Physics 472 Lecture 18

Semiclassical (WKB) Approx.

In classical mechanics, one has in

1D:

$$E = \frac{p^2}{2m} + V(x)$$

$$p^2 = 2m(E - V(x))$$

$$p(x) = \pm\sqrt{2m(E-V(x))}$$

In the <u>semiclassical approximation</u>, one assigns a local wavevector following de Broglie:

$$k(x) = \frac{p(x)}{\hbar} = \pm\sqrt{\frac{2m}{\hbar^2}(E-V(x))}$$

and takes

$$\psi(x) = \sqrt{\rho(x)}\, e^{i\int^x k(x')dx'}.$$

Let $A(x) = \sqrt{\rho(x)}$, $\theta(x) = \int^x k(x')dx'$.

$$\psi(x) = A(x)\, e^{i\theta(x)}$$

$$\frac{d\psi}{dx} = A'(x)e^{i\theta} + ik(x)\, A e^{i\theta}$$

$$\frac{d^2\psi}{dx^2} = A''(x)e^{i\theta} + 2ik(x)A'(x)e^{i\theta} + ik'(x)\, Ae^{i\theta} - k^2(x)\, A\, e^{i\theta}$$

$$= \psi(x)\left[\frac{A''}{A} + 2ik(x)\frac{A'}{A} + ik'(x) - k^2(x)\right]$$

Schrödinger's eq. in 1D is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$$

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}(E - V(x))\psi = -k^2(x)\psi$$

The semiclassical approx. satisfies the Sch. eq. if

$$\frac{A''}{A} = 0 \quad \left(\text{actually, if } \frac{A''}{A} \ll k^2(x)\right)$$

and

$$2k(x)\frac{A'}{A} + k'(x) = 0$$

$$\frac{A'}{A} = -\frac{1}{2}\frac{k'(x)}{k(x)}$$

$$d \ln A(x) = -\frac{1}{2}\, d \ln k(x)$$

$$\ln A(x) = \ln k(x)^{-1/2} + C'$$

$$A(x) = \frac{e^{C'}}{\sqrt{k(x)}} = \frac{C}{\sqrt{k(x)}}$$

$$\Rightarrow \quad \psi(x) = \frac{C}{\sqrt{|k(x)|}}\, e^{\pm i \int^{x} k(x')\,dx'} \, ,$$

where $k(x) = \frac{1}{\hbar}\sqrt{2m\left(E - V(x)\right)}$

The condition for validity of this so-called WKB (= Wenzel-Kramers-Brillouin) approximation is that

$$\frac{A''}{A} \ll k^2(x)$$

or $$\frac{1}{\sqrt{\rho(x)}} \frac{d^2}{dx^2} \sqrt{\rho(x)} \ll k^2(x),$$

i.e., provided the density $\rho(x)$ doesn't vary much in one wavelength of the de Broglie wave.

Actually, this analysis is a bit too naive, because the semiclassical approx. is an <u>asymptotic approximation</u>, which is not quite the same as dropping higher terms in a Taylor series!

The WKB method can also be used to describe the wavefunction in the classically forbidden regime $E < V(x)$:

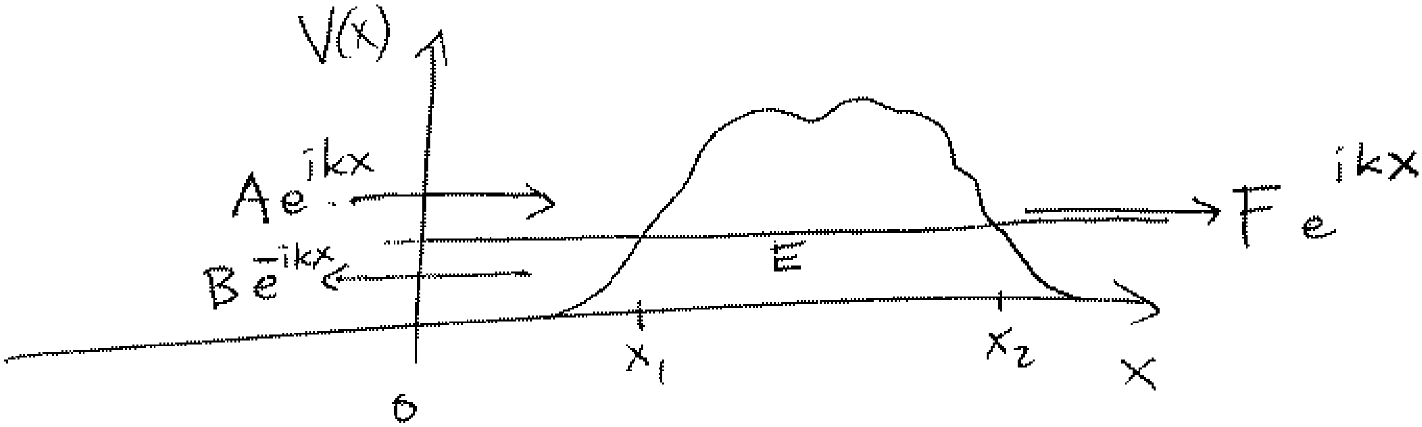
$$k(x) = \pm\sqrt{2m(E-V(x))} = \pm i\sqrt{2m(V(x)-E)}$$

$$\psi(x) = \frac{C}{\sqrt{|k(x)|}} e^{\pm \int^x |k(x')| dx'}$$

<u>Application to tunneling</u>

Consider a potential barrier of

arbitrary shape but finite length in 1D:



$$T = \frac{|j_{tr}|}{|j_{in}|} = \frac{\frac{\hbar k}{m}|F|^2}{\frac{\hbar k}{m}|A|^2} = \frac{|F|^2}{|A|^2}$$

In the tunneling region, $V(x) > E$, the WKB wavefunction is

$$\psi(x) = \frac{C}{\sqrt{|k(x)|}} e^{+\int_{x_1}^{x} |k(x')| dx'} + \frac{D}{\sqrt{|k(x)|}} e^{-\int_{x_1}^{x} |k(x')| dx'}$$

If the barrier is very high or wide, then the coefficient of the exponentially growing term must be zero.

Then

$$\frac{|F|}{|A|} \sim e^{-\int_{x_1}^{x_2} dx\,|k(x')|\,dx'}$$

$$T = \frac{|F|^2}{|A|^2} \sim e^{-2\int_{x_1}^{x_2} dx\,|k(x')|\,dx'}$$

WKB result for the tunneling probability

See application to α decay: Example 8.2, Griffiths pp. 322-325.

General derivation

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(\vec{r})\psi = i\hbar\frac{\partial\psi}{\partial t}$$

let $\psi(\vec{r},t) = A(\vec{r},t)\, e^{\frac{i}{\hbar}R(\vec{r},t)}$,

where $A, R \in \mathbb{R}$ and $A^2 = \rho(\vec{r},t)$.

Inserting this expression for ψ into the Sch. eq., and taking the real and imaginary parts, gives two equations

$$-\frac{\partial R}{\partial t} = \frac{(\nabla R)^2}{2m} + V(\vec{r}) - \frac{\hbar^2}{2m}\frac{\nabla^2\sqrt{\rho}}{\sqrt{\rho}}$$

$$\frac{\partial \rho}{\partial t} + \nabla\cdot\left(\rho\frac{\nabla R}{m}\right) = 0$$

The second equation is the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{J} = 0$$

(Note: no approximations have been made yet!)

If we define $\vec{J} = \rho \vec{V}$, then we can identify

$$\frac{\nabla R}{m} = \vec{V} = \text{velocity of particle}.$$

The first equation, aside from the last term

$$V_B \equiv -\frac{\hbar^2}{2m} \frac{\nabla^2 \sqrt{\rho}}{\sqrt{\rho}} = \text{"quantum potential"},$$

is the Hamilton-Jacobi eq., 11
which you can find in any advanced text on classical mechanics.

(The term $-\frac{\partial R}{\partial t} = E$ for time indep. problems.) The 3D WKB approx. results if we neglect the quantum potential $V_B(\vec{r})$, which gives a contribution to $R(\vec{r},t)$ that is higher-order in $\hbar$:

$$R(\vec{r},t) = R_0(\vec{r},t) + \hbar^2 R_2(\vec{r},t) + \cdots,$$

where $R_0(\vec{r},t)$ is the sol'n

of $$\frac{\partial R_0}{\partial t} = \frac{(\nabla R_0)^2}{2m} + V(\vec{r})$$

and
$$-\frac{\partial R_2}{\partial t} = \frac{\nabla R_0}{m} \nabla R_2 - \frac{1}{2m} \frac{\nabla^2 \sqrt{\rho_0}}{\sqrt{\rho_0}},$$

where $$\frac{\partial \rho_0}{\partial t} = \nabla \cdot \left(\rho_0 \frac{\nabla R_0}{m} \right), \text{etc.}$$

Also $\rho = \rho_0 + \hbar^2 \rho_2 + \cdots$, where

$$\frac{\partial \rho_2}{\partial t} + \nabla \cdot \left(\rho_0 \frac{\nabla R_2}{m} + \rho_2 \frac{\nabla R_0}{m} \right) = 0.$$

It ends up that ρ_2 is not necessarilly smaller than ρ_0, but it is a rapidly oscillating function that averges to zero.