TTP2
Lecture 5

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5 Path integral in Quantum Mechanics

The standard formulation of Quantum Mechanics involves Hamilton operator H that, for a system with one degree of freedom, reads

$$H = \frac{p^2}{2m} + V(q). \tag{5.1}$$

The variables p and q are momentum and position operators that satisfy the following quantization condition

$$[p, q] = -i\hbar. \tag{5.2}$$

Together with the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}|\Psi\rangle = H|\Psi\rangle, \tag{5.3}$$

and the interpretation of the function $\Psi(q) = \langle q|\Psi\rangle$ as a probability amplitude, the above equations provide the foundation for quantum mechanics.

On the contrary, in classical mechanics, we usually start with the Lagrangian formalism where dynamics of a mechanical system follows from the minimum of an action

$$S = \int \mathrm{d}t L(q, \dot{q}, t). \tag{5.4}$$

The function $L(q, \dot{q}, t)$ is the Lagrange function with $\dot{q}$ being the velocity. One can also study classical mechanics using the Hamilton formalism but it is clearly not as prominent there as in Quantum Mechanics where it appears to be the only game in town. Hence, one may wonder if there is a place for the Lagrange formalism in Quantum Mechanics?

To answer this question, we consider a quantum mechanical system described by the Hamiltonian in Eq.(5.1). We assume that at a time $t = t_i$ the system is in a state with a definite coordinate $x = x_i$; we would like to find a probability amplitude that at $t = t_f$ the system is in a state with a definite coordinate $x = x_f$. These states are formally defined as eigenstates of the q-operator

$$q|x_{i,f}\rangle = x_{i,f}|x_{i,f}\rangle, \tag{5.5}$$

We compute the probability amplitude by solving the Schrödinger equation Eq.(5.3)

$$|\Psi(t)\rangle = e^{-iH(t-t_i)/\hbar}|\Psi(t_i)\rangle, \tag{5.6}$$

identifying $|\Psi(t_i)\rangle$ with $|x_i\rangle$ and projecting $|\Psi(t_f)\rangle$ on $|x_f\rangle$. The desired probability amplitude then reads

$$U(x_f, x_i; t_f, t_i) = \langle x_f | e^{-iH(t_f - t_i)/\hbar} | x_i \rangle. \tag{5.7}$$

Our goal is to rewrite the expression Eq.(5.7) in a particular way. To this end, we split the time interval $[t_f, t_i]$ into $N+1$ segments where eventually N will be considered to be large, $N \to \infty$. The length of a single segment is

$$\delta t = \frac{(t_f - t_i)}{N+1}. \tag{5.8}$$

We then write the time evolution operator as a product of $N+1$ time evolution operators, one for each segment

$$e^{-iH(t_f - t_i)/\hbar} = \underbrace{e^{-iH\delta t/\hbar} e^{-iH\delta t/\hbar} \ldots\ldots e^{-iH\delta t/\hbar}}_{N+1 \text{ times}}. \tag{5.9}$$

As the next step, we insert complete set of states at intermediate times. To do so, we use the completeness relation for eigenstates of the q-operator

$$1 = \int \mathrm{d}x_k |x_k\rangle \langle x_k|. \tag{5.10}$$

Eigenstates of the position operator are normalized as

$$\langle x | y \rangle = \delta(x - y). \tag{5.11}$$

We obtain

$$\begin{aligned} U(x_f, x_i; t_f, t_i) &= \langle x_f | e^{-iH\delta t/\hbar} e^{-iH\delta t/\hbar} \ldots\ldots e^{-iH\delta t/\hbar} | x_i \rangle \\ &= \int \prod_{k=1}^{N} \mathrm{d}x_k \langle x_f | e^{-iH\delta t/\hbar} | x_N \rangle \langle x_N | e^{-iH\delta t/\hbar} | x_{N-1} \rangle \ldots\ldots \langle x_1 | e^{-iH\delta t/\hbar} | x_i \rangle. \end{aligned} \tag{5.12}$$

We see that the primary object to explore is the matrix element

$$\langle x_a | e^{-iH\delta t/\hbar} | x_b \rangle, \tag{5.13}$$

with δt being arbitrary small because of the $N \to \infty$ limit. Since δt is small, we replace the exponential with its expansion through first order in δt. We write

$$e^{-iH\delta t/\hbar} \approx 1 - i\frac{H\delta t}{\hbar}. \tag{5.14}$$

Since

$$\langle x_a|1|x_b\rangle = \delta(x_a - x_b), \quad \langle x_a|V(q)|x_b\rangle = V((x_a + x_b)/2)\delta(x_a - x_b), \quad (5.15)$$

the only non-trivial matrix element is $\langle x_a|p^2/(2m)|x_b\rangle$. To compute it, we make use of the complete set of momentum eigenstates and write

$$\begin{aligned}\langle x_a|\frac{p^2}{2m}|x_b\rangle &= \int \frac{\mathrm{d}p_a}{2\pi\hbar}\frac{\mathrm{d}p_b}{2\pi\hbar}\langle x_a|p_a\rangle\langle p_a|\frac{p^2}{2m}|p_b\rangle\langle p_b|x_b\rangle \\ &= \int \frac{\mathrm{d}p_a}{2\pi\hbar}\frac{\mathrm{d}p_b}{2\pi\hbar}\langle x_a|p_a\rangle\frac{p_a^2}{2m}2\pi\hbar\delta(p_a - p_b)\langle p_b|x_b\rangle = \int \frac{\mathrm{d}p_a}{2\pi\hbar}\,\frac{p_a^2}{2m}e^{ip_a(x_a-x_b)/\hbar},\end{aligned} \quad (5.16)$$

In deriving this result, we have used

$$1 = \int \frac{\mathrm{d}p_a}{2\pi\hbar}|p_a\rangle\langle p_a|, \quad \langle p_a|p_b\rangle = 2\pi\hbar\delta(p_a - p_b), \quad \langle x_a|p_a\rangle = e^{ip_a x_a/\hbar}, \quad (5.17)$$

and $\langle p_a|x_a\rangle = \langle x_a|p_a\rangle^*$. We will further use

$$\delta(x_a - x_b) = \int \frac{\mathrm{d}p_a}{2\pi\hbar}e^{ip_a(x_a-x_b)/\hbar}, \quad (5.18)$$

to write the matrix element of e.g. the potential energy $V(q)$ and of the kinetic energy in a similar way.

We exponentiate back the matrix elements of $H\delta t/\hbar$ operator and write

$$\langle x_a|e^{-iH\delta t/\hbar}|x_b\rangle = \int \frac{\mathrm{d}p_a}{2\pi\hbar}e^{ip_a(x_a-x_b)/\hbar - \frac{i\delta t}{\hbar}\left(\frac{p_a^2}{2m}+V((x_a+x_b)/2)\right)}. \quad (5.19)$$

We now put this result back into a formula for the time evolution operator $U(x_f, x_i; t_f, t_i)$, Eq.(5.12). We find

$$\begin{aligned}U(x_f, x_i; t_f, t_i) &= \int \prod_{k=1}^{N}\mathrm{d}x_k \prod_{k=1}^{N+1}\frac{\mathrm{d}p_k}{2\pi\hbar}\;\prod_{k=1}^{N+1}\left[e^{\frac{ip_k(x_k-x_{k-1})}{\hbar}}e^{-\frac{i\delta t}{\hbar}\left(\frac{p_k^2}{2m}+V((x_k+x_{k-1})/2)\right)}\right] \\ &= \int \prod_{k=1}^{N}\mathrm{d}x_k \prod_{k=1}^{N+1}\frac{\mathrm{d}p_k}{2\pi\hbar}\;\; e^{\sum_{k=1}^{N+1}\left[\frac{ip_k(x_k-x_{k-1})}{\hbar} - \frac{i\delta t}{\hbar}\left(\frac{p_k^2}{2m}+V((x_k+x_{k-1})/2)\right)\right]},\end{aligned} \quad (5.20)$$

where we identified x_0 with x_i and x_{N+1} with x_f.

All integrals over momenta p_k in Eq.(5.20) are Gaussian and it is straightforward to compute them. We find

$$\int \frac{\mathrm{d}p_k}{2\pi\hbar} e^{\frac{ip_k\xi_k}{\hbar} - \frac{i\delta t}{\hbar}\frac{p_k^2}{2m}} = \sqrt{\frac{mi}{2\pi\delta t\hbar}}\; e^{i\frac{m\xi_k^2}{2\delta t\hbar}}, \tag{5.21}$$

where $\xi_k = x_k - x_{k-1}$. We use this result in a formula for U, Eq.(5.20), and arrive at

$$U(x_f, x_i; t_f, t_i) = \left[\frac{mi}{2\pi\delta t\hbar}\right]^{\frac{N+1}{2}} \int \prod_{k=1}^{N} \mathrm{d}x_k\; e^{i\hat{\mathcal{O}}}, \tag{5.22}$$

where

$$\begin{aligned}
\mathcal{O} &= \sum_{k=1}^{N+1}\left[\frac{im(x_k - x_{k-1})^2}{2\delta t\hbar} - \frac{i\delta t}{\hbar}V\left(\frac{x_k + x_{k-1}}{2}\right)\right] \\
&= \frac{i}{\hbar}\sum_{k=1}^{N+1}\delta t\left[\frac{m}{2}\left(\frac{x_k - x_{k-1}}{\delta t}\right)^2 - V\left(\frac{x_k + x_{k-1}}{2}\right)\right] \\
&= \frac{i}{\hbar}\int_{t_i}^{t_f} \mathrm{d}\tau L(x(\tau), \dot{x}(\tau)).
\end{aligned} \tag{5.23}$$

We note that in the last step we replaced the sum over k with an integral over time τ and recognized that the summand in next-to-last equation is the Lagrange function. The integral over τ is supposed to be taken over trajectories that start at $x = x_i$ at $t = t_i$, end at $x = x_f$ at $t = t_f$ and go through points $x_1, x_2, ..., x_N$ at $\tau = t_i + \delta t, t_i + 2\delta t$, etc. Hence,

$$\begin{aligned}
U(x_f, x_i, t_f, t_i) &= \left[\frac{mi}{2\pi\delta t\hbar}\right]^{\frac{N+1}{2}} \int \prod_{k=1}^{N} \mathrm{d}x_k\; e^{\frac{i}{\hbar}\int_{t_i}^{t_f} \mathrm{d}\tau L(\dot{x}(\tau), x(\tau))} \\
&= \left[\frac{mi}{2\pi\delta t\hbar}\right]^{\frac{N+1}{2}} \int \prod_{k=1}^{N} \mathrm{d}x_k\; e^{\frac{i}{\hbar}S[t_f, t_i, x(\tau)]},
\end{aligned} \tag{5.24}$$

where in the last step we replaced the integral of the Lagrange function by the action S. Note that the integration over x_k implies that we obtain the time evolution operator in quantum mechanics by adding contributions of all possible trajectories with fixed initial and final points with weights proportional to the *complex exponential* of the *classical* action.

We now formally take the limit $N \to \infty$, write the integration measure and a prefactor as

$$\lim_{N\to\infty}\left[\frac{mi}{2\pi\delta t\hbar}\right]^{\frac{N+1}{2}}\prod_{k=1}^{N}\mathrm{d}x_k = [\mathcal{D}x(t)], \tag{5.25}$$

and obtain the final expression for the time evolution operator in quantum mechanics

$$U(x_f, x_i, t_f, t_i) = \int [\mathcal{D}x(t)]\ e^{\frac{i}{\hbar}S[t_f,t_i,x(\tau)]}|_{x(t_f)=x_f, x(t_i)=x_i}. \tag{5.26}$$

Eq.(5.26) provides the "path integral representation" of the time-evolution operator in quantum mechanics. We call this object path integral or an integral over paths because we have to integrate over *all* trajectories that connect points $x = x_f$ and $x = x_i$ but are, otherwise, arbitrary. We note that Eq.(5.26) does what we wanted to accomplish since it provides us with the formulation of quantum mechanics where Lagrange functions and classical actions play a prominent role. Note also that in contrast to classical mechanics, where "true" trajectories follow from the action minima $\delta S = 0$, i.e. the *least action principle*, in quantum mechanics the time evolution is determined by *all* directories each with the weight $e^{\frac{i}{\hbar}S}$.

This result Eq.(5.26) also explains why classical trajectories are special. Indeed, classical mechanics corresponds to the $\hbar \to 0$ limit; in that case $S/\hbar \to \infty$ and the integrand in Eq.(5.26) oscillates very rapidly and averages to zero. The largest contributions to the integral come from trajectories where the phase is *stationary* (methods of steepest descent etc. in complex analysis). Such trajectories are exactly the ones that minimize the action S, i.e. from trajectories that lead to $\delta S = 0$.

Often, we need to know a transition amplitude from the state $|i\rangle$ to the state $|f\rangle$ which are different from eigenstates of the position operator. Then we write

$$\begin{aligned}\langle f|e^{-iH(t_f-t_i)/\hbar}|i\rangle &= \int \mathrm{d}x_f\mathrm{d}x_i\langle f|x_f\rangle\langle x_i|i\rangle\langle x_f|e^{\frac{-iH(t_f-t_i)}{\hbar}}|x_i\rangle \\ &= \int \mathrm{d}x_f\mathrm{d}x_i\Psi_f^*(x_f)\Psi_i(x_i)U(x_f, x_i; t_f, t_i). \\ &= \int \mathrm{d}x_f\mathrm{d}x_i\Psi_f^*(x_f)\Psi_i(x_i)\int[\mathcal{D}x(t)]\ e^{\frac{i}{\hbar}S[t_f,t_i,x(\tau)]}|_{x(t_f)=x_f,x(t_i)=x_i}.\end{aligned} \tag{5.27}$$

We can also write the last formula as

$$\langle f|e^{-iH(t_f-t_i)/\hbar}|i\rangle = \int [\mathcal{D}x(t)]\ \Psi_f^*(x_f)\Psi_i(x_i)\ e^{\frac{i}{\hbar}S[t_f,t_i,x(\tau)]}, \tag{5.28}$$

where now the integration over initial and final points of the path is also included in the measure.

The two wave functions $\Psi_f(x_f)$ and $\Psi_i(x_i)$ are somewhat annoying although they are needed if we are interested in the matrix element of the time evolution operator. However, as we move to quantum field theory we will be interested in a transition from the ground state of the theory to the ground state of the theory that occurs over infinitely long time, i.e. $|i\rangle \to |0\rangle$, $|f\rangle \to |0\rangle$, $t_i \to -\infty$ and $t_f \to +\infty$, as well as the Green's functions. As we will now show, it is possible to omit the wave functions in Eq. (5.28) in such a case. Indeed, we can write

$$\langle x_f|e^{-iH(t_f-t_i)/\hbar}|x_i\rangle = \langle x_f|e^{-iHt_f}\ e^{iHt_i/\hbar}|x_i\rangle = \langle x_f, t_f|x_i, t_i\rangle, \tag{5.29}$$

where

$$|x_i, t_i\rangle = e^{iHt_i/\hbar}|x_i\rangle, \quad \langle x_f, t_f| = \langle x_f|e^{-iHt_f/\hbar}. \tag{5.30}$$

We insert full set of states of the Hamiltonian H

$$|x_i, t_i\rangle = e^{iHt_i/\hbar}|x_i\rangle = \sum e^{iHt_i/\hbar}|n\rangle\langle n|x_i\rangle = \sum e^{iE_nt_i/\hbar}\Psi_n^*(x_i). \tag{5.31}$$

We will assume that the energy of the ground state is zero and energies of all other states are positive.

We now consider a special limit of this formula, i.e. we take $t_i \to -T(1-i\epsilon)$, $T \to \infty$, and $\epsilon > 0$ and small. We find

$$\lim_{T\to\infty}|x_i, t_i\rangle = \Psi_0^*(x_i)e^{-iHT(1-i\epsilon)/\hbar}|0\rangle, \tag{5.32}$$

and with $t_f = T(1-i\epsilon)$

$$\lim_{T\to\infty}\langle x_f, t_f| = \langle 0|e^{-iHT(1-i\epsilon)/\hbar}\Psi_0(x_f). \tag{5.33}$$

Then,

$$\begin{aligned}\lim_{T\to\infty}\langle x_f|e^{-iH(t_f-t_i)/\hbar}|x_i\rangle &= \lim_{T\to\infty} U(x_f, x_i, t_f, t_i) \\ &= \Psi_0(x_f)\Psi_0^*(x_i)\langle 0|e^{-iH(t_f-t_i)/\hbar}|0\rangle,\end{aligned} \tag{5.34}$$

where $t_f = T(1-i\epsilon)$ and $t_i = -T(1-i\epsilon)$.

The time evolution operator $U(x_f, x_i, t_f, t_i)$ is computed through an integral over paths that start at $x = x_i$ and end at $x = x_f$. Suppose we integrate over x_f, x_i also considering limits as shown in the above equation. Then

$$N\langle 0|0\rangle = \lim_{t_{f,i}\to\pm T(1-i\epsilon)} \int [\mathcal{D}x(t)]\ e^{\frac{i}{\hbar}S[t_f,t_i,x(\tau)]}, \tag{5.35}$$

where

$$N = \left|\int \mathrm{d}x \Psi_0(x)\right|^2 \tag{5.36}$$

Absorbing the normalization factor N into the measure and omitting $i\epsilon$, we finally write

$$\lim_{t_{f,i}\to\pm\infty} \langle 0|e^{-iH(t_f-t_i)/\hbar}|0\rangle = \lim_{t_{f,i}\to\pm\infty} \int [\mathcal{D}x(t)]\ e^{\frac{i}{\hbar}S[t_f,t_i,x(\tau)]}. \tag{5.37}$$

Since vacuum states on the l.h.s. of this equation are eigenstates of the Hamiltonian H, the above equation is not very interesting since it tells us that the path integral on the r.h.s., with all normalizations included, should evaluate to 1. However, this form is important since it allows us to study Green's functions.

To see this, let us generalize the previous discussion to the following matrix element

$$\langle x_f, t_f|q(t_1)|x_i, t_i\rangle. \tag{5.38}$$

Here $q(t_1)$ is the position operator in Heisenberg representation; it is given by

$$q(t_1) = e^{iHt_1/\hbar} q e^{-iHt_1/\hbar}. \tag{5.39}$$

We use this respresentation in Eq.(5.38), insert a completeness relation in two strategic places and find

$$\begin{aligned} &\langle x_f, t_f|q(t_1)|x_i, t_i\rangle = \langle x_f|e^{-iH(t_f-t_1)/\hbar} q e^{-iH(t_1-t_i)/\hbar}|x_i\rangle \\ &\int \mathrm{d}x_1\ x_1 \langle x_f|e^{-iH(t_f-t_1)/\hbar}|x_1\rangle\langle x_1 e^{-iH(t_1-t_i)/\hbar}|x_i\rangle \end{aligned} \tag{5.40}$$

It is easy to realize now that the product of two matrix elements of the time evolution operators can be written as a path integral with additional factor in the integrand i.e.

$$\langle x_f, t_f|q(t_1)|x_i, t_i\rangle = \int [\mathcal{D}x(t)]\ x(t_1)\ e^{iS/\hbar}|_{x(t_f)=x_f, x(t_i)=x_i}. \tag{5.41}$$

To generalize this further, we can consider an integral

$$\int [\mathcal{D}x(t)]\ x(t_1)\ x(t_2)\ e^{iS/\hbar}|_{x(t_f)=x_f, x(t_i)=x_i}. \tag{5.42}$$

To write this in the form of a matrix element of time-dependent position operators, we need to know what time is larger t_1 or t_2.[1] To keep all the options open, we introduce the time-ordering operator T and write

$$T q(t_1) q(t_2) = \theta(t_1 - t_2)\ q(t_1) q(t_2) + \theta(t_2 - t_1)\ q(t_2) q(t_1). \tag{5.43}$$

Then, it is straightforward to see following the discussion of the matrix element in Eq.(5.38) that

$$\langle x_f, t_f | T q(t_1) q(t_2) | x_i, t_i \rangle = \int [\mathcal{D}x(t)]\ x(t_1)\ x(t_2)\ e^{iS/\hbar}|_{x(t_f)=x_f, x(t_i)=x_i}. \tag{5.44}$$

It is now clear that we can generalize the above formula to the Green's function with arbitrary number of q-insertions. We find

$$\langle 0 | T q(t_1) .... q(t_n) | 0 \rangle = \int [\mathcal{D}x]\ x(t_1)\ x(t_2) .... x(t_n)\ e^{iS/\hbar}. \tag{5.45}$$

There is another interesting way to write a representation for *all* such Green's functions. Consider the following functional

$$Z[j] = \langle 0|0 \rangle_j = \int [\mathcal{D}x]\ e^{i(S + \int \mathrm{d}\tau\, j(\tau) x(\tau))/\hbar}, \tag{5.46}$$

defined for an arbitrary function $j(t)$. Physically, it is introduced to study the response of the system that we want to study to an external force $j(t)$ in the linear approximation. Apart from physics, $Z[j]$ provides us with a tool to compute all the correlation functions. Indeed, taking the functional derivative of $Z[j]$ w.r.t. $j(t_1)$, we obtain

$$\frac{\hbar \delta Z[j]}{i \delta j(t_1)} = \int [\mathcal{D}x]\ x(t_1)\ e^{i(S + \int \mathrm{d}\tau j(\tau) x(\tau))/\hbar}. \tag{5.47}$$

Taking this derivative n times, we find

$$\begin{aligned} \frac{\hbar^n \delta^n Z[j]}{i\delta j(t_1) i\delta j(t_2) ... i\delta j(t_n)} &= \int [\mathcal{D}x]\ x(t_1)\ x(t_2) .... x(t_n)\ e^{iS/\hbar} \\ &= \langle 0 | T q(t_1) .... q(t_n) | 0 \rangle. \end{aligned} \tag{5.48}$$

Hence, $Z[j]$ is a *generating functional* for the Green's functions of the theory.

[1] The order of operators is important since $q(t_1)$ and $q(t_2)$ do not commute in general.