operatorname{Tr} e^{-\tau H}$$

$$= -\lim_{\tau\to\infty}\frac{1}{\tau}\log \int dx\, \langle x -i\hbar\tau | x\, 0\rangle \qquad (8.83)$$

The first line is easy to understand: in the "long Euclidean time" limit, all higher energy levels will be exponentially suppressed in $e^{-\tau H}$.
In the second line, we represented $\operatorname{Tr} e^{-\tau H}$ by the time evolution operator in imaginary time.

For the HO, we get from (8.82):

$$\int dx\, \langle x\, t | x\, 0\rangle = \sqrt{\frac{m\omega}{2\pi i\hbar \sin\omega t}} \int dx\, e^{\frac{im\omega}{2\hbar\sin\omega t}2x^2(\cos\omega t - 1)}$$

$$= \frac{1}{2i}\left(\sin\frac{\omega t}{2}\right)^{-1}$$

$$= \frac{e^{-\frac{i}{2}\omega t}}{1-e^{-i\omega t}} = e^{-\frac{1}{2}i\omega t}\sum_{n=0} e^{-in\omega t} \qquad (8.84)$$

$$\Rightarrow \int dx\, \langle x -i\hbar\tau | x\, 0\rangle = e^{-\frac{1}{2}\hbar\omega\tau}\sum_{n=0}^{\infty} e^{-n\hbar\omega\tau} \qquad (8.85)$$

From the Feynman-Kac formula, we get

$$E_0 = \frac{1}{2} \hbar \omega \qquad (8.86)$$

We also get the full spectrum from isolating the subleading behavior of (8.83) in the limit $\tau \to \infty$,

$$E_n = \hbar \omega \left(n + \frac{1}{2}\right), \qquad n = 0, 1, 2, \ldots \qquad (8.87)$$