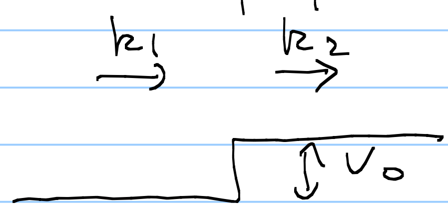
WKB Approximation

Note Title

Earlier, we have learned that a free particle can be written by wave functions

$$\psi(x) = Ae^{\pm ikx}, \text{ with } k = \frac{\sqrt{2m(E-V)}}{\hbar}$$

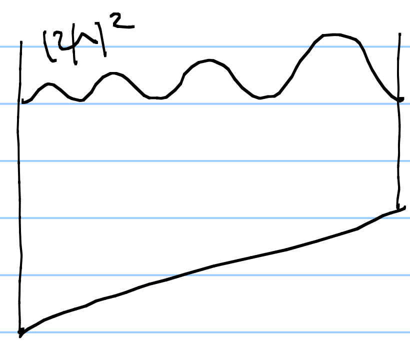
We used this formulation in the context of the step potential.



$$k_1 = \frac{\sqrt{2mE}}{\hbar}$$

$$k_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar}$$

Now if we consider a situation where $V(x)$ continuously changes as a function of x, as in the mid term problem



$$k = \frac{2\pi}{\lambda}$$

k-large $\longrightarrow$ k-small [k-large = λ-small]

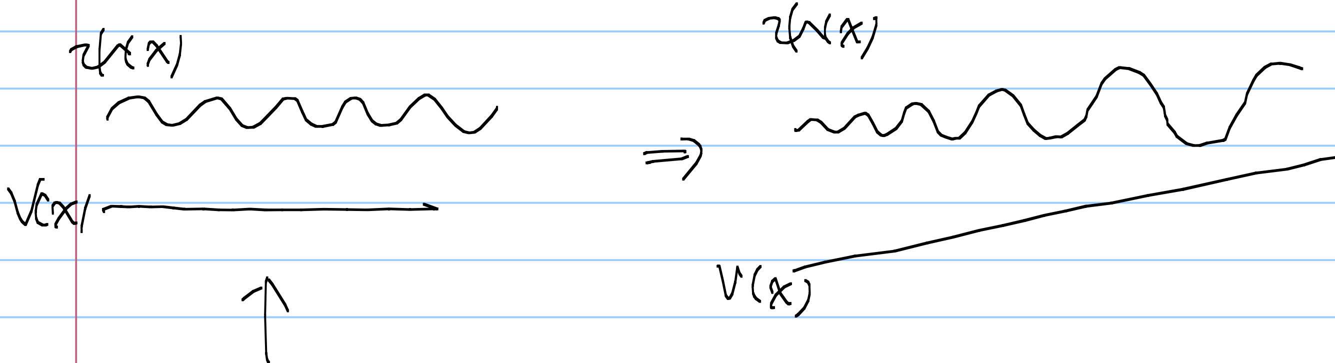
$|\psi|$-small $|\psi|$-large

In such a case, we can approximately write

$$\psi(x) \approx \frac{C}{\sqrt{k(x)}} e^{\pm i\int k(x)\,dx}, \text{ with}$$

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

$|\psi(x)|^2 \propto \frac{1}{k(x)} \propto \frac{1}{p(x)}$; implying that the faster the particle is, the lower the propability of finding the particle at that location.

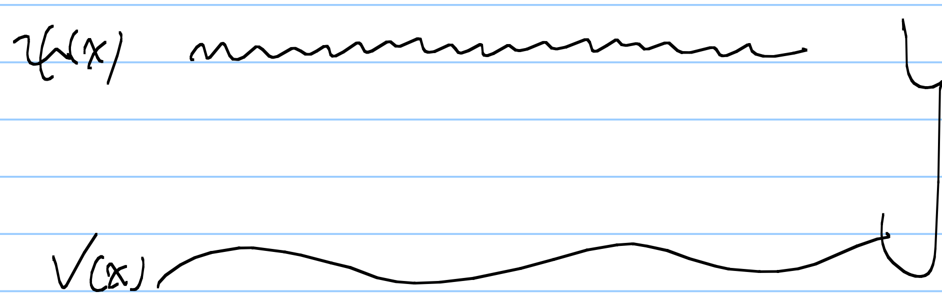


Free particle

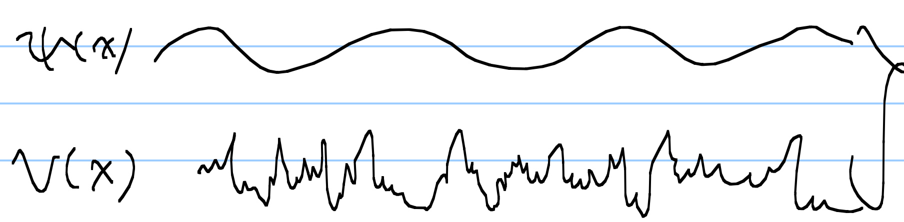
This approximation is called WKB approximation.

The WKB approximation is valid when the potential energy changes slowly compared to the wave length λ.

In other words,



WKB works

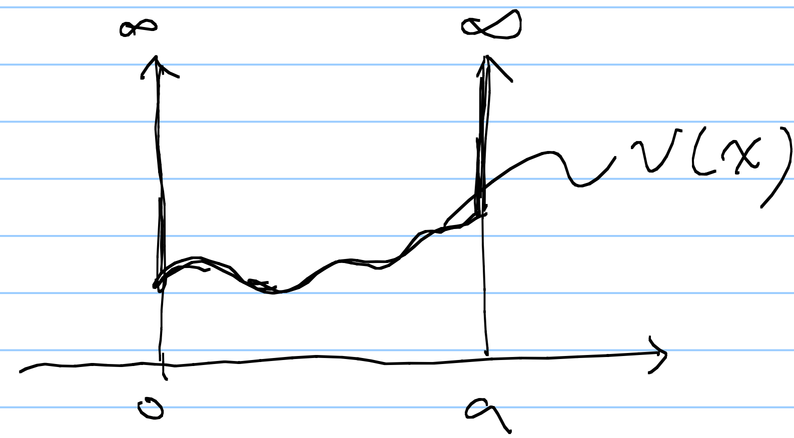


WKB does not work

So WKB approximation works well for large k values: in other words, when E is large compared to $V(x)$.

Large E case is usually called semi-classical regime.

$\boxed{\text{Ex 1}}$



Using the WKB approximation,

$$\psi(x) = \frac{1}{\sqrt{k(x)}}\left(C_+ e^{i\phi(x)} + C_- e^{-i\phi(x)}\right)$$

$$\text{or} = \frac{1}{\sqrt{k(x)}}\left(C_1 \sin\phi(x) + C_2 \cos\phi(x)\right)$$

, where $\phi(x) = \int_0^x k(x')dx' > 0$

$\psi(x=0) = \psi(x=a) = 0$

$\Rightarrow C_1 \sin(0) + C_2 \cos(0) = 0$

$\Rightarrow C_2 = 0$

, $C_1 \sin(\phi(a)) = 0 \Rightarrow \phi(a) = n\pi$

, $n = 1, 2, 3, \ldots$

$$\Rightarrow \quad \phi(a) = \boxed{\int_0^a k(x)\,dx = n\pi}$$

with $k(x') = \dfrac{\sqrt{2m(E - V(x'))}}{\hbar}$

For a special case of $V(x) = 0$, i.e, the standard infinite square well case,

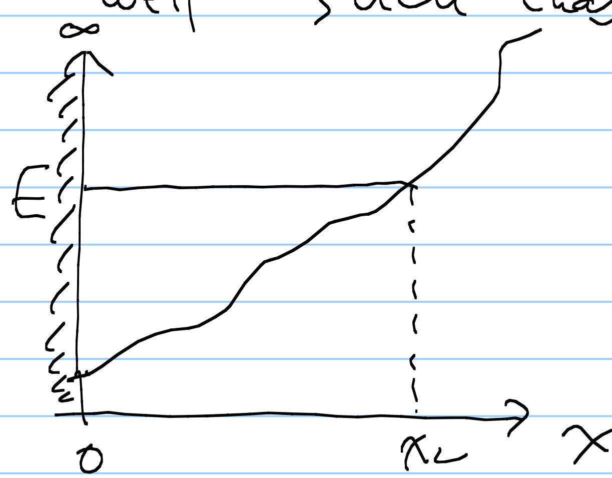
$$\int_0^a \frac{\sqrt{2mE}}{\hbar}\, dx' = n\pi$$

$$\Rightarrow \quad \frac{\sqrt{2mE}}{\hbar} \cdot a = n\pi$$

$$\Rightarrow \quad E = \frac{1}{2m}\left(\frac{n\pi}{a}\hbar\right)^2 = \frac{\hbar^2}{2m}\left(\frac{n\pi}{a}\right)^2$$

, which is exactly what we have obtained previously by solving the Schrödinger equation.

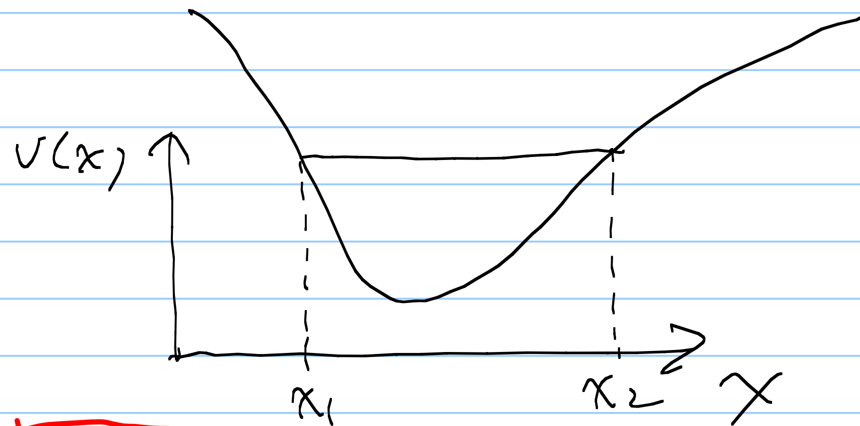
Now if one side of the infinite potential well is replaced by a non-vertical well such that



Then using the so-called connection formulas described in 8.3, the WKB approximation yields

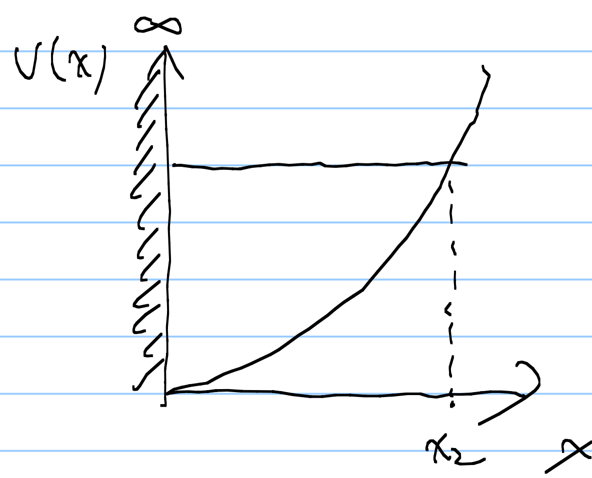
$$\boxed{\int_0^{x_2} k(x)\,dx = \left(n-\frac{1}{4}\right)\pi}$$

Similarly for a potential well with no vertical walls such that



$$\boxed{\int_{x_1}^{x_2} k(x)\,dx = \left(n-\frac{1}{2}\right)\pi}$$

$\boxed{\text{Ex. 2}}$



$$V(x) = \begin{cases} \frac{1}{2} m\omega^2 x^2, & \text{if } x > 0 \\ 0, & \text{else} \end{cases}$$

Since only one side has a vertical well we need to use the second condition from above

$$\int_0^{x_2} k(x)\,dx = (n - \tfrac{1}{4})\pi$$

$$k(x) = \frac{\sqrt{2m(E-U(x))}}{\hbar} = \frac{\sqrt{2m(E-\frac{1}{2}m\omega^2 x^2)}}{\hbar}$$

$$= \frac{1}{\hbar}\sqrt{2m \cdot \tfrac{1}{2}m\omega^2\left(E \cdot \tfrac{2}{m\omega^2} - x^2\right)}$$

$$= \frac{m\omega}{\hbar}\sqrt{x_2^2 - x^2}$$

, with $x_2 = \frac{1}{\omega}\sqrt{\frac{2E}{m}}$

So $\frac{m\omega}{\hbar}\int_0^{x_2}\sqrt{x_2^2 - x^2}\,dx = (n - \tfrac{1}{4})\pi$

$$\Rightarrow \int_0^{\frac{\pi}{2}} x_2^2 \sqrt{1-\sin^2\theta}\,\cos\theta\,d\theta = x_2^2\int_0^{\frac{\pi}{2}}\cos^2\theta\,d\theta$$

$[x = x_2 \sin\theta \Rightarrow dx = x_2 \cos\theta\,d\theta]$

$[\cos^2\theta = \frac{\cos 2\theta + 1}{2}]$

$$\Rightarrow x_2^2 \int_0^{\frac{\pi}{2}} \frac{\cos 2\theta + 1}{2}\,d\theta$$

$$= \frac{x_2^2}{2}\left[-\frac{\sin 2\theta}{2} + x\right]_0^{\frac{\pi}{2}}$$

$$= \frac{\pi}{4}x_2^2$$

So $\frac{\pi}{4}x_2^2 \cdot \frac{m\omega}{\hbar} = (n - \tfrac{1}{4})\pi$

$$\Rightarrow \frac{\cancel{\pi} m\cancel{\omega}}{\cancel{4}_{2}\hbar} \cdot \frac{1}{\omega\cancel{^2}} \frac{\cancel{2}E}{\cancel{m}} = (n - \tfrac{1}{4})\cancel{\pi}$$

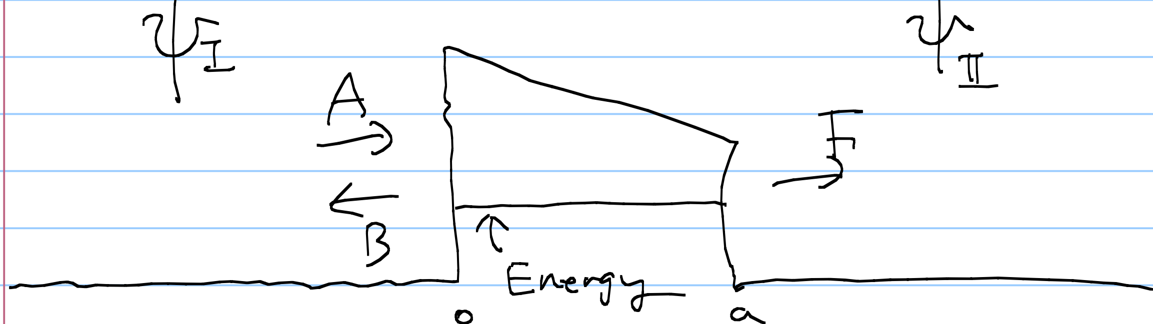
$$\Rightarrow E = 2\hbar\omega(n - \tfrac{1}{4}) = \hbar\omega(2n - \tfrac{1}{2})$$

$$= \left(\frac{3}{2}, \frac{7}{2}, \frac{11}{2}, \cdots\right)\hbar\omega$$

which are the odd energies of the full harmonic oscillator.

* $\boxed{\text{Tunneling}}$

Even if WKB approximation can be used for bound states as discussed above, its most popular application is for tunneling problems

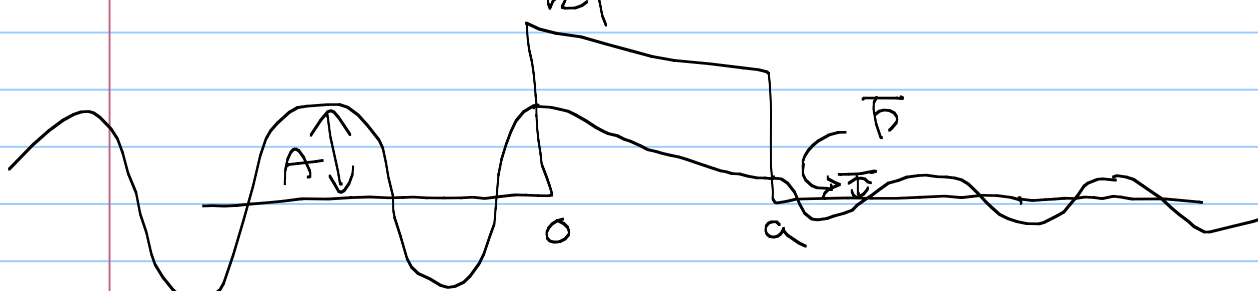


$$\psi_{I} = \frac{1}{\sqrt{k_1}}\left(A e^{ik_1x} + B e^{-ik_1x}\right)$$

$$\psi_{II} = \frac{1}{\sqrt{k_2}} F e^{-ik_2x}$$

$$\Rightarrow T = \frac{\frac{|F|^2}{k_2}}{\frac{|A|^2}{k_1}} = \frac{|F|^2}{|A|^2}$$

if $k_1 = k_2 = k$



Between 0 and a, the WKB approximation leads to

$$\psi(x) = \frac{C}{\sqrt{\kappa(x)}} e^{\int_0^x \kappa(x')dx'} + \frac{D}{\sqrt{\kappa(x)}} e^{-\int_0^x \kappa(x')dx'}$$

, where $\kappa(x) = \frac{k(x)}{i} = \frac{\sqrt{2m(E-V(x))}}{i\hbar}$

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

If the tunneling barrier is very high or very wide, that is, if the tunneling probability is very low, then the exponentially diverging first term should have a negligible coefficient (C), then we can approximately keep only the exponentially decaying second term.

In this case, $\frac{|F|}{|A|} \sim e^{-\int_0^a \kappa(x)dx}$

$$\Rightarrow \boxed{T = \left|\frac{F}{A}\right|^2 \approx e^{-2\int_0^a \kappa(x)dx}}$$

with $\kappa(x) \equiv \frac{\sqrt{2m(V(x)-E)}}{\hbar}$

This expression is widely used to describe a variety of tunneling behaviours, such as tunnel junctions, scanning tunneling microscopes