Physics 731 Lecture Notes 5

Summary: WKB Approximation, Path Integral Approach to QM

These notes summarize the WKB (semiclassical) approximation and Feynman's path integral method. References for the WKB approximation are **S1r**, **S3** 2.5, **S2**, 2.6; Shankar 6, Merzbacher 7 (particularly recommended), and Gottfried 8. References for the path integral include **S1r** 2.5, **S2**, **S3** 2.6, Shankar 8, 16, 21, and the text by Feynman and Hibbs; we will largely follow Shankar's treatment.

Semiclassical limit, WKB approximation. The WKB (sometimes called WKBJ or JWKB) method, named after Wentzel, Kramers, Brillouin, (and Jeffreys), is a semiclassical approximation based on an asymptotic expansion in powers of $\hbar$, which has its domain of validity in the $\hbar \to 0$ limit. The method is based on the idea that if V is slowly varying, the wavefunction approximately takes the free-particle form $\sim e^{\pm ikx}$ (or $\sim e^{\pm\kappa x}$), with a slowly varying k (or κ) vector, with $k^2(x) = 2m(E-V(x))/\hbar^2$, $\kappa^2 = 2m(V(x)-E)/\hbar^2$. More precisely, taking the following ansatz for energy eigenstates,

$$\Psi(x,t) \sim e^{iW(x,t)/\hbar} = e^{i(S(x)-Et)/\hbar} = \psi(x)e^{-iEt/\hbar}, \tag{1}$$

and using it in the Schrödinger equation, it is straightforward to obtain the following equation for $S(x)$:

$$i\hbar S(x)'' - (S(x)')^2 + 2m(E-V(x)) = 0, \tag{2}$$

in which the primes denote differentiation by x. Expanding $S(x)$ in powers of $\hbar$:

$$S(x) = S_0(x) + \hbar S_1(x) + \ldots, \tag{3}$$

and inserting this expansion into Eq. (2), by matching powers of $\hbar$, we obtain for order $\hbar^0$ and order $\hbar$:

$$O(\hbar^0): \quad -(S_0')^2 + 2m(E-V(x)) = 0, \qquad O(\hbar): \quad iS_0'' - 2S_0'S_1' = 0.$$

Solving the $O(\hbar^0)$ condition yields $S_0' = \pm\sqrt{2m(E-V(x))}$, such that

$$\frac{S_0}{\hbar} = \pm\int^x \frac{\sqrt{2m(E-V(x'))}}{\hbar}dx' = \begin{cases} \pm\int^x k(x')dx' & E > V(x) \\ \pm i\int^x \kappa(x')dx' & E < V(x). \end{cases}$$

Using this result, we then solve the $O(\hbar)$ equation to obtain

$$S_1' = (i/2)S_0''/S_0' = \begin{cases} (i/2)k'(x)/k(x) & E > V(x) \\ (i/2)\kappa'(x)/\kappa(x) & E < V(x). \end{cases}$$

Using these results in Eq. (1), for which $\psi(x) \sim e^{iS(x)/\hbar} = e^{i(S_0+\hbar S_1)/\hbar}$, we obtain the following forms for the WKB wavefunctions :

• $E > V(x)$ (the classical region):

$$\psi_{\rm WKB}(x) \sim \frac{1}{\sqrt{k(x)}}\exp\left[\pm i\int^x k(x')dx'\right] \sim \frac{1}{(E-V(x))^{1/4}}\exp\left[\pm\frac{i}{\hbar}\int^x \sqrt{2m(E-V(x'))}dx'\right]. \tag{4}$$

• $E < V(x)$ (the classically forbidden region):

$$\psi_{\rm WKB}(x) \sim \frac{1}{\sqrt{\kappa(x)}}\exp\left[\pm\int^x \kappa(x')dx'\right] \sim \frac{1}{(V(x)-E)^{1/4}}\exp\left[\pm\frac{1}{\hbar}\int^x \sqrt{2m(V(x')-E)}dx'\right]. \tag{5}$$

The approach is valid in the limit that

$$\left|k'/k^2\right| \ll 1,$$

where $k' = dk(x)/dx$, and $O(1)$ numerical factors have been dropped. This condition can also be expressed as (again dropping $O(1)$ numerical factors):

$$\left|\frac{dV/dx}{k(x)(E-V(x))}\right| \ll 1, \tag{6}$$

From the form of the WKB wavefunctions, it is straightforward to see that the approximation breaks down at the classical turning points x_i ($E = V(x_i)$). These regions are handled by matching to exact solutions of the Schrödinger equation that results upon a Taylor expansion of the potential in the neighborhood of the turning point. For the case in which the leading term of this expansion is the linear term, one solves the Schrödinger equation with a linear potential, which can be expressed as the Airy equation

$$\frac{d^2\psi}{dy^2} - y\psi = 0, \tag{7}$$

in which y is a function of the distance from the turning point. More precisely, for the turning point $x = x_1$ where the potential has a negative slope ($V'(x_1) < 0$), we have

$$y = -\left(\frac{2m|V'(x_1)|}{\hbar^2}\right)^{1/3}(x - x_1), \tag{8}$$

and for the turning point $x = x_2$, where the potential has a positive slope ($V'(x_2) > 0$), we have

$$y = \left(\frac{2m|V'(x_2)|}{\hbar^2}\right)^{1/3}(x - x_2). \tag{9}$$

The general solution to Eq. (7) is given by a linear combination of Airy functions $\mathrm{Ai}(y)$ and $\mathrm{Bi}(y)$. Using the asymptotic forms of these functions, one obtains the connection rules for matching the WKB wavefunctions around the turning point regions. These connection rules are as follows:

- $V'(x_2) > 0$ at the turning point $x = x_2$ (the linearized potential has a positive slope):

$$\frac{2}{\sqrt{k(x)}}\cos\left[\int_x^{x_2} k(x')dx' - \frac{\pi}{4}\right] \quad\longleftrightarrow\quad \frac{1}{\sqrt{\kappa(x)}}\exp\left[-\int_{x_2}^{x}\kappa(x')dx'\right] \tag{10}$$

$$\frac{1}{\sqrt{k(x)}}\sin\left[\int_x^{x_2} k(x')dx' - \frac{\pi}{4}\right] \quad\longleftrightarrow\quad -\frac{1}{\sqrt{\kappa(x)}}\exp\left[\int_{x_2}^{x}\kappa(x')dx'\right]. \tag{11}$$

- $V'(x_1) < 0$ at the turning point $x = x_1$ (the linearized potential has a negative slope):

$$\frac{1}{\sqrt{\kappa(x)}}\exp\left[\int_{x_1}^{x}\kappa(x')dx'\right] \quad\longleftrightarrow\quad \frac{2}{\sqrt{k(x)}}\cos\left[\int_{x_1}^{x} k(x')dx' - \frac{\pi}{4}\right] \tag{12}$$

$$-\frac{1}{\sqrt{\kappa(x)}}\exp\left[-\int_{x_1}^{x}\kappa(x')dx'\right] \quad\longleftrightarrow\quad \frac{1}{\sqrt{k(x)}}\sin\left[\int_{x_1}^{x} k(x')dx' - \frac{\pi}{4}\right]. \tag{13}$$

In each case, it is important to avoid instabilities that can result in regions with large $|x|$. In Eq. (10), the matching is best done proceeding to the left, while in Eq. (11), to the right (and conversely for Eqs. (12-13)). The reason is that the decaying exponential is subdominant compared to the growing exponential, but neglecting it can lead to an $O(1)$ shift in the phase of the sine or cosine term.

The method, when valid, can be used in bound and scattering problems. The idea is to write down a general WKB solution for each region, and match using the connection formulae. This entails rewriting the solution obtained by matching at one turning point to the form needed to match at the other turning point, which results in prefactors that depend on the integral of k or κ between the turning points.

For bound state problems consisting of a single well (without any infinite barriers), connecting the WKB solutions in the classical region of a binding potential between turning points x_1 and x_2 leads to the energy quantization condition:

$$\int_{x_1}^{x_2} k(x)dx = \left(n + \frac{1}{2}\right)\pi, \qquad n = 0, 1, 2, \ldots. \tag{14}$$

Note the similarity to the Bohr-Sommerfeld quantization condition:

$$\oint p\, dx = nh, \qquad n = 1, 2, \ldots, \tag{15}$$

after expressing Eq. (14) in terms of p to obtain

$$\oint p\, dx = \left(n + \frac{1}{2}\right)h. \tag{16}$$

Eq. (14) does not generalize to the case of more intricate potentials, e.g. with multiple wells or infinite walls. The WKB method can also be used to find the transmission and reflection probabilities at a potential barrier.

Path Integral Approach to Quantum Mechanics. For Hamiltonians of the form (in 1d for simplicity)

$$H = \frac{p^2}{2m} + V(x), \tag{17}$$

the propagator $K(x, t; x', 0)$, which takes a state from position x' at time $t = 0$ to position x at time t, can be expressed as

$$K(x, t; x', 0) = \langle x|\mathcal{U}|x'\rangle = \sum_n e^{-iE_n t/\hbar}\psi_n(x)\psi_n^*(x'), \tag{18}$$

in which the $\psi_n(x)$ are the position-space energy eigenfunction of H.

Feynman, based on early ideas of Dirac, instead proposed the following expression for the propagator as the sum over all histories of the exponential of the action (times $i/\hbar$), as follows:

$$K(x, t; x', 0) = \langle x|\mathcal{U}|x'\rangle = \int_{x'}^{x} \mathcal{D}[x(t)]e^{iS[x(t)]/\hbar}, \tag{19}$$

in which the functional integral is taken over all paths $[x(t)]$ with endpoints $x(t) = x$ and $x(0) = x'$, and $S = \int_0^t L dt$, where L is the Lagrangian ($L = p\dot{x} - H(x, p)$).

In practice, this is computed by discretizing $x(t)$ at N points, with $\epsilon = \Delta t = t/N$, and taking the limit $\epsilon \to 0$, $N \to \infty$, with $N\epsilon \to t$, which leads to the following explicit expression for the meaning of the functional integral:

$$\int \mathcal{D}[x(t)] = \lim_{\epsilon\to 0, N\to\infty} \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{1/2} \int_{-\infty}^{\infty} dx_{N-1} \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{1/2} \ldots \int_{-\infty}^{\infty} dx_1 \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{1/2}. \tag{20}$$

It is straightforward to verify, for example, that for the free particle, this prescriptions gives the correct result. In the cases in which $V(x) \neq 0$, there is a question of where to sample $V(x)$ when discretizing $S[x(t)]$. A standard approach is to take the "midpoint prescription" for V:

$$S[x(t)] = \sum_{n=0}^{N-1} \left[\frac{m}{2} \frac{(x_{n+1} - x_n)^2}{\epsilon} - V\left(\frac{x_{n+1} + x_n}{2} \right) \epsilon \right]. \tag{21}$$

A particularly useful result is that for potentials of the form $V(x) = a + bx + cx^2$, the propagator can be obtained (up to a dimensionful prefactor) by evaluating the action only along the classical path:

$$K(x, t; x', 0) = A(t) e^{iS_{\text{classical}}/\hbar}. \tag{22}$$

For this class of potentials, expanding the action about the classical path truncates at second order, which yields this simple result. For $V = a + bx$ (that is, taking $c = 0$), the $A(t)$ factor can be obtained easily by considering the fact that for $t \to 0$, the propagator should result in the delta function $\delta(x - x')$. For $c \neq 0$ (*i.e.*, the simple harmonic oscillator), to obtain $A(t)$ we need to compute

$$A(t) = \int_0^0 \mathcal{D}[y(t)] e^{\frac{i}{\hbar} \int_0^t (\frac{1}{2} m \dot{y}^2 - c y^2) dt}, \tag{23}$$

which can be done using Fourier analysis (done in class). This method also applies if the potentials depend on $\dot{x}$ at linear order (for example, via terms proportional to $\dot{x}$ or $x\dot{x}$), for the same reason that the expansion around the classical path truncates.

To justify the path integral approach, recall that for time-independent Hamiltonians of the form $H = p^2/(2m) + V(x)$, the propagator is given by

$$K(x, t; x', 0) = \langle x | e^{-iHt/\hbar} | x' \rangle. \tag{24}$$

If we break up the time interval, as before: $\epsilon = t/N$, then for an infinitesimal time increment ϵ,

$$e^{-i\epsilon H/\hbar} = e^{-\frac{i\epsilon}{\hbar}\left(\frac{p^2}{2m} + V(x)\right)} = e^{-\frac{i\epsilon}{\hbar}\frac{p^2}{2m}} e^{-\frac{i\epsilon}{\hbar} V(x)} + O(\epsilon^2) \tag{25}$$

(we will drop terms of $O(\epsilon^2)$ and higher). Therefore, we have

$$K(x, t; x', 0) = \langle x | e^{-\frac{i\epsilon}{\hbar}\frac{p^2}{2m}} e^{-\frac{i\epsilon}{\hbar} V(x)} \dots e^{-\frac{i\epsilon}{\hbar}\frac{p^2}{2m}} e^{-\frac{i\epsilon}{\hbar} V(x)} | x' \rangle. \tag{26}$$

Inserting a complete set of $|x\rangle$ states, we obtain

$$K(x, t; x', 0) = \int \prod_{n=1}^{N-1} \langle x | e^{-\frac{i\epsilon}{\hbar}\frac{p^2}{2m}} e^{-\frac{i\epsilon}{\hbar} V(x)} | x_{n-1} \rangle \langle x_{n-1} | e^{-\frac{i\epsilon}{\hbar}\frac{p^2}{2m}} e^{-\frac{i\epsilon}{\hbar} V(x)} | x_{n-2} \rangle \dots \langle x_1 | e^{-\frac{i\epsilon}{\hbar}\frac{p^2}{2m}} e^{-\frac{i\epsilon}{\hbar} V(x)} | x' \rangle. \tag{27}$$

For a separable Hamiltonian which is at most quadratic in derivatives, we can evaluate the matrix element

$$\langle x_n | e^{-\frac{i\epsilon}{\hbar}\frac{p^2}{2m}} e^{-\frac{i\epsilon}{\hbar} V(x)} | x_{n-1} \rangle = \left(\frac{m}{2\pi i \hbar \epsilon} \right)^{1/2} e^{\frac{im(x_n - x_{n-1})^2}{2\hbar\epsilon}} e^{-\frac{i\epsilon}{\hbar} V(x)}. \tag{28}$$

Collecting the factors, the propagator takes the form

$$K(x, t; x', 0) = \left(\frac{m}{2\pi i \hbar \epsilon} \right)^{1/2} \int \prod_{n=1}^{N-1} \left(\frac{m}{2\pi i \hbar \epsilon} \right)^{1/2} dx_n \exp\left(\sum_{n=1}^{N} \frac{i\epsilon}{\hbar} \left[\frac{m}{2} \left(\frac{(x_n - x_{n-1})}{\epsilon} \right)^2 - V(x_{n-1}) \right] \right). \tag{29}$$

This is just the discretized form of the path integral as given above (note the slight difference in notation regarding the index n, which of course is equivalent to Eqs. (20)-(21)). Furthermore, rather than working out Eq. (28) explicitly, we can insert a complete set of $|p\rangle$ states in between each pair of terms consisting of $e^{-\frac{i\epsilon}{\hbar}\frac{p^2}{2m}}$ and $e^{-\frac{i\epsilon}{\hbar}V(x)}$, to obtain the following form of the path integral:

$$K(x,t;x',0) = \int \prod_{n'=1}^{N} \frac{dp_{n'}}{2\pi\hbar} \prod_{n=1}^{N-1} \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{1/2} dx_n \, \exp\left(\frac{i}{\hbar}\sum_{n=1}^{N}\left[-\frac{i\epsilon p_n^2}{2m\hbar} + \frac{ip_n(x_n - x_{n-1})}{\hbar} - \frac{i\epsilon V(x_{n-1})}{\hbar}\right]\right). \tag{30}$$

In the continuum limit, this takes the form

$$K(x,t;x',0) = \int \mathcal{D}p \, \mathcal{D}x \, e^{i\int_0^t (p\dot{x} - H(x,p))dt}. \tag{31}$$

This form is of more general applicability; in the case in which the p integrations can be performed (for example, in the standard case when the Hamiltonian is quadratic in p), the standard Feynman path integral form involving the action is recovered.