

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 semiclassical approximation,
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

(2)

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

$$\text{Let } A(x) = \sqrt{p(x)}, \quad \theta(x) = \int^x k(x') dx'$$

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

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

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

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

Schrödinger's eq. in 1D is

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

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

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

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

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

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

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

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

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

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

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

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

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

i.e., provided the density $S(x)$ 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 asymptotic approximation, 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

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$$E < V(x) :$$

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

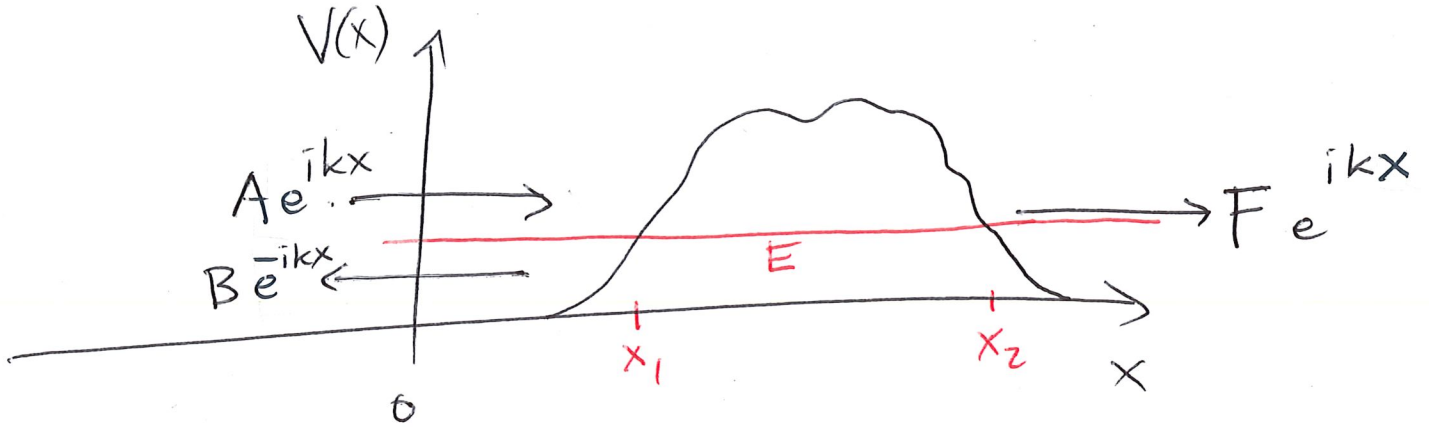
$$\Psi(x) = \frac{C}{\sqrt{|k(x)|}} e^{\pm \int^x |k(x')| dx'}$$

Application to tunneling

Consider a potential barrier of

arbitrary shape but finite 7

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. 8

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

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

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

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 (10)
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 :

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

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

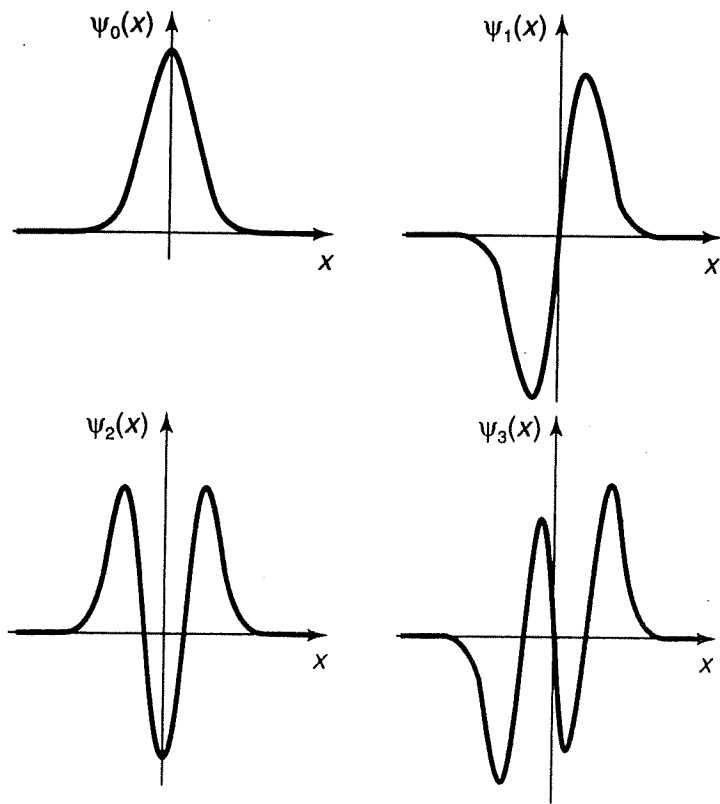
$$-\frac{\partial R_2}{\partial t} = \frac{\nabla R_0 \cdot \nabla R_2}{m} - \frac{1}{2m} \frac{\nabla^2 \sqrt{S_0}}{\sqrt{S_0}}$$

where
$$\frac{\partial S_0}{\partial t} = \nabla \cdot \left(S_0 \frac{\nabla R_0}{m} \right), \text{ etc.}$$

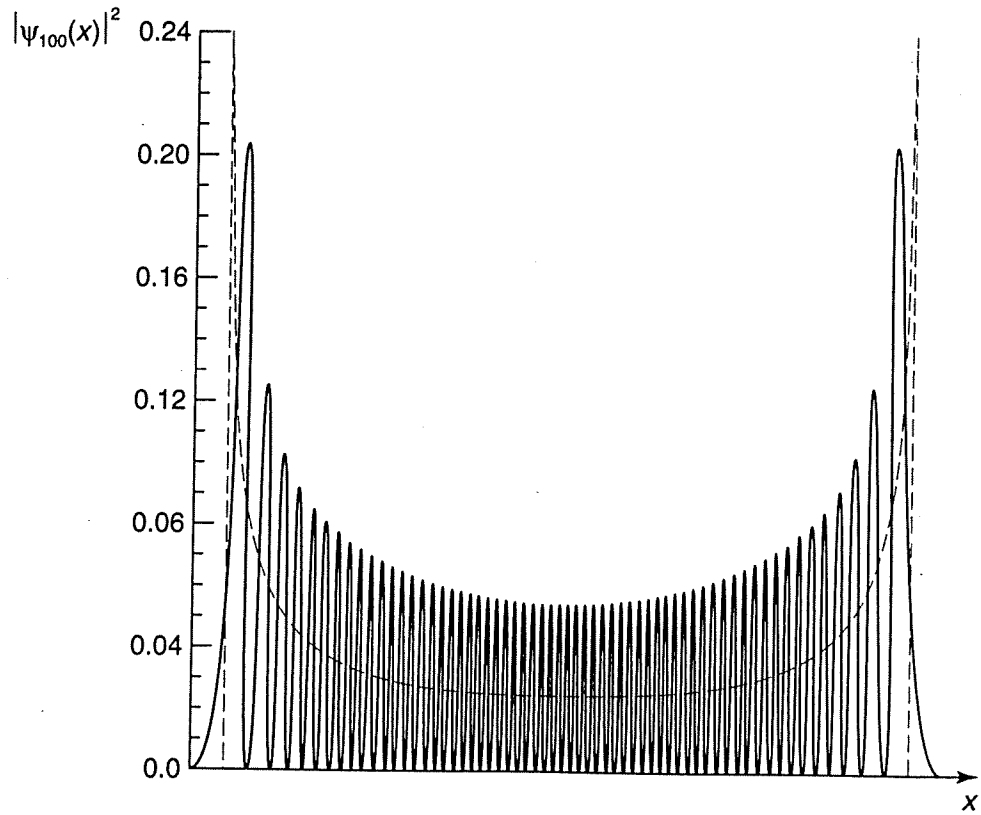
Also $S = S_0 + \hbar^2 S_2 + \dots$, where

$$\frac{\partial S_2}{\partial t} + \nabla \cdot \left(S_0 \frac{\nabla R_2}{m} + S_2 \frac{\nabla R_0}{m} \right) = 0.$$

It ends up that S_2 is not necessarily smaller than S_0 , but it is a rapidly oscillating function that averages to zero.



(a)



(b)

Figure 2.5: (a) The first four stationary states of the harmonic oscillator. (b) Graph of $|\psi_{100}|^2$, with the classical distribution (dashed curve) superimposed.