Path integrals

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In the study of quantum mechanical many-body systems it is not so useful to write down the Schrödinger equation of $N \sim 10^{23}$ particles and attempt to solve it. Even if we somehow managed to obtain such a solution, the amount of detail in $\psi(\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots \boldsymbol{x}_N)$ would too much information to make sense of.

A successful approach to quantum mechanical many-body physics is the approach through second quantization. However, this technique, although very useful, can be at times quite clumsy to work with. It is useful to have a different mathematical tool to deal with the same problem. The mathematical tool that is discussed here is the path integral approach. This technique is intimately related to the second-quantization approach and in particular both ways of describing a physical many-body system are equivalent. This means that anything that can be achieved by second quantization must also be achievable by the path integral method and the other way around. Sometimes, however, it is much easier to work out a problem one way than the other. So it is useful to know both techniques.

Before we discuss the many-body problem, we go back to the single-particle problem. The path integral is most easily understood in this setting. The path integral is closely connected to the concept of *action* from classical mechanics. We therefore begin with a review of this concept.

Review of the action concept

Consider a classical particle of mass m that lives in one dimension and is subject to a potential $V(x)$. We can describe this problem by means of a Lagrangian, which is the kinetic minus the potential energy,

$$L(x, \dot{x}) = \frac{m}{2}\dot{x}^2 - V(x).$$

A striking and beautiful result is that the particle always moves such that it minimizes the *classical action*. Let us imagine that the particle starts at position x_i at time t_i and is at position x_f at a later time t_f. The action is a number that we obtain by integrating the Lagrangian between the start and end times for the actual curve $x(t)$

$$S = \int_{t_i}^{t_f} dt\ L(x, \dot{x}).$$

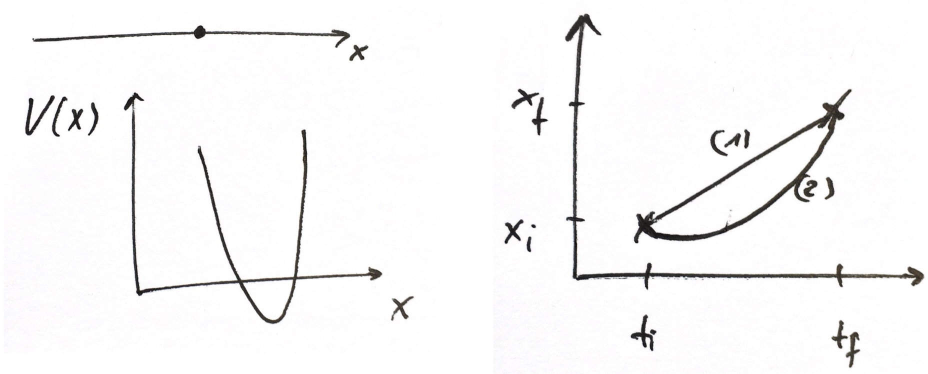

Figure 1: Left: Particle moving in 1 dimension inside a potential $V(x)$ Right: paths connecting start and end points

Actually, we could plug in any curve $x(t)$ into the Lagrangian and evaluate the action. The principle of least action states that this value will be least (actually only extremal) when the true path of the particle is chosen. We can use the calculus of variations to find the curve $x(t)$ that makes the action stationary. The result is of course the equation of motion of the particle

$$\frac{\partial L(x,\dot{x})}{\partial x} - \frac{d}{dt}\frac{\partial L(x,\dot{x})}{\partial \dot{x}} = 0,$$

which tells us how the particle actually moves from x_i to x_f in the given time.

The sum over all paths

Let us now look at the same setting in the quantum context. The Hamiltonian is

$$H = \frac{P^2}{2m} + V(X),$$

where P and X are now operators and the physics of the particle is governed by the Schrödinger equation

$$H|\psi\rangle = i\hbar\frac{\partial}{\partial t}|\psi\rangle.$$

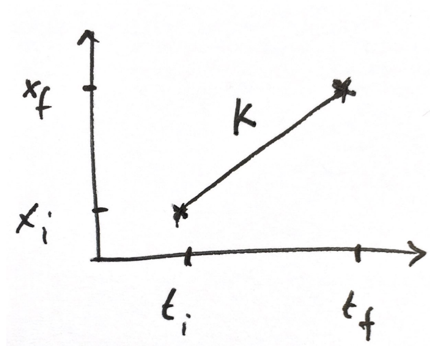

Figure 2: Spacetime diagram of the propagator

A particle that is localized at position x_i is described quantum mechanically by the ket $|\psi\rangle = |x_i\rangle$. We can ask what is the probability amplitude to find it in the state $|x_f\rangle$ at a time $t_f - t_i$ later. We get the answer by time-evolving the state $|x_i\rangle$ and computing the overlap with $|x_f\rangle$. The answer is the probability amplitude

$$K(x_f, t_f; x_i, t_i) = \langle x_f | e^{-\frac{i}{\hbar} H \cdot (t_f - t_i)} | x_i \rangle,$$

where the object K is called the *propagator* sometimes, since it propagates a wave function $\psi(x, t_i)$ at time t_i to a wave function at time t_f:

$$\int dx' \; K(x, t_f; x', t_i) \psi(x', t_i) = \psi(x, t_f)$$

Of course, this is not a big surprise, after all $K(x_f, t_f; x_i, t_i)$ is just the time-evolution operator expressed in the x-basis. We draw a diagram for the propagator as shown in the figure. A straight edge indicates the propagator K. Of course this edge does not represent the particle's trajectory (which is not defined sharply), but rather it is to be understood as an abstract representation of the probability amplitude K.

There is a composition law rule for this propagator, that we look at next.

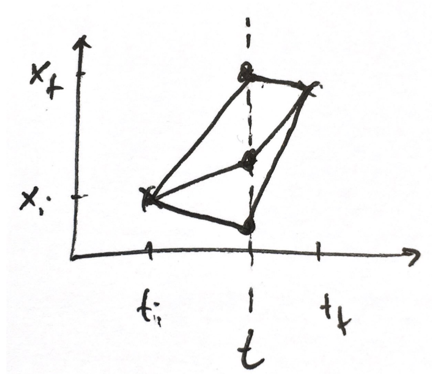

Figure 3: Composition rule for propagators

Imagine we pick a time t between t_i and t_f. Then we can write

$$\begin{aligned} K(x_f, t_f; x_i, t_i) &= \langle x_f | e^{-\frac{i}{\hbar} H\cdot(t_f - t)} e^{-\frac{i}{\hbar} H\cdot(t-t_i)} | x_i \rangle \\ &= \int dx \ \langle x_f | e^{-\frac{i}{\hbar} H\cdot(t_f - t)} | x \rangle \langle x | e^{-\frac{i}{\hbar} H\cdot(t-t_i)} | x_i \rangle \\ &= \int dx \ K(x_f, t_f; x, t) K(x, t; x_i, t_i), \end{aligned}$$

where in the second line we used the resolution of identity $\mathbb{1} = \int dx \ |x\rangle\langle x|$ and in the last line the result was rexpressed in terms of propagators. Let us interpret the result. The propagator for the particle to travel from x_i at t_i to x_f at t_f is the sum (integral) over the product of propagators with an intermediate point x at time t. We can show this too in a diagram.

Imagine decomposing each of the two $K's$ into two $K's$ and introducing more and more intermediate times. The result is shown in the figure. In the limit of an infinite number of intermediate points, the broken lines become a smooth curve and we end up with an integral over all curves connecting points x_i, t_i and x_f, t_f. Notice that the number of integrals, which comes from putting in resolutions of the identity, tends to infinity. This is what is called a path integral, an integral over all curves connecting given points. In the next section

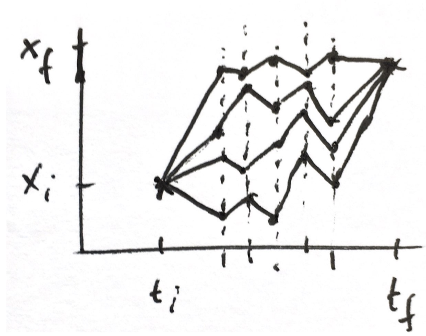

Figure 4: One can introduce many intermediate times and integrate over the corresponding positions

we find that the propagator can be expressed as

$$K(x_f, t_f; x_i, t_i) \sim \sum_{\text{all paths } x(t)} e^{\frac{i}{\hbar} S[x(t)]},$$

where by 'all paths' we mean all paths connecting the two boundary points. In the exponential the action S has to be computed for every path that appears in the sum. Clearly this sum is a new kind of mathematical object and when we derive this result below, we will see how it has to be understood.

A nice feature of this result can be seen right away. A slight change in a path $x(t) \to x(t) + \delta x(t)$ will result in a slight change in the action $S \to S + \delta S$. If the action is large compared to $\hbar$, which is the case if the mass of the particle is macroscopic, then even for a small change δS, a large change in $\frac{i}{\hbar} S[x(t)]$ will result. As a consequence the exponential oscillates very fast and all the different paths that appear in the sum will cancel. However, for classical paths $\delta S = 0$, thus these paths will survive in the sum. In this way the classical laws (equation of motion) emerge from the quantum laws. Clearly whether a system behaves classically or quantum mechanically is governed by how the value of the action compares to $\hbar$. Treating $\hbar$ like a small parameter, we will see below that it is possible to develop a semiclassical approximation to quantum mechanics through the path integral.

Derivation of the path integral

The composition rule for the propagator allows us to work out the propagator for an infinitesimal time $\Delta t = \frac{t_f - t_i}{N}$ and to later combine N such tiny propagators to get the full propagator. Therefore we consider

$$K(x', t + \Delta t; x, t) = \langle x'|e^{-\frac{i}{\hbar}H \cdot \Delta t}|x\rangle$$

and expand the exponential for small Δt:

$$\langle x'|e^{-\frac{i}{\hbar}H \cdot \Delta t}|x\rangle = \langle x'| \left[1 - \frac{i}{\hbar}H \cdot \Delta t + \mathcal{O}(\Delta t)^2\right] |x\rangle = \langle x'| \left[1 - \frac{i}{\hbar}[\frac{P^2}{2m} + V(X)] \cdot \Delta t + \mathcal{O}(\Delta t)^2\right] |x\rangle.$$

Here P and X are of course operators. However, when $V(X)$ acts on the position ket to the right it will become $V(x)$ and the operator turns into a regular number. We can do the same to the kinetic energy term when we insert the resolution of identity in the momentum basis $\mathbb{1} = \int dp \; |p\rangle\langle p|$:

$$\begin{aligned}
\langle x'|e^{-\frac{i}{\hbar}H \cdot \Delta t}|x\rangle &= \int dp \; \langle x'|p\rangle\langle p| \left[1 - \frac{i}{\hbar}[\frac{P^2}{2m} + V(X)] \cdot \Delta t + \mathcal{O}(\Delta t)^2\right] |x\rangle \\
&= \int dp \; \langle x'|p\rangle\langle p|x\rangle \left[1 - \frac{i}{\hbar}[\frac{p^2}{2m} + V(x)] \cdot \Delta t + \mathcal{O}(\Delta t)^2\right] \\
&= \int dp \; \langle x'|p\rangle\langle p|x\rangle \exp\left(-\frac{i}{\hbar}[\frac{p^2}{2m} + V(x)] \cdot \Delta t\right) \qquad (1)
\end{aligned}$$

In the last line we rexponentiated, which is allowed since Δt can be made arbitrarily small. Now we use that $|p\rangle$ is a normalzied plane wave state, i.e. $\langle x|p\rangle = e^{ipx/\hbar}/\sqrt{2\pi\hbar}$. This brings the propagator into the form

$$K(x', t + \Delta t; x, t) = \int dp \; \frac{e^{ip(x'-x)/\hbar}}{2\pi\hbar} \exp\left(-\frac{i}{\hbar}[\frac{p^2}{2m} + V(x)] \cdot \Delta t\right).$$

The integral over p is Gaussian and can be carried out, we find:

$$\begin{aligned}
K(x', t + \Delta t; x, t) &= \sqrt{\frac{m}{2\pi i\hbar\Delta t}} \; \exp\left(-\frac{m}{2i\hbar}\frac{(x'-x)^2}{\Delta t}\right) [\exp\left(-\frac{i}{\hbar}[V(x)] \cdot \Delta t\right) \\
&= \sqrt{\frac{m}{2\pi i\hbar\Delta t}} \; \exp\frac{i\Delta t}{\hbar}\left(\frac{m}{2}\frac{(x'-x)^2}{\Delta t^2} - V(x)\right).
\end{aligned}$$

This is the form of the propagator for infinitesimal times Δt.

Now we can decompose the full propagator by splitting the time between t_f and t_i into N parts of size $\Delta t = (t_f - t_i)/N$:

$$K(x_f, t_f; x_i, t_i) = \int dx_{N-1} \ldots dx_1 K(x_f, t_f; x_{N-1}, t_{N-1}) K(x_{N-1}, t_{N-1}; x_{N-2}, t_{N-2}) \ldots K(x_1, t_1; x_i, t_i)$$

Notice the following peculiarity. The number of integrals is $N-1$ and we will let $N \to \infty$, i.e. we have to do an infinite number of integrations.

In the limit where N is large, Δt is small and we can express the K's on the right hand side in terms of the infinitesimal time propagator (1). Inserting the result that we found for the latter, we get:

$$K(x_f,t_f;x_i,t_i) = \int dx_{N-1}\dots dx_1 \left[\sqrt{\frac{m}{2\pi i\hbar\Delta t}}\right]^N \exp\frac{i\Delta t}{\hbar}\sum_{i=0}^{N-1}\left(\frac{m}{2}\frac{(x_{i+1}-x_i)^2}{\Delta t^2} - V(x_i)\right),$$

where we have put

$$\begin{aligned} x_0 &= x_i \\ t_0 &= t_i \\ x_N &= x_f \\ t_N &= t_f. \end{aligned}$$

Let us now look more closely at what stands inside the exponential. In the limit of $N \to \infty$, i.e. an infinite subdivision of the time interval, the sum corresponds to the definition of the Riemann integral:

$$\frac{i\Delta t}{\hbar}\sum_{i=0}^{N}\left(\frac{m}{2}\frac{(x_{i+1}-x_i)^2}{\Delta t^2} - V(x_i)\right) \to \frac{i}{\hbar}\int dt\, \left[\frac{m}{2}\dot{x}^2 - V(x)\right],$$

Quite amazingly we see that the action familiar to us from classical mechanics appears here.

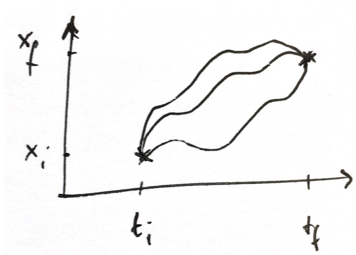

Figure 5: The zig-zag lines go over into paths as $N \to \infty$

In the limit of $N \to \infty$ the jagged, zig-zag lines become continuous curves, see figure. We write the propagator as

$$K(x_f, t_f; x_i, t_i) = \int\limits_{\substack{x(t_i)=x_i \\ x(t_f)=x_f}} Dx(t)\; e^{\frac{i}{\hbar}S[x(t)]},$$

the differential sign under the integral stands for an infinite number of integrals:

$$\int Dx(t) = \lim_{N\to\infty} \left[\sqrt{\frac{m}{2\pi i\hbar\Delta t}}\right]^N \int dx_{N-1} \dots dx_1$$

The mathematician would not be very happy with such a definition. But the path integral has been shown to be an incredibly useful and a fully valid tool in the exploration of physical systems. The only way to get comfortable with this strange mathematical object is to practise it on many example problems and convince oneself that the answers obtained from quantum mechanics are the same as those obtained with the path integral.