Chapter 2

Feynman path integral

The Feynman path integral provides a way to express quantum mechanics in terms of trajectories reminding of classical mechanics. Specifically it expresses the propagator as

$$K(\boldsymbol{r}_f, \boldsymbol{r}_0, t) = \int D[\boldsymbol{r}] e^{\frac{i}{\hbar} S[\boldsymbol{r}]} \tag{2.1}$$

Here the integral is taken over all trajectories that go from from $\boldsymbol{r}_0$ to $\boldsymbol{r}_f$ during the time t. These trajectories are described by functions $\boldsymbol{r}(t')$ with $\boldsymbol{r}(0) = \boldsymbol{r}_0$ and $\boldsymbol{r}(t) = \boldsymbol{r}_f$. Hence we have functions as integration variables! This is unusual and we we will give a proper definition of such integrals including the integration measure $D[\boldsymbol{r}]$ only at a later stage.

The integrand, i.e., the weight attributed to each trajectory, depends on the action of each trajectory.

We stress that the integral is taken over *all* trajectories from $\boldsymbol{r}_0$ to $\boldsymbol{r}_f$, not just those obeying the classical laws of motion. In hindsight this is not surprising as quantum mechanics goes beyond classical mechanics so its formulation should involve elements not present in classical mechanics. However we still expect that in some sense the contributions from trajectories obeying the classical laws of motion should dominate. We will come back to this point at a later stage.

2.1 Propagator for small times

We start by deriving the path integral. We first consider the case of small times t and then proceed to arbitrary times. We will concentrate on systems with a Hamiltonian of the form

$$\hat{H} = \underbrace{\frac{\hat{\boldsymbol{p}}^2}{2m}}_{=\hat{T}} + \hat{U}(\hat{\boldsymbol{r}}),$$

i.e. a standard kinetic energy plus potential. The propagator is then given by

$$K(\boldsymbol{r}_f, \boldsymbol{r}_0, t) = \langle \boldsymbol{r}_f | e^{-\frac{i}{\hbar}\hat{H}t} | \boldsymbol{r}_0 \rangle$$

where $e^{-\frac{i}{\hbar}\hat{H}t} = e^{-\frac{i}{\hbar}(\hat{T}+\hat{U})t}$. It would be very nice if we could write this as $e^{-\frac{i}{\hbar}\hat{T}t}e^{-\frac{i}{\hbar}\hat{U}t}$ as application of the exponentiated potential to the position eigenstate $|\boldsymbol{r}_0\rangle$ would simply amount to multiplication with $e^{-\frac{i}{\hbar}U(\boldsymbol{r}_0)t}$. However in general it is not correct to replace an exponentiated sum of *operators* by the product of the exponentiated summands. (Instead one has to use the so-called Baker-Campbell-Hausdorff formula which also involves the commutator if the two operators.) However in the present case we are only interested in small t, and we get through with the above replacement up to corrections of quadratic and higher orders in t. We have

$$\begin{aligned}
\langle \boldsymbol{r}_f | e^{-\frac{i}{\hbar}\hat{H}t} | \boldsymbol{r}_0 \rangle &\approx \langle \boldsymbol{r}_f | (1 - \frac{i}{\hbar}\hat{H}t) | \boldsymbol{r}_0 \rangle \\
&\approx \langle \boldsymbol{r}_f | (1 - \frac{i}{\hbar}\hat{T}t)(1 - \frac{i}{\hbar}\hat{U}t) | \boldsymbol{r}_0 \rangle \\
&\approx \langle \boldsymbol{r}_f | e^{-\frac{i}{\hbar}\hat{T}t} \underbrace{e^{-\frac{i}{\hbar}\hat{U}t} | \boldsymbol{r}_0 \rangle}_{= e^{-\frac{i}{\hbar}U(\boldsymbol{r}_0)t} | \boldsymbol{r}_0 \rangle} \\
&= \underbrace{\langle \boldsymbol{r}_f | e^{-\frac{i}{\hbar}\hat{T}t} | \boldsymbol{r}_0 \rangle}_{=: A} e^{-\frac{i}{\hbar}U(\boldsymbol{r}_0)t} \qquad (2.2)
\end{aligned}$$

Here we used first used a Taylor expansion, then we included a negligible error proportional to $\hat{T}\hat{U}t^2$, then we made a Taylor expansion 'in reverse', and finally we just applied to operator $\hat{U}$.

Evaluation of A. If we write out the delta functions for $|\boldsymbol{r}_f\rangle$ and $|\boldsymbol{r}_0\rangle$ in position representation we get

$$A = \int_{\mathbb{R}^n} \delta(\boldsymbol{r} - \boldsymbol{r}_f) e^{-\frac{i}{\hbar}\hat{T}t} \delta(\boldsymbol{r} - \boldsymbol{r}_0) d^n r$$

Using the integral representation (1.4) for the second delta function this turns into

$$\begin{aligned}
A &= \int_{\mathbb{R}^n} \delta(\boldsymbol{r} - \boldsymbol{r}_f) e^{-\frac{i}{\hbar}\hat{T}t} \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^n} e^{i\boldsymbol{p}\cdot(\boldsymbol{r}-\boldsymbol{r}_0)/\hbar} d^n p \\
&= \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^n} d^n r \; \delta(\boldsymbol{r} - \boldsymbol{r}_f) \int_{\mathbb{R}^n} d^n p \; e^{-\frac{i}{\hbar}\hat{T}t} e^{i\boldsymbol{p}\cdot(\boldsymbol{r}-\boldsymbol{r}_0)/\hbar}
\end{aligned}$$

Our expression involves both momentum operators $\hat{\boldsymbol{p}}$ inside $\hat{T}$ and momenta $\boldsymbol{p}$ brought in through the integral representation of the delta function. However given the way the expression is arranged now we can replace $\hat{\boldsymbol{p}}$ by $\boldsymbol{p}$. This is possible because

$$\hat{\boldsymbol{p}} e^{i\boldsymbol{p}\cdot(\boldsymbol{r}-\boldsymbol{r}_0)/\hbar} = \frac{\hbar}{i} \frac{\partial}{\partial \boldsymbol{r}} e^{i\boldsymbol{p}\cdot(\boldsymbol{r}-\boldsymbol{r}_0)/\hbar} = \boldsymbol{p} e^{i\boldsymbol{p}\cdot(\boldsymbol{r}-\boldsymbol{r}_0)/\hbar}.$$

Analogous results apply for any power of $\hat{\boldsymbol{p}}$ and hence also for exponentials involving $\boldsymbol{p}$. As a consequence we have

$$e^{-\frac{i}{\hbar}\hat{T}t} e^{i\boldsymbol{p}\cdot(\boldsymbol{r}-\boldsymbol{r}_0)/\hbar} = e^{-\frac{i}{\hbar}\frac{\hat{\boldsymbol{p}}^2}{2m}t} e^{i\boldsymbol{p}\cdot(\boldsymbol{r}-\boldsymbol{r}_0)/\hbar} = e^{-\frac{i}{\hbar}\frac{\boldsymbol{p}^2}{2m}t} e^{i\boldsymbol{p}\cdot(\boldsymbol{r}-\boldsymbol{r}_0)/\hbar}$$

If we insert this into A we get

$$\begin{aligned} A &= \frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^n} d^n r\; \delta(\boldsymbol{r}-\boldsymbol{r}_f)\int_{\mathbb{R}^n} d^n p\; e^{-\frac{i}{\hbar}\frac{\boldsymbol{p}^2}{2m}t} e^{i\boldsymbol{p}\cdot(\boldsymbol{r}-\boldsymbol{r}_0)/\hbar} \\ &= \frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^n} d^n p\; e^{-\frac{i}{\hbar}\frac{\boldsymbol{p}^2}{2m}t} e^{i\boldsymbol{p}\cdot(\boldsymbol{r}_f-\boldsymbol{r}_0)/\hbar} \\ &= \prod_{k=1}^{n}\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dp_k e^{-\frac{i}{\hbar}\frac{p_k^2}{2m}t+ip_k(r_{fk}-r_{0k})/\hbar}. \end{aligned} \tag{2.3}$$

Here we used the definition of the delta function and afterwards wrote the integral in terms of the components of $\boldsymbol{p}$.

The remaining integral over p_k is quite similar to a Gaussian one and can be done easily with the following results about integrals of this type:

- The **Gauss integral** gives

  $$\int_{-\infty}^{\infty} e^{-ax^2}dx = \sqrt{\frac{\pi}{a}}$$

  for $a > 0$.

- The **Fresnel integral** involves an additional i and is evaluated as

  $$\int_{-\infty}^{\infty} e^{\mp iax^2}dx = \sqrt{\frac{\pi}{\pm ia}} = \sqrt{\frac{\pi}{|a|}}e^{\mp i\frac{\pi}{4}\,\mathrm{sign}\,a}. \tag{2.4}$$

  Heuristically these results follow from the Gauss integral by replacing $a \to \pm ia$, using $i = e^{i\frac{\pi}{2}}$, and hoping for the best. The rigorous derivation involves contour integration in the complex plane.

- Our p_k-integral also involves linear terms in the exponent. Hence we have to evaluate a shifted Fresnel integral $\int_{-\infty}^{\infty} e^{-iax^2+ibx}dx$. By completing the square as in

  $$-iax^2 + ibx = -ia\left(x-\frac{b}{2a}\right)^2 + ia\frac{b^2}{4a^2}$$

  and substituting $y = x - \frac{b}{2a}$ this integral can be evaluated as

  $$\int_{-\infty}^{\infty} e^{-iax^2+ibx}dx = \int_{-\infty}^{\infty} e^{-iay^2}dy\; e^{i\frac{b^2}{4a}} = \sqrt{\frac{\pi}{ia}}\,e^{i\frac{b^2}{4a}}. \tag{2.5}$$

If we apply (2.5) to (2.3) with $a = \frac{t}{2m\hbar}$, $b = \frac{r_{fk}-r_{ik}}{\hbar}$ we finally get

$$A = \prod_{k=1}^{n}\left(\frac{m}{2\pi i\hbar t}\right)^{1/2}\exp\left(\frac{i}{\hbar}\frac{1}{2}m\left(\frac{r_{fk}-r_{0k}}{t}\right)^2 t\right).$$

After simplification and combination with (2.2) this gives our final result for the short-time propagator:

$$K(\boldsymbol{r}_f,\boldsymbol{r}_0,t) \approx \left(\frac{m}{2\pi i\hbar t}\right)^{n/2}\exp\left(\frac{i}{\hbar}\left[\frac{1}{2}m\left(\frac{\boldsymbol{r}_f-\boldsymbol{r}_0}{t}\right)^2 - U(\boldsymbol{r}_0)\right]t\right) \tag{2.6}$$

This result is reassuring given our final goal (2.1): If we moved with constant velocity from $\boldsymbol{r}_0$ to $\boldsymbol{r}_f$ in time t that velocity would be given by $\frac{\boldsymbol{r}_f-\boldsymbol{r}_0}{t}$. For a different (differentiable) motion between these points it is still a good approximation of the velocity for small times t. Hence the expression in the square brackets is a good approximation for the Lagrangian $L = T - U$. Multiplied with t we get a good approximation for action over a small time interval during which the Lagrangian does not change much.

2.2 Propagator for arbitrary times

The propagator for arbitrary times t can be evaluated using our preceding result if we split the time interval t into N intervals of size $\tau = \frac{t}{N}$. If we then apply the limit $N \to \infty$ we can make use of the result for small times. We thus write

$$K(\boldsymbol{r}_f, \boldsymbol{r}_0, t) = \langle \boldsymbol{r}_f | e^{-\frac{i}{\hbar}\hat{H}\tau} \dots e^{-\frac{i}{\hbar}\hat{H}\tau} | \boldsymbol{r}_0 \rangle$$

(with N factors). We now insert resolutions of unity $1 = \int |\boldsymbol{r}\rangle\langle\boldsymbol{r}| d^n r$ between the factors. As there are N factors we need $N - 1$ integrals. We thus obtain

$$\begin{aligned} K(\boldsymbol{r}_f, \boldsymbol{r}_i, t) &= \int \dots \int \langle \boldsymbol{r}_f | e^{-\frac{i}{\hbar}\hat{H}\tau} | \boldsymbol{r}_{N-1} \rangle \langle \boldsymbol{r}_{N-1} | e^{-\frac{i}{\hbar}\hat{H}\tau} | \boldsymbol{r}_{N-2} \rangle \langle \boldsymbol{r}_{N-2} | \dots | \boldsymbol{r}_2 \rangle \\ &\quad \langle \boldsymbol{r}_2 | e^{-\frac{i}{\hbar}\hat{H}\tau} | \boldsymbol{r}_1 \rangle \langle \boldsymbol{r}_1 | e^{-\frac{i}{\hbar}\hat{H}\tau} | \boldsymbol{r}_0 \rangle \; d^n r_1 \dots d^n r_{N-1}. \end{aligned}$$

To simplify notation in the following it is helpful to set $\boldsymbol{r}_N = \boldsymbol{r}_f$; however like $\boldsymbol{r}_0$, $\boldsymbol{r}_N$ will remain fixed and is not an integration variable. Now we can use (2.6) for all N factors. For each of them we obtain one power of the prefactor in (2.6) with time $\frac{t}{N}$; the exponents are all added and in these exponents the positions turn into $\boldsymbol{r}_j$ and $\boldsymbol{r}_{j+1}$. We thus obtain

$$\begin{aligned} K(\boldsymbol{r}_f, \boldsymbol{r}_0, t) &= \int d^n r_1 \dots d^n r_{N-1} \left(\frac{mN}{2\pi i \hbar t} \right)^{nN/2} \\ &\quad \exp\left(\frac{i}{\hbar} \sum_{j=0}^{N-1} \left[\frac{1}{2} m \left(\frac{\boldsymbol{r}_{j+1} - \boldsymbol{r}_j}{\tau} \right)^2 - U(\boldsymbol{r}_j) \right] \tau \right) \end{aligned}$$

We can now imagine the points $\boldsymbol{r}_j$ to arise from a discretisation of a trajectory, with $\boldsymbol{r}_j$ being the position at time $j\tau$, see Fig. 2.1. (This is consistent with our derivation as the resolution of the identity with integration variable $\boldsymbol{r}_j$ was inserted after j factors $e^{-\frac{i}{\hbar}\hat{H}\tau}$ each describing evolution over a time τ.) Then, given our earlier discussion, $\frac{1}{2}m\left(\frac{\boldsymbol{r}_{j+1}-\boldsymbol{r}_j}{\tau}\right)^2 - U(\boldsymbol{r}_j)$ is a good approximation for the Lagrangian during the motion from $\boldsymbol{r}_j$ to $\boldsymbol{r}_{j+1}$, and its product with τ is a good approximation for the action associated to that piece of trajectory. The sum over j leads to a summation over all pieces of trajectory and hence to a good approximation for the overall action. The approximation gets better and better the finer we make our discretisation, i.e., the larger we make N. In the limit $N \to \infty$ we indeed obtain the action,

$$\sum_{j=0}^{N-1}\left[\frac{1}{2}m\left(\frac{\boldsymbol{r}_{j+1}-\boldsymbol{r}_j}{\tau}\right)^2 - U(\boldsymbol{r}_j)\right]\tau \to \int_0^t \left(\frac{1}{2}m\dot{\boldsymbol{r}}(t')^2 - U(\boldsymbol{r}(t'))\right)dt' = S[\boldsymbol{r}] \qquad (N\to\infty)$$

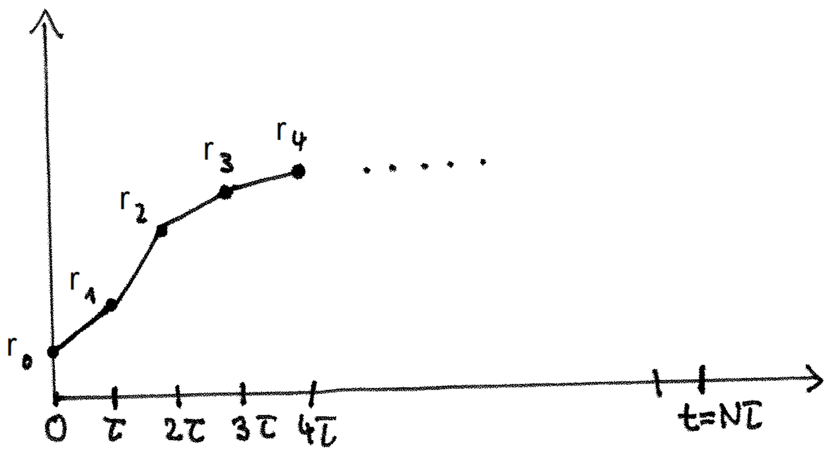

Figure 2.1: A discretised trajectory.

Now it is important that we *integrate* over $\boldsymbol{r}_1, \ldots, \boldsymbol{r}_{N-1}$. I.e. we take into account all discretised versions of trajectories, and in the limit $N \to \infty$, we take into account all possible trajectories or in other words all functions $\boldsymbol{r}(t')$. The only restriction is that we have to start at $\boldsymbol{r}_0$ and end at $\boldsymbol{r}_N = \boldsymbol{r}_f$. For our function this implies the anticipated boundary conditions $\boldsymbol{r}(0) = \boldsymbol{r}_0$ and $\boldsymbol{r}(t) = \boldsymbol{r}_f$. There are no further restrictions on these function, in particular they don't have to be solutions for the classical equations of motion.

If we simply define our integration measure on the space of functions by the limit

$$\int D[\boldsymbol{r}]\ldots = \lim_{N\to\infty}\left(\frac{mN}{2\pi i\hbar t}\right)^{nN/2}\int d^n r_1 \ldots d^n r_{N-1}\ldots$$

we get the expected path integral

$$K(\boldsymbol{r}_f, \boldsymbol{r}_0, t) = \int_{\substack{\boldsymbol{r}(0)=\boldsymbol{r}_0,\\ \boldsymbol{r}(t)=\boldsymbol{r}_f}} D[\boldsymbol{r}]e^{\frac{i}{\hbar}S[\boldsymbol{r}]}. \qquad (2.7)$$

Remarks.

- The Feynman path integral provides a **link between quantum mechanics and trajectories** which are the essential objects in classical mechanics. As it also involves trajectories that don't obey the classical laws of motion it goes beyond classical mechanics. This is to be expected as quantum mechanics is the deeper theory and should involve corrections to classical behaviour.

- However **trajectories satisfying the classical laws of motion dominate** in the following sense: These trajectories are stationary points of the action. Hence varying a trajectory compared to a classical one does not change the action to linear order in the deviation. Changes to the original action appear only in quadratic or higher orders. So trajectories close to a classical one have very similar actions and give very similar contributions to the path integral. By contrast the actions of trajectories further away from a classical one already show deviations from each other already in a linear approximation. As an action difference of $\pi\hbar$ already leads to a change in sign this means that the contributions of such trajectories have a tendency to cancel. This leaves contributions close to classical trajectories as the dominant ones.

  One can use this idea for approximations of the path integral in terms of classical trajectories. These approximations are used e.g. in Quantum Chaos.

- For a **rigorous** theory one would have to pay more attention to the definition of the integration measure and to trajectories that are not differentiable. The rigorous formulation of path integrals is still not complete.

- We assumed that all positions $\boldsymbol{r} \in \mathbb{R}^n$ are possible. If some $\boldsymbol{r}$ are ruled out and this leads to a 'not simply connected' position space (for example a two dimensional space with a hole) a similar result applies. But there is an additional phase factor depending on how often each trajectory winds around the hole.

- In our derivation we introduced an integral over $\boldsymbol{p}$ in order to represent a delta function, but we got rid of this integral again because it was a shifted Fresnel integral that could be evaluated explicitly. However, one could have just left this integral. As it appeared in the formula for the short time propagator one would then obtain momentum integrals for each of the N time steps in the propagator for arbitrary times. These integrals can be treated very similarly to the integrals in position space, so that in the end we would obtain a path integral in **phase space** with integrations over functions $\boldsymbol{r}$ and $\boldsymbol{p}$. This integral, to be derived in problem sheet 1, question 2, has the form

$$K(\boldsymbol{r}_f, \boldsymbol{r}_0, t) = \int \mathcal{D}[\boldsymbol{r}]\mathcal{D}[\boldsymbol{p}] \exp\left(\frac{i}{\hbar}\int_0^t (\boldsymbol{p}(t') \cdot \dot{\boldsymbol{r}}(t') - H(\boldsymbol{r}(t'), \boldsymbol{p}(t'))dt'\right)$$

  where the integration measure $\int \mathcal{D}[\boldsymbol{r}]\mathcal{D}[\boldsymbol{p}]\ldots$ is different from the one in the position space path integral. The exponent involves the natural generalisation of the action to phase space, using that $H = \boldsymbol{p} \cdot \dot{\boldsymbol{r}} - L \;\Rightarrow\; L = \boldsymbol{p} \cdot \dot{\boldsymbol{r}} - H$.

2.3 Example: Harmonic oscillator

As an example we want to evaluate the path integral for the (one-dimensional) harmonic oscillator with the Lagrangian

$$L = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2 x^2 \ .$$

The action is

$$S[x] = \int_0^t \left(\frac{1}{2}m\dot{x}(t')^2 - \frac{1}{2}m\omega^2 x(t')^2\right) dt'.$$

It is helpful to split $x(t')$ into the classical solution (the stationary point of the action subject to our boundary conditions $x(0) = x_0$, $x(t) = x_f$) $x_{\rm cl}(t')$ and the deviation from the classical solution $\delta x(t')$,

$$x(t') = x_{\rm cl}(t') + \delta x(t').$$

As $x_{\rm cl}$ satisfies the same boundary conditions as x the deviation δx must vanish at the boundaries, $\delta x(0) = \delta x(t) = 0$. If we insert this decomposition of x into $S[x]$ we get

$$\begin{aligned} S[x] \ &= \int_0^t \left(\frac{1}{2}m\dot{x_{\rm cl}}(t')^2 - \frac{1}{2}m\omega^2 x_{\rm cl}(t')^2\right) dt' \\ &+ \int_0^t \left(m\dot{x_{\rm cl}}(t')\dot{\delta x}(t') - m\omega^2 x_{\rm cl}(t')\delta x(t')\right) dt' \\ &+ \int_0^t \left(\frac{1}{2}m\dot{\delta x}(t')^2 - \frac{1}{2}m\omega^2 \delta x(t')^2\right) dt'. \end{aligned}$$

Here we have arranged the terms as in a Taylor expansion in δx: the first line contains terms independent of δx (i.e. the action evaluated at $x_{\rm cl}$), the second line contains linear terms, and the third line contains quadratic terms. Now it is important that we are expanding around a stationary point of the action. As always, in a Taylor expansion around a stationary point the linear term vanishes because the derivative[1] vanishes. In the special case of the harmonic oscillator it also turns out that the quadratic term can just be written as $S[\delta x]$. We thus have

$$S[x] = S[x_{\rm cl}] + S[\delta x].$$

Classical solution. To proceed we compute $S[x_{\rm cl}]$. $x_{\rm cl}(t')$ is the solution of Lagrange's equation,

$$\frac{\partial L}{\partial x} = \frac{d}{dt'}\frac{\partial L}{\partial \dot{x}}$$

which for the harmonic oscillator boils down to

$$-m\omega^2 x_{\rm cl}^2 = m\ddot{x_{\rm cl}}.$$

Hence we have

$$x_{\rm cl}(t') = A\sin\omega t' + B\cos\omega t'.$$

[1]In our case this is a functional derivative as discussed in Mechanics 2/23.

If we insert this result into the action (2.3) we obtain

$$S[x_{\rm cl}] = \frac{m\omega}{2}\left((A^2 - B^2)\frac{\sin 2\omega t}{2} + 2AB\frac{\cos 2\omega t - 1}{2}\right).$$

To satisfy the boundary condition at 0 we need $x_{\rm cl}(0) = B = x_0$. The boundary condition at t is satisfied if

$$x_{\rm cl}(t) = A\sin\omega t + B\cos\omega t = x_f \;\Rightarrow\; A = \frac{x_f - B\cos\omega t}{\sin\omega t} = \frac{x_f - x_0\cos\omega t}{\sin\omega t}$$

Inserting these values into $S[x_{\rm cl}]$ gives

$$S[x_{\rm cl}] = \frac{m\omega}{2\sin\omega t}\left((x_0^2 + x_f^2)\cos\omega t - 2x_0 x_f\right).$$

Integration measure. We now have the intermediate result

$$K(x_f, x_0, t) = \int D[x] e^{\frac{i}{\hbar}(S[x_{\rm cl}] + S[\delta x])} \tag{2.8}$$

with $S[x_{\rm cl}]$ as above. It would be very nice if we could replace $D[x]$ by $D[\delta x]$. This is permitted because it just amounts to a shift of the integration variable by a constant amount, but because we are dealing with a functional integral we want to work it out explicitly. We have

$$\begin{aligned}
\int D[x]\dots &= \lim_{N\to\infty}\left(\frac{mN}{2\pi i\hbar t}\right)^{nN/2}\int dx_1 \int dx_2 \dots \int dx_{N-1}\dots \\
&= \lim_{N\to\infty}\left(\frac{mN}{2\pi i\hbar t}\right)^{nN/2}\int d\delta x_1 \int d\delta x_2 \dots \int d\delta x_{N-1}\dots \\
&= \int D[\delta x]\dots
\end{aligned}$$

Here we made, for each step j, the variable substitution $x_j \to \delta x_j$ where $x_j = x_{{\rm cl},j} + \delta x_j$. As $x_{{\rm cl},j}$ is not an integration variable the Jacobian for this transformation is 1.

As noted earlier the boundary conditions for δx are $\delta x(0) = \delta x(t) = 0$. After the variable transformation the propagator can thus be written as

$$\begin{aligned}
K(x_f, x_0, t) &= \underbrace{\left(\int_{\delta x(0)=\delta x(t)=0} D[\delta x] e^{\frac{i}{\hbar}S[\delta x]}\right)}_{=A(t)} e^{\frac{i}{\hbar}S[x_{\rm cl}]} \\
&= A(t)\exp\left(\frac{i}{\hbar}\frac{m\omega}{2\sin\omega t}\left((x_0^2 + x_f^2)\cos\omega t - 2x_0 x_f\right)\right).
\end{aligned} \tag{2.9}$$

Here the δx integral does not depend on x_0 and x_f at all (not even through the boundary conditions) but only on t.

How to determine $A(t)$? To get $A(t)$ we could use the discretised version of the path integral and integrate over $\delta x_1, \delta x_2, \ldots$ but this calculation becomes a little messy – this method works better for the propagator with vanishing potential which we are leaving for the homework. Instead we are employing a shortcut to determine $A(t)$, and we will only consider the case $0 < \omega t < \pi$.[2]

Using the resolution of the identity we can derive the following result for integrals of products of propagators

$$\begin{aligned} & \int K(x_f, x, t_2) K(x, x_0, t_1) dx \\ = & \int \langle x_f | e^{-\frac{i}{\hbar}\hat{H}t_2} | x \rangle \langle x | e^{-\frac{i}{\hbar}\hat{H}t_1} | x_0 \rangle dx \\ = & \langle x_f | e^{-\frac{i}{\hbar}\hat{H}(t_1+t_2)} | x_0 \rangle \\ = & K(x_f, x_0, t_1 + t_2). \end{aligned}$$

Intuitively this result means that time evolution according to the Schrödinger equation over time t_1 followed by time evolution over time t_2 gives time evolution over the combined time $t_1 + t_2$. For our present argument we just need the special case $x_0 = x_f = 0$,

$$\int K(0, x, t_2) K(x, 0, t_1) dx = K(0, 0, t_1 + t_2). \tag{2.10}$$

Now the $A(t)$ in (2.9) has to be picked such that (2.10) is satisfied. The r.h.s. gives $A(t_1 + t_2)$. For the l.h.s. we obtain

$$\begin{aligned} & \int K(0, x, t_2) K(x, 0, t_1) dx \\ = & \int A(t_2) \exp\left(\frac{i}{\hbar} \frac{m\omega}{2\sin\omega t_2} x^2 \cos\omega t_2\right) A(t_1) \exp\left(\frac{i}{\hbar} \frac{m\omega}{2\sin\omega t_1} x^2 \cos\omega t_1\right) \\ = & A(t_1) A(t_2) \int \exp\left(\frac{i}{\hbar} \frac{m\omega}{2} \frac{\sin\omega t_1 \cos\omega t_2 + \sin\omega t_2 \cos\omega t_1}{\sin\omega t_1 \sin\omega t_2} x^2\right) dx \\ = & A(t_1) A(t_2) \sqrt{\frac{2\pi\hbar}{m\omega} \frac{\sin\omega t_1 \sin\omega t_2}{\sin\omega(t_1 + t_2)}}\, e^{i\frac{\pi}{4}} \end{aligned}$$

where in the final step we used a trigonometric identity and the Fresnel integral. Now the equation can be rearranged into terms associated to the times t_1, t_2, and $t_1 + t_2$. If we do this, and also multiply through with $\sqrt{\frac{2\pi\hbar}{m\omega}\sin\omega(t_1 + t_2)}e^{i\frac{\pi}{4}}$, we obtain

$$\begin{aligned} & \sqrt{\frac{2\pi\hbar}{m\omega}\sin\omega(t_1 + t_2)}e^{i\frac{\pi}{4}} A(t_1 + t_2) \\ = & \left(\sqrt{\frac{2\pi\hbar}{m\omega}\sin\omega t_1} e^{i\frac{\pi}{4}} A(t_1)\right) \left(\sqrt{\frac{2\pi\hbar}{m\omega}\sin\omega t_2} e^{i\frac{\pi}{4}} A(t_2)\right) \end{aligned}$$

The easiest way to satisfy this equation is to set the l.h.s., the two factors on the r.h.s., and any term of the same form, to 1. This means that for all times t under

[2] Actually there is even a third way to do this calculation. This is based on a Fourier transform and briefly outlined in the Altland & Simons book.

consideration,

$$\sqrt{\frac{2\pi\hbar}{m\omega}\sin\omega t}e^{i\frac{\pi}{4}}A(t) \;\Rightarrow\; A(t) = \sqrt{\frac{m\omega}{2\pi\hbar\sin\omega t}}e^{-i\frac{\pi}{4}} \tag{2.11}$$

and hence

$$K(x_f, x_0, t) = \sqrt{\frac{m\omega}{2\pi\hbar\sin\omega t}}\exp\left(\frac{i}{\hbar}\frac{m\omega}{2\sin\omega t}\left((x_0^2 + x_f^2)\cos\omega t - 2x_0 x_f\right) - i\frac{\pi}{4}\right)$$

Note that we have just seen that our choice of $A(t)$ is the simplest way to satisfy (2.11) but we did not look for other solutions. Hence to be really sure one still has to plug our result into the Schrödinger equation and check that it works – indeed it does (see problem sheet 2).

We have just considered $0 < \omega t < \pi$ as in this case $\sin\omega t$ is positive. For arbitrary ωt one has to be more careful with the phase factor appearing in the Fresnel integral (a complication that is often ignored in the literature).

2.4 Elastic chain

We want to present a further example for a path integral. An interesting feature of this path integral is that in a certain limit it allows for a representation in terms of a field. This will serve as a simple illustration for the use of path integrals in the context of fields; more involved uses of path integrals with fields originate from quantum field theory and condensed matter theory.

We consider a chain of $N+1$ masses m connected by springs with spring constant k and natural length 0. We take the length of the chain as C. The positions along the chain will be denoted by Φ_i. We require that the initial mass is fixed at $\Phi_0 = 0$ and the final one is fixed at $\Phi_N = C$. The positions Φ_i of the remaining masses ($i = 1 \ldots N-1$) will be assembled into a vector $\mathbf{\Phi}$. Then the Lagrangian is

$$L(\mathbf{\Phi}, \dot{\mathbf{\Phi}}) \;=\; \sum_{i=1}^{N-1}\frac{1}{2}m\dot{\Phi}_i^2 - \sum_{i=0}^{N-1}\frac{1}{2}k(\Phi_{i+1} - \Phi_i)^2. \tag{2.12}$$

The vector $\mathbf{\Phi}$ can now be treated just like the position $\boldsymbol{r}$ considered earlier and hence we obtain the propagator of our system as the path integral

$$K(\mathbf{\Phi}_f, \mathbf{\Phi}_0, t) = \langle\mathbf{\Phi}_f|e^{-\frac{i}{\hbar}\hat{H}t}|\mathbf{\Phi}_0\rangle = \int_{\mathbf{\Phi}(0)=\mathbf{\Phi}_0, \mathbf{\Phi}(t)=\mathbf{\Phi}_f} D[\mathbf{\Phi}]e^{\frac{i}{\hbar}S[\mathbf{\Phi}]}.$$

This propagator describes the time evolution of a quantum mechanical chain with springs. The states $|\mathbf{\Phi}_0\rangle$ and $|\mathbf{\Phi}_f\rangle$ are eigenstates where the positions of all the masses in the system are fixed and $K(\mathbf{\Phi}_f, \mathbf{\Phi}_0, t)$ gives the wavefunction that started with initial condition $\mathbf{\Phi}_0\rangle$ and is then evaluated at $\mathbf{\Phi}_f$ after time evolution over time t. The integral goes over all $\mathbf{\Phi}(t')$ with the appropriate conditions at 0 and t, and we have

$$S[\mathbf{\Phi}] = \int_0^t dt' L(\mathbf{\Phi}(t'), \dot{\mathbf{\Phi}}(t')). \tag{2.13}$$

Continuum limit

We are now interested in the limit where the length C stays fixed but the number of masses and springs N is taken to infinity. This limit describes a string or rubber band whose different parts can be compressed or expanded independently and are thus modelled by separate springs instead of modelling the whole system by just one spring; the only constraint when expanding and contracting the different parts is that the total length has to stay fixed.

In our limit it is convenient to replace i by a continuous parameter. To choose a convenient parameter we use that at equilibrium the masses will be equally spaced with distance $a = \frac{C}{N}$, such that each mass i has the position ia. We thus replace the index i as a parameter by the equililibrium position $x = ia$. For finite N this means that Φ is parameterised by a real parameter that can still only assume discrete values $a, 2a, \dots$. However in the limit $N \to \infty$ it can really assume continuous values. Φ thus becomes a function $\Phi(x, t')$ of positions x as well as times t', or in other words a field.

It is natural to expect that the discrete sum over i in the Lagrangian will then also be replaced by an integral. To show this we show that each summand in L (see Eq. (2.12)) can be replaced by an integral from ia to $(i+1)a$ implying that the whole sum can be replaced by an integral from 0 to C. We start by making the replacement

$$\Phi_i(t') = \Phi(ia, t')$$

in the summand, leading to

$$\frac{1}{2}m\dot{\Phi}(ia,t')^2 - \frac{1}{2}k\underbrace{\left(\Phi((i+1)a,t') - \Phi(ia,t')\right)^2}_{\approx(\Phi'(ia,t')a)^2}$$

where we Taylor expanded denoting the derivative w.r.t. x by a prime. Now the summand can be approximated further by

$$\frac{1}{2}\frac{m}{a}\int_{ia}^{(i+1)a} dx\dot{\Phi}(x,t')^2 - \frac{1}{2}ka\int_{ia}^{(i+1)a} dx\Phi'(x,t)^2$$

where we the integrands are almost constant in integration interval (exactly constant in the limit $a \to 0$). Hence integration only leads to multiplication with a which is compensated by dividing out a. Combining all summands we obtain

$$L(\mathbf{\Phi}, \dot{\mathbf{\Phi}}) \approx \int_0^C dx \left(\frac{1}{2}\frac{m}{a}\dot{\Phi}(x,t')^2 - \frac{1}{2}ka\Phi'(x,t')^2\right) \tag{2.14}$$

where the approximation turns into an identity as $N \to \infty$.

The path integral thus turns into

$$K(\Phi_f, \Phi_0, t) = \int D[\Phi]e^{iS[\Phi]/\hbar}$$

where all occurrences of indices i are replaced by the continuous variable x. Hence the initial and final conditions are now given by functions $\Phi_0(x)$ and $\Phi_f(x)$ and the integral is taken over fields $\Phi(x,t')$ with

$$\Phi(x,0) = \Phi_0(x), \quad \Phi(x,t) = \Phi_f(x)$$

for all x. Moreover our earlier requirements $\Phi_0 = 0$ and $\Phi_N = C$ now turn into the boundary conditions

$$\Phi(0,t') = 0$$

and

$$\Phi'(C,t') = C$$

for all t'.

Substituting the integral for the Lagrangian (2.14) into (2.13) we obtain the double integral for the action

$$S[\Phi] = \int_0^C dx \int_0^t dt' \underbrace{\left(\frac{1}{2}\frac{m}{a}\dot{\Phi}(x,t')^2 - \frac{1}{2}ka\Phi'(x,t')^2\right)}_{=\mathcal{L}(\Phi,\dot{\Phi},\Phi')}$$

Here position and time are treated on the same footing, and it is natural to interpret the integrand $\mathcal{L}$ as a Lagrangian density whose role is analogous to the one played by the Lagrangian in usual Lagrangian mechanics. (However note that the Lagrangian for the problem is still (2.14).) In addition to the dependence on the field (absent here) and its time derivative the Lagrangian density also depends on the spacial derivative. However time is still singled out as we consider time evolution and we take initial and final conditions at specified times 0 and t.

To keep the coefficients from going to zero and infinity as $N \to \infty$ and $a \to 0$ we have to let m go to zero at the same rate as $a = \frac{C}{N}$, and k has to diverge. Indeed this is the appropriate limit for our physical system. In particular it means that the overall mass of the system stays fixed[3] as it should if we take a given string or rubber band and just discretise it in a finer and finer way.

2.5 Path integrals in Statistical Mechanics

Path integrals also have important applications in Statistical Mechanics. In this case it is not the propagator that is written as a path integral, but a slightly different quantity that we are about to introduce. In Statistical Mechanics one is often interested in systems that can exchange energy with the environment. Hence the energy of the system is not fixed. One can show that the statistical probability to find it in the j-th energy eigenstate is proportional to

$$e^{-\frac{1}{k_B T}E_j}$$

where T is the temperature and k_B is called the Botzmann constant; one often uses the abbreviation $\beta = \frac{1}{k_B T}$. In order to normalise these probabilities we need to

[3]To be precise, if we choose M as the fixed overall mass we have $m = \frac{M}{N+1}$ i.e. m shrinks like $\frac{1}{N+1}$ rather than $\frac{1}{N}$ but the difference between these is negligible as $N \to \infty$.

compute the **partition function** given by

$$Z = \sum_j e^{-\beta E_j}.$$

The partition function can also be written as

$$Z = \operatorname{tr} e^{-\beta \hat{H}},$$

using that the eigenvalues of $e^{-\beta\hat{H}}$ are $e^{-\beta E_j}$ and that the trace is the sum of the eigenvalues. Now $e^{-\beta\hat{H}}$ looks formally very similar to the time-evolution operator, and it is natural to look for a corresponding path integral. One possibility is to determine a path integral for the partition function itself, which involves a trace. However in order to increase the similarity with what we have done before, we instead consider the matrix elements

$$\langle \boldsymbol{r}_f | e^{-\beta\hat{H}} | \boldsymbol{r}_0 \rangle.$$

We note that here $\boldsymbol{r}_f$ and $\boldsymbol{r}_0$ could also be collections of the positions of many particles, and one can easily construct the trace from the matrix elements.

Path integral. The path integral for $\langle \boldsymbol{r}_f | e^{-\beta\hat{H}} | \boldsymbol{r}_0 \rangle$ can be obtained from the path integral for $\langle \boldsymbol{r}_f | e^{-\frac{i}{\hbar}\hat{H}t} | \boldsymbol{r}_0 \rangle$ by replacing $\frac{i}{\hbar}t$ by β. This is somewhat heuristic but the result is the same as obtained with a more careful approach. Recalling that

$$\langle \boldsymbol{r}_f | e^{-\frac{i}{\hbar}\hat{H}t} | \boldsymbol{r}_0 \rangle = \int D[\boldsymbol{r}] \exp\left[\frac{i}{\hbar}\int_0^t \left(\frac{1}{2}m\dot{\boldsymbol{r}}(t')^2 - U(\boldsymbol{r}(t'))\right) dt'\right]$$

we also have to make an analogous change for the integration variable t', replacing $\frac{i}{\hbar}t'$ by β' which runs from 0 to β. Then $\frac{i}{\hbar}dt'$ is replaced by β', simplifying the exponential. This leads to

$$\langle \boldsymbol{r}_f | e^{-\beta\hat{H}} | \boldsymbol{r}_0 \rangle = \int D[\boldsymbol{r}] \exp\left[\int_0^\beta \left(\frac{1}{2}m\left(\frac{i}{\hbar}\frac{d\boldsymbol{r}}{d\beta'}\right)^2 - U(\boldsymbol{r}(\beta'))\right) d\beta'\right]$$

where in the kinetic energy we had to replace the time derivative $\frac{d}{dt'}$ (indicated by the dot) by $\frac{i}{\hbar}\frac{d}{d\beta'}$. This result can be rewritten as

$$\langle \boldsymbol{r}_f | e^{-\beta\hat{H}} | \boldsymbol{r}_0 \rangle = \int D[\boldsymbol{r}] \exp\Bigg[-\int_0^\beta \underbrace{\left(\frac{1}{2}m\left(\frac{1}{\hbar}\frac{d\boldsymbol{r}}{d\beta'}\right)^2 + U(\boldsymbol{r}(\beta'))\right) d\beta'}_{=S_E[\boldsymbol{r}]}\Bigg].$$

Here we have used that due to the squared factor i the kinetic energy contributes with a negative sign. It can be combined with the potential which contributed with a negative sign anyway. The integrand is now (up to the scaling with $\hbar$) the energy, and its integral over the parameter β' taking the role of time is called the **Euclidian action**.

Extracting the ground state energy. A nice feature of $\langle \boldsymbol{r}_f | e^{-\beta \hat{H}} | \boldsymbol{r}_0 \rangle$ is that it allows to determine the energy of the ground state. Using the spectral decomposition of $e^{-\beta \hat{H}}$ in terms of energy levels E_j and energy eigenstates $|\psi_j\rangle$,

$$e^{-\beta \hat{H}} = \sum_j e^{-\beta E_j} |\psi_j\rangle\langle\psi_j|,$$

we can write

$$\langle \boldsymbol{r}_f | e^{-\beta \hat{H}} | \boldsymbol{r}_0 \rangle = \sum_j e^{-\beta E_j} \langle \boldsymbol{r}_f | \psi_j \rangle \langle \psi_j | \boldsymbol{r}_0 \rangle.$$

In the limit $\beta \to \infty$ all summands decrease exponentially but the summand corresponding to the ground state decreases most slowly as this state has the lowest energy. Denoting the ground state energy by E_0 we see that for $\beta \to \infty$, $\langle \boldsymbol{r}_f | e^{-\beta \hat{H}} | \boldsymbol{r}_0 \rangle$ is dominated by a term proportional to $e^{-\beta E_0}$.

We show for the **harmonic oscillator** how this can be used to determine E_0. The propagator for the harmonic oscillator is

$$\langle x_f | e^{-\frac{i}{\hbar}\hat{H}t} | x_0 \rangle = \sqrt{\frac{m\omega}{2\pi\hbar \sin \omega t}} \exp\left(\frac{i}{\hbar} \frac{m\omega}{2 \sin \omega t} ((x_0^2 + x_f^2) \cos \omega t - 2 x_0 x_f) - i\frac{\pi}{4} \right).$$

However we can work with the propagator for $x_0 = x_f = 0$,

$$\langle 0 | e^{-\frac{i}{\hbar}\hat{H}t} | 0 \rangle = \sqrt{\frac{m\omega}{2\pi\hbar \sin \omega t}} \exp\left(-i\frac{\pi}{4} \right).$$

Replacing $\frac{i}{\hbar}t$ by β gives

$$\begin{aligned}
\langle 0 | e^{-\beta \hat{H}} | 0 \rangle &= \sqrt{\frac{m\omega}{2\pi\hbar \sin\left(\omega \frac{\hbar}{i}\beta\right)}} \exp\left(-i\frac{\pi}{4} \right) \\
&\propto \left(\sin\left(\omega \frac{\hbar}{i} \beta \right) \right)^{-1/2} \\
&= \left(\frac{e^{i\omega\frac{\hbar}{i}\beta} - e^{-i\omega\frac{\hbar}{i}\beta}}{2i} \right)^{-1/2}
\end{aligned}$$

In the limit $\beta \to \infty$ the first term in the numerator dominates. In this limit the leading contribution is thus proportional to

$$(e^{\omega\hbar\beta})^{-1/2} = e^{-\beta\frac{1}{2}\hbar\omega}$$

which leads to a ground state energy of

$$E_0 = \frac{1}{2}\hbar\omega.$$

This is of course in line with the result from third-year Quantum Mechanics. In the next chapter we will come back to this way of computing ground state energies for the harmonic oscillator with a perturbation.