Path integral formulation. Evolution operator in real space for harmonic oscillator

Let us have another look at the dynamic solution for an arbitrary quantum state written as
\[ \chi(x, t) = \sum_n \langle \psi_n | \chi(t = 0) \rangle e^{-itE_n} \psi_n(x), \]
in terms of the energy eigenbasis. We can rewrite it identically as
\[ \chi(x, t) = \int dx' U(x, t; x', t = 0) \chi(x', t = 0), \quad U(x, t; x', t = 0) = \sum_n e^{-itE_n} \psi_n(x) \psi_n^*(x'), \]
where all information about a particular quantum system is encoded in the \( U \)-function. If the first expression forces you to do the calculation for every state \( \chi \) from scratch by doing all integrals \( \langle \psi_n | \chi(t = 0) \rangle \) and then a sum over states, the second formulation allows you do the sum for a given system only once and then use \( U \)-function to get the final result by doing only one integral.

[This method is known in math. as the Green’s-function method.] There are many alternative ways to get the \( U \)-function; the most obvious one is to do the sum over the basis as in the second equation, e.g. for the harmonic oscillator one has to evaluate
\[ U(x, t; x', t = 0) = \sum_{n=0}^{\infty} e^{-it\omega(n+1/2)} N_n^2 e^{-[(x')^2 + x^2]m\omega/2} H_n(\sqrt{m\omega}x') H_n(\sqrt{m\omega}x), \]
This is doable with some effort. One may also solve an appropriately formulated differential equation for \( U \). Here I will discuss yet another method invented by Feynman—the path integral formulation of quantum mechanics.

Path integrals offer a remarkable new way to look at things in quantum mechanical systems making the most intuitive link between the classical and quantum behavior. They do not resemble Schrödinger Equation at all, but ultimately lead to exactly the same final results. One starts from the most basic expression for time evolution
\[ \chi(t) = e^{-i\hat{H}t} \chi(t = 0), \]
and writes it in the real-space representation as (all integrals and variables are \( D \)-dimensional)
\[ \chi(x, t) = \langle x | \chi(t) \rangle = \int dx' \langle x | e^{-i\hat{H}t} | x' \rangle \langle x' | \chi(t = 0) \rangle = \int dx' \langle x | e^{-i\hat{H}t} | x' \rangle \chi(x', t = 0), \]
leading to
\[ U(x, t; x', t = 0) = \langle x | e^{-i\hat{H}t} | x' \rangle. \]
Next, we slice the time interval \( (0, t) \) into large number \( N \rightarrow \infty \) of very short intervals of duration \( d\tau = t/N \rightarrow 0 \) and write identically
\[ \langle x | e^{-i\hat{H}t} | x' \rangle = \langle x | \prod_{j=1}^{N} e^{-i\hat{H}d\tau} | x' \rangle = \langle x | e^{-i\hat{H}_d\tau} e^{-i\hat{H}_d\tau} \ldots e^{-i\hat{H}_d\tau} | x' \rangle = \]
\[ \int dx_{N-1} \ldots \int dx_2 \cdot \cdot \cdot \int dx_1 \langle x | e^{-i\hat{H}_d\tau} | x_{N-1} \rangle \langle x_{N-1} | e^{-i\hat{H}_d\tau} | x_{N-2} \rangle \ldots \langle x_2 | e^{-i\hat{H}_d\tau} | x_1 \rangle \langle x_1 | e^{-i\hat{H}_d\tau} | x' \rangle, \]
where in the last expression we used completeness relation to express the calculation of matrix elements over an arbitrary time \( t \) in terms of short time evolution only. The advantage of doing so is obvious: in the limit of \( d\tau \to 0 \) we can write approximately
\[
e^{-i\hat{H}d\tau} \approx e^{-i\hat{V}d\tau} e^{-i\hat{K}d\tau},
\]
where \( \hat{V} = V(x) \) is the potential energy operator, and \( \hat{K} = p^2/2m \) is the kinetic energy operator. Corrections to the approximate relation above are proportional to \( d\tau^2 \) and can be neglected in the considered limit. It also makes sense to introduce notation \( x' \equiv x_0 \), and \( x = x_N \) to label all space points with one ordered index.

After we split each exponential into two, we face the following expression (real-space representation is an eigenbasis of the potential energy operator)
\[
\int dx_{N-1} \cdots \int dx_{1} \prod_{j=N}^{1} e^{-iV(x_j)d\tau} \langle x_{j}|e^{-i\hat{K}d\tau}|x_{j-1}\rangle.
\]  

(1)

The only matrix elements left to calculate refer to the particle propagation in free space, i.e. no potential, which are obviously easy to deal with (using now completeness relation in momentum space)
\[
\langle y|e^{-i\hat{K}d\tau}|x\rangle = \int \frac{dp}{(2\pi)^D} \langle y|p\rangle e^{-i(p^2/2m)d\tau} \langle p|x\rangle = \int \frac{dp}{(2\pi)^D} e^{-i(p^2/2m)d\tau + ip(y-x)}.
\]

By evaluating the Gaussian integral we get for the propagation in free space
\[
\langle y|e^{-i\hat{K}d\tau}|x\rangle = (\frac{m}{2\pi id\tau})^{D/2} e^{i(y-x)^2m/2d\tau}.
\]

Substituting this expression back to Eq. (1) we get
\[
U(x_N, t; x_0, t = 0) = (\frac{m}{2\pi id\tau})^{D/2} \int dx_{N-1} \cdots \int dx_{1} \prod_{j=N}^{1} e^{-iV(x_j)d\tau + i(x_j-x_{j-1})^2m/2d\tau}.
\]  

(2)

To complete the calculation we take the limit of \( d\tau \to 0 \). At this point we introduce the notion of a ‘trajectory’
\[x_N, x_{N-1}, \ldots, x_j, \ldots, x_0 \equiv x(t = Nd\tau), x((N - 1)d\tau), \ldots, x(jd\tau), \ldots, x(0) \equiv [x(\tau)],\]
to describe the sequence of coordinates starting from \( x_0 \) and followed by \( x_1 \), etc. all the way to \( x_N \).

By the same token, the combination \( [x_j-x_{j-1}]/d\tau = [x(jd\tau) - x((j-1)d\tau)]/d\tau = dx(\tau)/d\tau \equiv \dot{x}(\tau) \) will be called particle velocity along the trajectory. Then
\[
\prod_{j=N}^{1} e^{-iV(x_j)d\tau + i(x_j-x_{j-1})^2m/2d\tau} = \exp \left\{ i \sum_{j=1}^{N} d\tau \left[ m\dot{x}^2(\tau)/2 - V(x(\tau)) \right] \right\} = \exp \left\{ i \int_{0}^{t} d\tau \left[ m\dot{x}^2(\tau)/2 - V(x(\tau)) \right] \right\}
\]  

(3)
With standard simplified notation for the set of integrals over all possible particle trajectories between points \( x_0 = x' \) and \( x_N = x \) (this is where the path-integral name comes from)

\[
\int_{x(0)=x'}^{x(t)=x} \mathcal{D}x \cdots = \left( \frac{m}{2\pi id\tau} \right)^{DN/2} \int dx_{N-1} \cdots \int dx_1 \cdots
\]

we finally arrive at Feynman’s formulation of quantum mechanics

\[
U(x, t; x', t = 0) = \int_{x(0)=x'}^{x(t)=x} \mathcal{D}x \, e^{iS},
\]

where \( S \) is the classical action

\[
S[x(\tau)] = \int_0^t d\tau \mathcal{L}[x(\tau), \dot{x}(\tau)] = \int_0^t d\tau \left[ m\dot{x}^2(\tau)/2 - V(x(\tau)) \right],
\]

related to the classical Lagrangian in the usual way!

This expression is straightforwardly generalized to many-body systems (with only one extra point to care - for identical particles the sets of coordinates at the initial and final times can be connected in a number of ways and all of them have to be accounted for in the path-integral). This is illustrated for the two particle example in the figure; the sign rule distinguishes between bosons and fermions.

Remarkably, we have our classical picture of particles moving along classical trajectories with well defined coordinates and trajectories back! Not quite so. There is no principle of minimal action attached to this calculation and you see that individually ANY trajectory is as good as any other because they all contribute with exactly the same amplitude, only phases are different. It means that individual trajectories barely make any sense. However, packs of trajectories with large and dissimilar phases cancel individual contributions very efficiently while packs with nearly identical phases contribute in ‘unison’. Thus if typical phases accumulated along trajectories are large, one has to look for trajectories which minimize action; in this case all nearby trajectories have nearly identical phases and their combined contribution to the answer is dominating. This is how classical equations of motion emerge in Feynman’s picture.

Before I complete this calculation for the harmonic oscillator let me also mention one connection to statistical mechanics. The main quantity of interest is the partition function

\[
Z = \sum_n e^{-\beta E_n}.
\]
We write it identically as

\[
Z = \sum_n \langle n | e^{-\beta \hat{H}} | n \rangle \equiv \sum_n \langle n | x \rangle \int dx \int dx' \langle x | e^{-\beta \hat{H}} | x' \rangle \langle x' | n \rangle \equiv \\
\int dx \int dx' \langle x' | x \rangle \langle x | e^{-\beta \hat{H}} | x' \rangle = \int dx \langle x | e^{-\beta \hat{H}} | x \rangle ,
\]

which is nothing but the trace of the matrix (same in any representation). Up to change of notations \( \beta = it \) we have to deal with the same expression as in dynamic evolution, but now in 'imaginary time' \( t = -i\beta \). With this we arrive at

\[
Z = \oint_{x(0)=x(\beta)} Dx \exp \left\{ - \int_0^\beta d\tau \left[ m\dot{x}^2(\tau)/2 + V(x(\tau)) \right] \right\} . \tag{7}
\]

This expression is extremely well suited for Monte Carlo simulations of bosonic systems, and is also a powerful theoretical tool to deal with quantum statistics questions.

Now back to harmonic oscillator. In this case the Lagrangian is quadratic in \( x(t) \) and all integrals are of the Gaussian form. This property leads to the exact procedure (ignoring pre-exponential factors for a while):

- Solve for the optimal classical trajectory subject to boundary conditions \( x(t=0) = x' \), \( x(t) = x \)
  which is the same calculation as in classical mechanics based on the minimal action principle

\[
\rightarrow \ddot{x} + \omega^2 x = 0 \quad \rightarrow \quad x(\tau) = x' \cos(\omega \tau) + \frac{x - x' \cos(\omega t)}{\sin(\omega t)} \sin(\omega \tau) .
\]

- Substitute this solution to the action \( S = \int_0^t d\tau \left[ m\dot{x}^2(\tau)/2 - m\omega^2 x^2(\tau)/2 \right] \) to get

\[
S = \frac{m\omega^2}{2} \int_0^t d\tau \left[ - x' \sin(\omega \tau) + \frac{x - x' \cos(\omega t)}{\sin(\omega t)} \cos(\omega \tau) \right]^2 - \left[ x' \cos(\omega \tau) + \frac{x - x' \cos(\omega t)}{\sin(\omega t)} \sin(\omega \tau) \right]^2 = \\
\]

\[
\frac{m\omega^2}{2} \int_0^t d\tau \left[ - (x')^2 + \left( \frac{x - x' \cos(\omega t)}{\sin(\omega t)} \right)^2 \right] \cos(2\omega \tau) - 2x' \frac{x - x' \cos(\omega t)}{\sin(\omega t)} \sin(2\omega \tau) \right] =
\]

integrate and re-arrange terms

\[
\frac{m\omega}{2} \left\{ - (x')^2 + \left( \frac{x - x' \cos(\omega t)}{\sin(\omega t)} \right)^2 \right\} \sin(\omega t) \cos(\omega t) - 2x' \frac{x - x' \cos(\omega t)}{\sin(\omega t)} \sin^2(\omega t) \right] =
\]

\[
S = \frac{m\omega}{2 \sin(\omega t)} \left\{ \cos(\omega t) \left[ x^2 + (x')^2 \right] - 2xx' \right\} .
\]

With this result we obtain

\[
U(x, t; x', t = 0) = f(t) e^{iS} ,
\]

where the pre-exponential factor can be determined as follows: Use identity

\[
\langle x | e^{-it\hat{H}} | x' \rangle = \int dy \langle x | e^{-i\hat{H}/2} | y \rangle \langle y | e^{-i\hat{H}/2} | x' \rangle ,
\]
to obtain a relation (the integral over $y$ is Gaussian)

$$f(t)e^{iS(x,x',t)} = f^2(t/2) \int_{-\infty}^{\infty} dy \, e^{i[S(x,y,t/2)+S(y,x',t/2)]} = f^2(t/2) \sqrt{\frac{i\pi \sin(\omega t/2)}{m\omega \cos(\omega t/2)}} e^{iS(x,x',t)} ,$$

with the solution (check by substituting)

$$f(t) = \sqrt{\frac{m\omega}{2\pi i \sin(\omega t)}} .$$

The final result reads

$$U(x,t;x',t=0) = \sqrt{\frac{m\omega}{2\pi i \sin(\omega t)}} \exp \left\{ i \frac{m\omega}{2 \sin(\omega t)} \left( \cos(\omega t) \left[ x^2 + (x')^2 \right] - 2xx' \right) \right\} . \quad (8)$$

With this we may solve any dynamics (and thermodynamics for $t = -i\beta$) problem in harmonic oscillator.

**Problem 29. Path-integrals**

As an example of how this can be used consider a particle which at time $t=0$ has the form

$$\chi(x,t=0) = \frac{1}{(2\pi \sigma^2)^{1/4}} e^{-(x-x_0)^2/4\sigma^2} .$$

Determine $|\chi(x,t)|$ (skip the phase factor) by taking the required Gaussian integrals. The answer will look awful unless you employ good intermediate notations. To check for mistakes compare to (you do the normalization)

$$|\chi(x,t)| \propto e^{-[x-x_0 \cos(\omega t)]^2/4\sigma(t)^2} , \quad |\sigma(t)|^2 = \sigma^2 \cos^2(\omega t) + \frac{1}{4m^2 \omega^2 \sigma^2} \sin^2(\omega t) .$$

What is the value of $\langle x \rangle$ as a function of time?

The outlined procedure is exact for the harmonic oscillator because when trajectories are parameterized as

$$x(\tau) = x_{opt}(\tau) + \delta(\tau) , \quad \text{with} \; \delta(0) = \delta(t) = 0 ,$$

the action splits into two independent terms

$$S = S_{opt}(x,t;x') + \int_0^t d\tau \left[ \frac{m\delta^2(\tau)}{2} - m\omega^2 \delta^2(\tau)/2 \right] .$$

Terms linear in $\delta(\tau)$ are identically zero by construction of the optimal trajectory: $\delta(\tau)$ is multiplied by $\ddot{x}_{opt} + \omega^2 x_{opt}$ which is zero. Thus,

$$U(x,t;x',t=0) = e^{iS_{opt}(x,t;x')} \oint_{\delta(0)=\delta(t)=0} D\delta \, e^{iS[\delta(\tau)]} \equiv f(t) \, e^{iS_{opt}(x,t;x')} ,$$

i.e. all meaningful dependence on $x$ and $x'$ is contained in $S_{opt}(x,t;x')$ while the rest of the path integral accounting for fluctuations can only be a function of time since it is independent of $x$ and $x'$. 

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