1 Semiclassical Approximation

The semiclassical approximation is a powerful approach to evaluating the propagator under the right conditions. Roughly speaking, we want a smooth potential and short de Broglie wavelengths. In the semiclassical approximation, the propagator takes the following form,

$$K_{sc}(x, x', t) = F \exp(\frac{i}{\hbar} S_c(x, x', t)), \tag{1}$$

where S_c is a strictly classical quantity, the action evaluated along the classical path from x to x'. The pre-factor F is an approximation to the path integral for paths other than the classical path. When the semiclassical approximation is working, most of the important physics is in S_c, not F. The semiclassical approximation is exact, that is not an approximation, for the free particle and the harmonic oscillator, among other examples. It is important to realize that the semiclassical approximation has to do with how close F is to the path integral around the classical path. Any path integral can be written in the form of Eq.(1). The semi-classical approximation then is an approximation to F. The general formula for F in semiclassical approximation is given at the end of these notes.

Classical Path and Classical Action Consider any path $x(t')$ which starts at x' and ends at x. This means $x(0) = x'$, and $x(t) = x$. Once we have a path, we can calculate the action for that path. This is just

$$S = \int_0^t L(x(t'))dt'.$$

The action certainly depends on the path used to calculate it. Now suppose we go to a nearby path,

$$x(t') \to x(t') + \delta(t')$$

where $\delta(t')$ is small and vanishes at the endponts, $\delta(0) = \delta(t) = 0$. In other words, we are considering only paths which start and end at our two points. It is of interest to see how the action varies to $O(\delta)$. Putting $x(t') \to x(t') + \delta(t')$ into the Lagrangian, we have

$$L \to \frac{m}{2} \left(\frac{d}{dt}(x + \delta) \right)^2 - V(x + \delta)$$

Expanding, we have

$$L = \frac{m}{2} (\frac{dx}{dt})^2 + m \frac{dx}{dt} \frac{d\delta}{dt} - V(x) - \delta \frac{\partial}{\partial x} V + \dots$$

Putting these terms in the action, we have for δS,

$$\delta S = \int_0^t dt' (\frac{dx}{dt} \frac{d\delta}{dt} - \delta \frac{\partial}{\partial x} V)$$

Integrating by parts, we have

$$\delta S = m\frac{dx}{dt}\delta\Big]_0^t - \int_0^t dt'\delta(t')(m\frac{d^2x}{dt^2} + \frac{\partial V}{\partial x})$$

The boundary term vanishes since $\delta(0) = \delta(t) = 0$. The coefficient of δ in the integral term is just the equation of motion, so if the equations of motion are satisfied, $\delta S = 0$, for any $\delta(t')$. Hence, we have the important result that:

The action is stationary against small changes in the path when the equations of motion are satisfied. Hamilton's Principle

Method of Stationary Phase To see why it is important to be near a stationary action in the path integral, consider an ordinary integral, not a path integral. Suppose we want to calculate

$$I \equiv \int dx \exp(i\lambda f(x)),$$

where λ is a very large parameter. The integrand is highly oscillatory and will be dominated by points of *stationary phase*. A stationary phase point is when $df/dx = 0$. Suppose x_c is such a point, and we set $x = x_c + x'$. Our integral becomes

$$I = \exp(i\lambda f(x_c)) \int dx' \exp(i\lambda f''(x_c)\frac{x'^2}{2} + \ldots)$$

The integral is then of the form

$$I = F \exp(i\lambda f(x_c)),$$

where F is the result of the integral on x'. When the method is working, this integrand can be gotten to a good approximation by keeping only the $O(x'^2)$ term in the exponent, which then becomes a standard Gaussian integral and is represented by the factor F.

The semiclassical approximation to the path integral is in the spirit of the method of stationary phase for ordinary integrals. The point x_c becomes the classical path $x_c(t')$. The role of the large parameter is played by $1/\hbar$. We are near the classical limit, so $\hbar$ is small (compared to any other quantity with dimension of action.) The factor F in Eq.(1) is supposed to account for the contributions of paths around the classical path, just as in the case of an ordinary integral, F accounts for the integral around the point of stationary phase.

For certain problems, the semiclassical approximation is not in fact an approximation. Examples are: the free particle, the harmonic oscillator, a particle in a constant field, etc.

Harmonic Oscillator The Lagrangian for a a simple harmonic oscillator is

$$L = \frac{m}{2}(\frac{dx}{dt})^2 - \frac{m}{2}\omega^2 x^2$$

We will denote final and initial points as x_a and x_b instead of x and x'. To find the classical action $S_c(x_a, x_b, t)$, we need to find the classical trajectory satisfying $x_c(t) = x_a$, and $x_c(0) = x_b$. We know the motion is sinusoidal, and it is easy to show that

$$x_c(t') = \frac{x_a \sin(\omega t') + x_b \sin(\omega(t - t'))}{\sin(\omega t)}$$

Note that t is the fixed time at the endpoint, while t' is the variable time along the path. Knowing $x_c(t')$, we then can calculate S_c. We have

$$S_c(x_a, x_b, t) = \int_0^t L(x_c(t'))dt' = \frac{m\omega[(x_a^2 + x_b^2)\cos(\omega t) - 2x_a x_b]}{2\sin(\omega t)},$$

where the elementary integration has been omitted. The quantity $S_c(x_a, x_b, t)$ goes up in the exponent. The prefactor F is a simple generalization of the factor used for a free particle. We have

$$\underbrace{\sqrt{\frac{m}{2\pi i\hbar t}}}_{free} \longrightarrow \underbrace{\sqrt{\frac{m\omega}{2\pi i\hbar \sin(\omega t)}}}_{harmonic\ oscillator}$$

Semiclassical Approximation and Schrödinger Equation The exact propagator is supposed to satisfy the Schrödinger equation,

$$\begin{aligned}
i\hbar\partial_t K(x_a, x_b, t) &= < x_a|H \exp(-\frac{iHt}{\hbar})|x_b > \\
&= (-\frac{\hbar^2}{2m}\partial_a^2 + V(x_a)) < x_a| \exp(-\frac{iHt}{\hbar})|x_b > \\
&= (-\frac{\hbar^2}{2m}\partial_a^2 + V(x_a))K(x_a, x_b, t)
\end{aligned}$$

Let us see how the Schrödinger might work out for a semiclassical approximation to K. We write

$$K_{sc}(x_a, x_b, t) = F(t)\exp(\frac{iS_c(x_a, x_b, t)}{\hbar}),$$

where we are not restricting ourselves to the harmonic oscillator at the moment. Acting on K with $i\hbar\partial_t$, we have

$$i\hbar\partial_t K = (-\frac{\partial S_c}{\partial t} + \frac{i\hbar}{F}\frac{\partial F}{\partial t})K$$

We note that there is a purely classical term ($\partial_t S_c$) with no factors of $\hbar$ in it, and another term which is $O(\hbar)$. The semiclassical approximation classifies terms by their order in $\hbar$. Looking at the right side of the Schrödinger equation, let us start with one derivative. We have

$$\frac{\hbar}{i}\frac{\partial K}{\partial x_a} = \frac{\partial S_c}{\partial x_a}K$$

Continuing to get the full right side of the Schrödinger equation, we have

$$(\frac{1}{2m}(\frac{\partial S_c}{\partial x_a})^2 + V(x_a))K + (\frac{\hbar}{2mi}\frac{\partial^2 S_c}{\partial^2 x_a})K.$$

We see the same pattern again, a term with no $\hbar$, and a term proportional to $\hbar$. It turns out that the terms without $\hbar$ on both sides of the equation automatically cancel, that is

$$-\frac{\partial S_c}{\partial t} = \frac{1}{2m}(\frac{\partial S_c}{\partial x_a})^2 + V(x_a).$$

This is an equation called the Hamilton-Jacobi equation and is satisfied by the classical action. It is really saying

$$E = \frac{p_a^2}{2m} + V(x_a),$$

where E is the energy, since $-\partial_t S = E$, and $\partial_x S = p$. While the energy is constant, the momentum is in general not constant. This is taken account of, since differentiating with respect to the final coordinate gives the final momentum, and differentiating with respect to the initial coordinate gives minus the initial momentum. A simple example where this can all be checked easily is the free particle, which in the present notation has a classical action given by

$$S_c = \frac{m(x_a - x_b)^2}{2t}$$

So if we can find the classical action $S_c(x_a, x_b, t)$ for a given problem, the semiclassical expression for the propagator automatically satisfies the part of the time-dependent Schrödinger equation independent of $\hbar$. We are left with the $O(\hbar)$ terms. If the Schrödinger equation is to be satisfied, we must have

$$\frac{i\hbar}{F}\frac{\partial F}{\partial t} = \frac{\hbar}{2mi}\frac{\partial^2 S_c}{\partial^2 x_a}.$$

For the harmonic oscillator, using the formulae given above for S_c and F, it is easy to check that this equation is indeed satisfied. So along with the free particle, the harmonic oscillator is an example where the semi-classical approximation to the propagator is exact. There are a few other problems where this is true as well.

Formula for F In the discussion above, we got the factor F for the oscillator by some guesswork from the free particle case. It turns out that there is a general formula for F. This is

$$F = \sqrt{\frac{1}{2\pi i\hbar}(-\frac{\partial^2 S_c}{\partial x_a \partial x_b})},$$

so in fact the full semiclassical approximation for K can be expressed in terms of the classical action. This is pleasing. In general semiclassical methods are useful in the limit of large quantum numbers, for example an electron in a high n orbit. The semiclassical method continues to develop. A sample of beautiful work on the subject is on the website of Eric Heller, a Harvard physicist.