Chapter 9: The WKB Approximation

Back to time independent problems. WKB stands for Wentzel, Kramers, Brillouin.

WKB is a technique to obtain approximate solutions to time independent problems, mainly in 1D or where only "r" matters in 3D.

Main intuitive idea: suppose you have a potential V(x) totally constant, no imperfections. Then, the solution if $E > V(x)$ is:

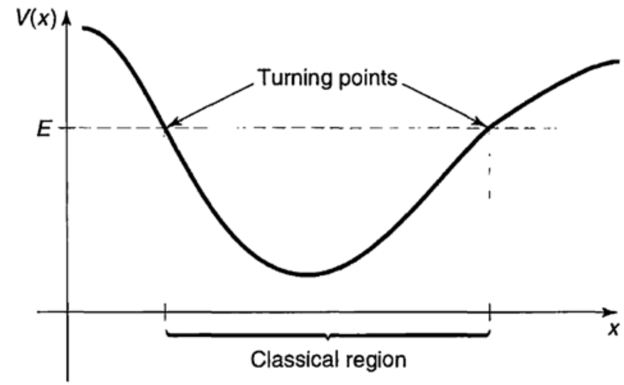
$$\psi(x) = Ae^{\pm ikx} \qquad k \equiv \sqrt{2m(E-V)}/\hbar \qquad \lambda = 2\pi/k$$

Of course, here *A* is constant, *k* is constant, λ is constant.

However, a perfect flat potential is unlikely. Suppose V(x) is "nearly" flat but changes very slowly with x, i.e. over distances much larger than λ. Then, the solution cannot be too different: A, k,… will now be smooth slowly varying functions of x.

9.1: The "Classical" Region

Let us first consider the case E>V(x), i.e. the classical region. First, we will not make any approximation and find exact equations for amplitude and phase. Then, we will make the WKB approximation.



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

Exactly, this can be written $\frac{d^2\psi}{dx^2} = -\frac{p^2}{\hbar^2}\psi$ where $p(x) \equiv \sqrt{2m[E - V(x)]}$

Propose $\psi(x) = A(x)e^{i\phi(x)}$, which is generic for any wave function. Here both *A(x)* and $\phi(x)$ are real functions, dependent on x.

$$\frac{d\psi}{dx} = (A' + iA\phi')e^{i\phi}$$

$$\frac{d\psi}{dx} = (A' + iA\phi')e^{i\phi} \longrightarrow \frac{d^2\psi}{dx^2} = [A'' + 2iA'\phi' + iA\phi'' - A(\phi')^2]e^{i\phi}$$

$$\frac{d^2\psi}{dx^2} = -\frac{p^2}{\hbar^2}\psi \longrightarrow A'' + 2iA'\phi' + iA\phi'' - A(\phi')^2 = -\frac{p^2}{\hbar^2}A$$

$$p(x) \equiv \sqrt{2m[E - V(x)]}$$

Real part:

$$A'' - A(\phi')^2 = -\frac{p^2}{\hbar^2}A$$

$$A'' = A\left[(\phi')^2 - \frac{p^2}{\hbar^2}\right]$$

Cannot be solved unless we assume $A''\sim 0$, i.e. amplitude varies slowly with x.

Imaginary part:

$$2A'\phi' + A\phi'' = 0$$

$$\left(A^2\phi'\right)' = 0$$

$$A^2\phi' = C^2$$

Exact: $$A = \frac{C}{\sqrt{\phi'}}$$

Again, the two exact eqs. are:

$$A'' = A\left[(\phi')^2 - \frac{p^2}{\hbar^2}\right] \qquad A = \frac{C}{\sqrt{\phi'}}$$

If A″~0, then:

$$(\phi')^2 \cong \frac{p^2}{\hbar^2}$$

$$\phi(x) = \pm\frac{1}{\hbar}\int p(x)\,dx$$

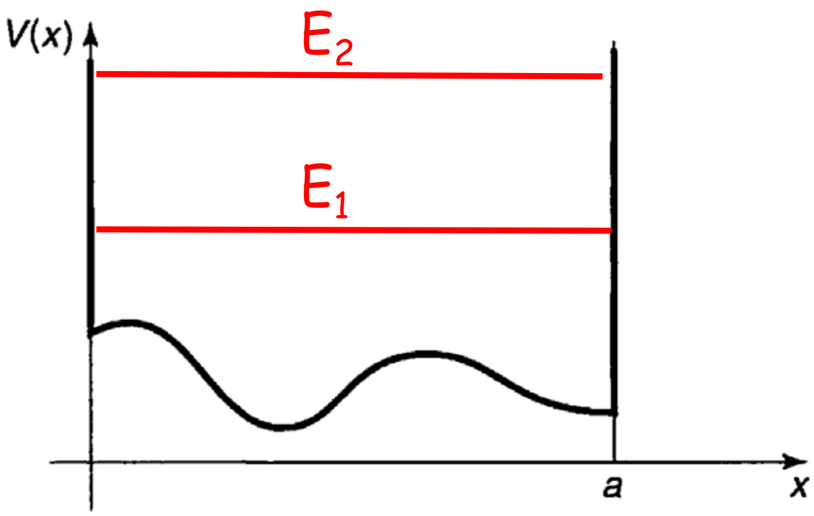
We started with $\psi(x) = A(x)e^{i\phi(x)}$ then we arrive to:

$$\psi(x) \cong \frac{C}{\sqrt{p(x)}} e^{\pm\frac{i}{\hbar}\int p(x)\,dx}$$

This is the WKB approximation to the wave function.

Note $\phi(x)$ is an indefinite integral i.e. x dependent.
We will need boundary conditions.

Example 9.1: Potential well with two vertical walls.



Assume $E > V(x)$ for all values of x (this may or may not be right, we have to be careful).

We found before:

$$\psi(x) \cong \frac{C}{\sqrt{p(x)}} e^{\pm \frac{i}{\hbar} \int p(x)\, dx}$$

In general, we have to make a linear combination:

$$\psi(x) \cong \frac{1}{\sqrt{p(x)}} \left[C_+ e^{i\phi(x)} + C_- e^{-i\phi(x)} \right]$$

where $\phi(x) = \frac{1}{\hbar} \int_0^x p(x')\, dx'$

$$\psi(x) \cong \frac{1}{\sqrt{p(x)}}\left[C_+ e^{i\phi(x)} + C_- e^{-i\phi(x)}\right]$$

$$\psi(x) \cong \frac{1}{\sqrt{p(x)}}\left[C_1 \sin\phi(x) + C_2 \cos\phi(x)\right]$$

Boundary conditions:

(1) $\psi(x) = 0$ at $x = 0$

This means $C_2 = 0$

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

This means $\phi(a) = n\pi$ $(n = 1, 2, 3, \ldots)$

$$\phi(a) = n\pi \quad (n = 1, 2, 3, \ldots)$$

means

$$\int_0^a p(x)\, dx = n\pi\hbar$$

$$\int_0^a \sqrt{2m[E - V(x)]}\, dx = n\pi\hbar$$

where E is the unknown for each "n".

The integral can be done analytically and an equation for E will be found, or we can find E numerically.

If V(x)=0 inside the well, then of course:

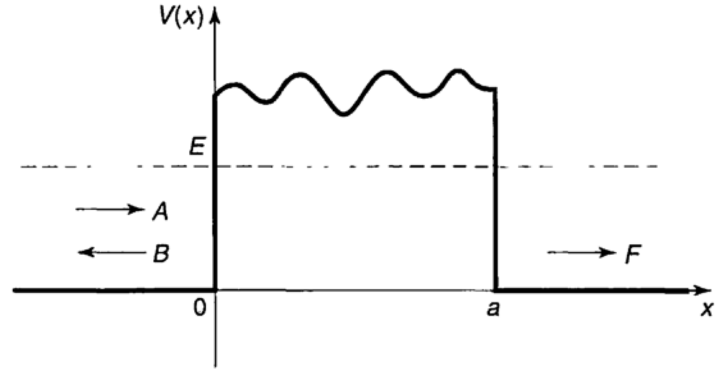
$$\int_0^a \sqrt{2m[E - V(x)]} = \int_0^a \sqrt{2m\ E}\ dx = n\pi\hbar$$

$$\sqrt{2m\ E}\ a = n\pi\hbar$$

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

which is the exact result.

9.2: "Tunneling"



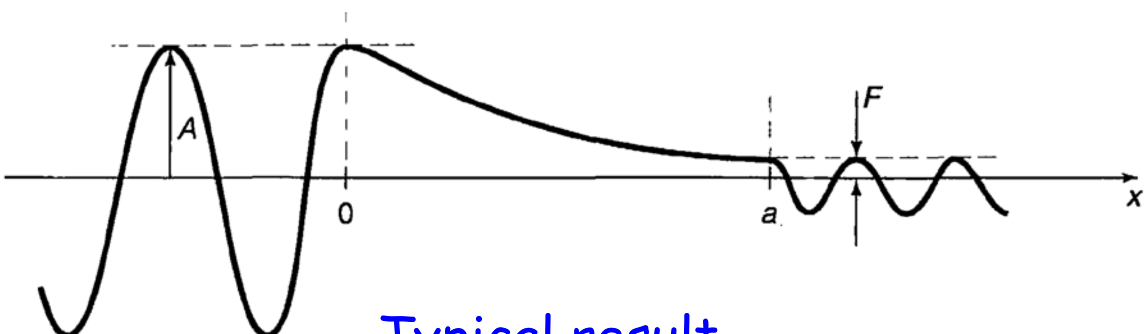
Now consider regions that are NOT classical i.e. E<V(x).

We can repeat all the same and we find:

Indefinite integral, i.e. x dependent

$$\psi(x) \cong \frac{C}{\sqrt{|p(x)|}} e^{\pm \frac{1}{\hbar} \int |p(x)|\, dx}$$

Note: no "*i*" in phase and |..| in *p(x)*



Typical result

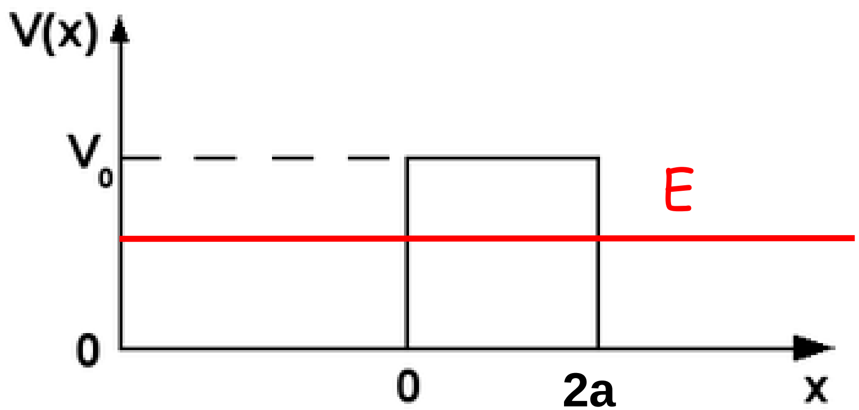
$$\frac{|F|}{|A|} \sim e^{-\frac{1}{\hbar} \int_0^a |p(x')|\, dx'}$$

The result of previous page is a general result:

$$\frac{|F|^2}{|A|^2} \sim e^{-\frac{1}{\hbar}2\int_0^a |p(x')|\,dx'}$$

$$T \cong e^{-2\gamma} \qquad \gamma \equiv \frac{1}{\hbar}\int_0^a |p(x)|\,dx$$

Example,
Problem 8.3:



This is the **exact** result from Ch. 2:

$$T_{\text{exact}} = \frac{1}{1 + \frac{V_0^2}{4E(V_0 - E)}\sinh^2\gamma}$$

where

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

General WKB approx. for tunneling through barrier of width *a*:

We pretend we do not know the exact result and try to use the WKB approximation:

$$T \cong e^{-2\gamma} \qquad \gamma \equiv \frac{1}{\hbar}\int_0^a |p(x)|\,dx$$

Width of barrier is 2*a* here:

$$\gamma = \frac{1}{\hbar}\int |p(x)|\,dx = \frac{1}{\hbar}\int_0^{2a} \sqrt{2m(V_0 - E)}\,dx = \frac{2a}{\hbar}\sqrt{2m(V_0 - E)}$$

Then, WKB prediction for tunneling is:

$$T \approx e^{-4a\sqrt{2m(V_0 - E)}/\hbar}$$

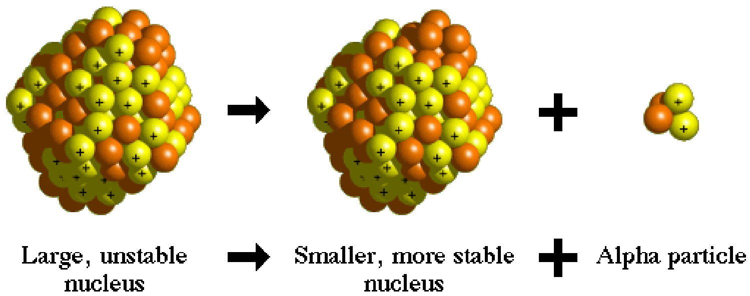
$$T_{\text{exact}} = \frac{1}{1 + \frac{V_0^2}{4E(V_0 - E)}\sinh^2\gamma} \quad \Bigg| \quad \sinh\gamma = \tfrac{1}{2}(e^{\gamma} - e^{-\gamma}) \approx \tfrac{1}{2}e^{\gamma} \quad \Bigg| \quad \sinh^2\gamma \approx \tfrac{1}{4}e^{2\gamma}$$

$$T_{\text{exact}} \approx \frac{1}{1 + \frac{V_0^2}{16E(V_0 - E)}e^{2\gamma}} \approx \left\{\frac{16E(V_0 - E)}{V_0^2}\right\} e^{-2\gamma}$$

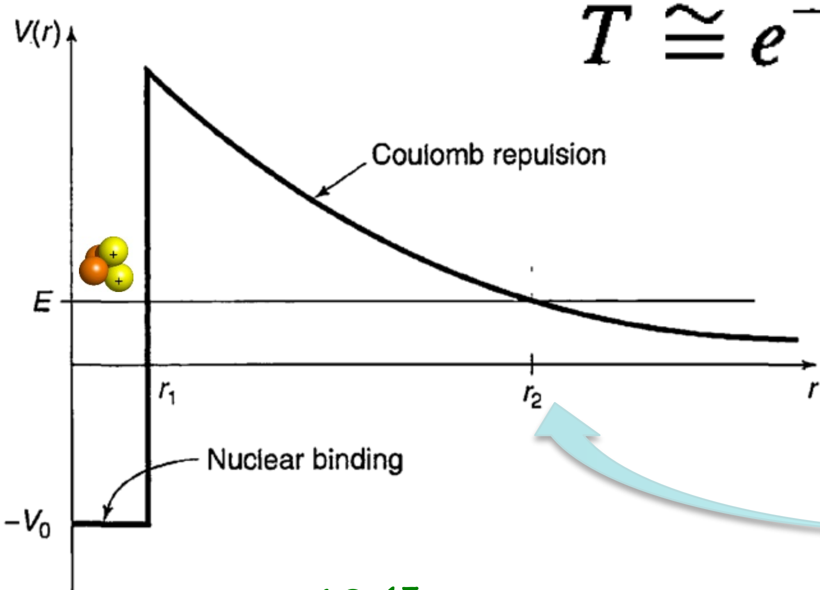
$$\gamma_{\text{exact}} = \frac{2a}{\hbar}\sqrt{2m(V_0 - E)}$$

Dominant exponential is properly reproduced by WKB

Famous example: Gamow's theory of alpha decay (1928)



$$T \cong e^{-2\gamma} \qquad \gamma \equiv \frac{1}{\hbar}\int_0^a |p(x)|\,dx$$



$$\frac{1}{4\pi\epsilon_0}\frac{2Ze^2}{r_2} = E$$

size $r_1 \sim 10^{-15}$ m

$$\gamma = \frac{1}{\hbar}\int_{r_1}^{r_2}\sqrt{2m\left(\frac{1}{4\pi\epsilon_0}\frac{2Ze^2}{r} - E\right)}\,dr$$

Turns out, the integral can be done exactly, and moreover it can be simplified considerably if $r_1 \ll r_2$

$$\gamma = \frac{1}{\hbar}\int_{r_1}^{r_2}\sqrt{2m\left(\frac{1}{4\pi\epsilon_0}\frac{2Ze^2}{r} - E\right)}\,dr \longrightarrow K_1\frac{Z}{\sqrt{E}} - K_2\sqrt{Zr_1}$$

Full integral

After some approximations

where

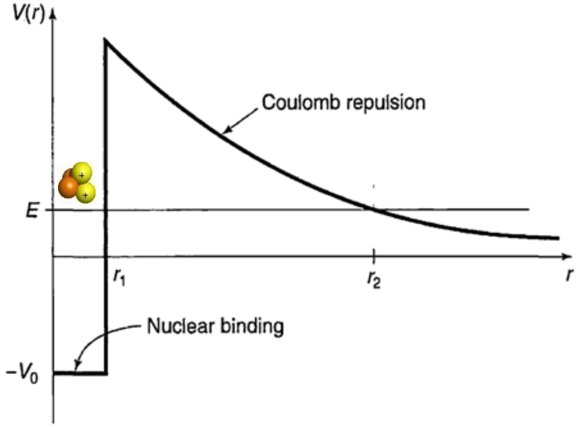
$$K_1 \equiv \left(\frac{e^2}{4\pi\epsilon_0}\right)\frac{\pi\sqrt{2m}}{\hbar} = 1.980\ \mathrm{MeV}^{1/2}$$

$$K_2 \equiv \left(\frac{e^2}{4\pi\epsilon_0}\right)^{1/2}\frac{4\sqrt{m}}{\hbar} = 1.485\ \mathrm{fm}^{-1/2}$$

1 fm = 10^{-15} m is the size of a typical nucleus

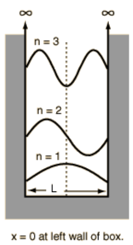
As "m" we use the mass of an alpha particle ~ 4 proton masses

Z is the positive charge of the nucleus



If alpha particles have an average velocity "v" inside the well, then to travel from r=0 to $r=r_1$ it takes $t=r_1/v$, i.e. hits the walls with a period $2r_1/v$. At each collision the probability of **remaining trapped** is $e^{+2\gamma}$ (or prob. of escape is $e^{-2\gamma}$)

The **lifetime** then is $\tau = (2r_1/v)\, e^{+2\gamma}$.

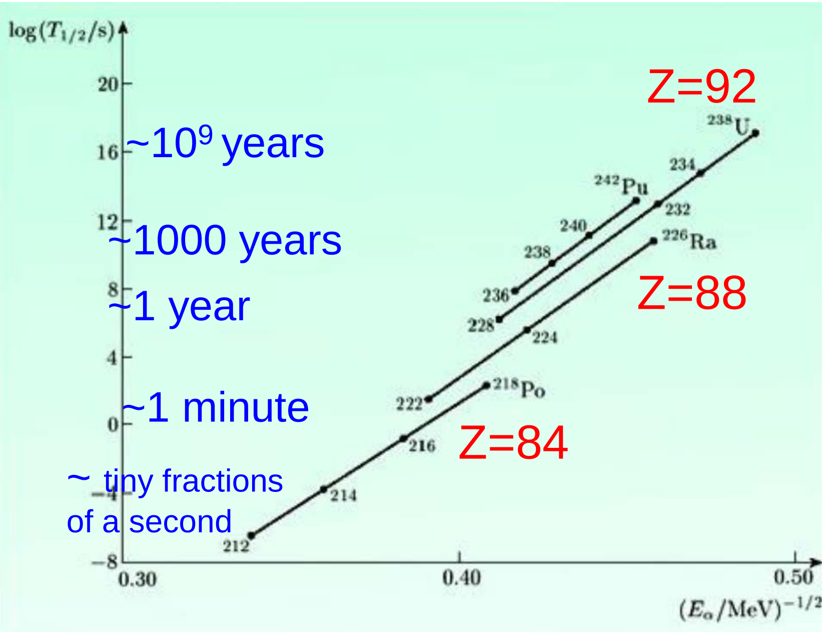


The energy of the alpha particle is not arbitrary but resembles that of a square well.

Then, $\ln(\tau)= \ln(2r_1/v) +2\gamma$ with

$$\gamma \sim K_1 \frac{Z}{\sqrt{E}} - K_2 \sqrt{Z r_1}$$

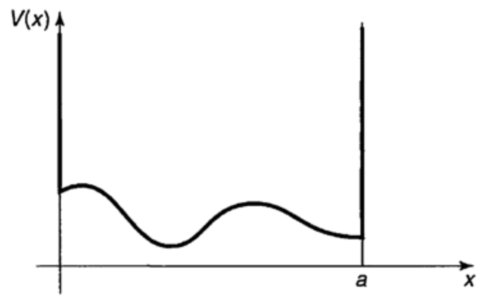
Experiments confirm that lifetime depends ~ linearly on 1/sqrt{Eα} on a range of lifetimes from 10^9 years to tiny fractions of seconds!
(Geiger-Nuttall law)

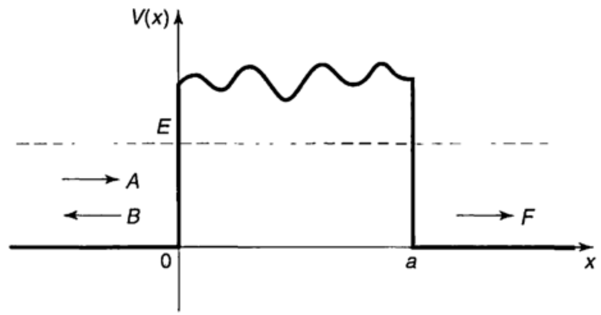


Lecture ended here. The next three pages are only for completeness. It is not material that you need to know for Test 3 (final exam).

9.3: The connection region

In many examples we use the WKB approximation in cases V(x) has vertical walls.

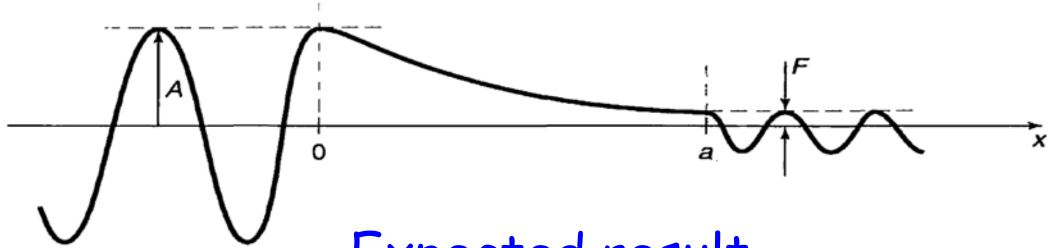




But in most real situations, this is not the case, such as in alpha decay. We may try the "usual" procedure:

$$\psi(x) \cong \begin{cases} \frac{1}{\sqrt{p(x)}}\left[Be^{\frac{i}{\hbar}\int_x^0 p(x')\,dx'} + Ce^{-\frac{i}{\hbar}\int_x^0 p(x')\,dx'}\right], & \text{if } x < 0, \\ \frac{1}{\sqrt{|p(x)|}} De^{-\frac{1}{\hbar}\int_0^x |p(x')|\,dx'}, & \text{if } x > 0. \end{cases}$$

Naively we may simply be tempted to try to match coefficients at the boundary.



Expected result

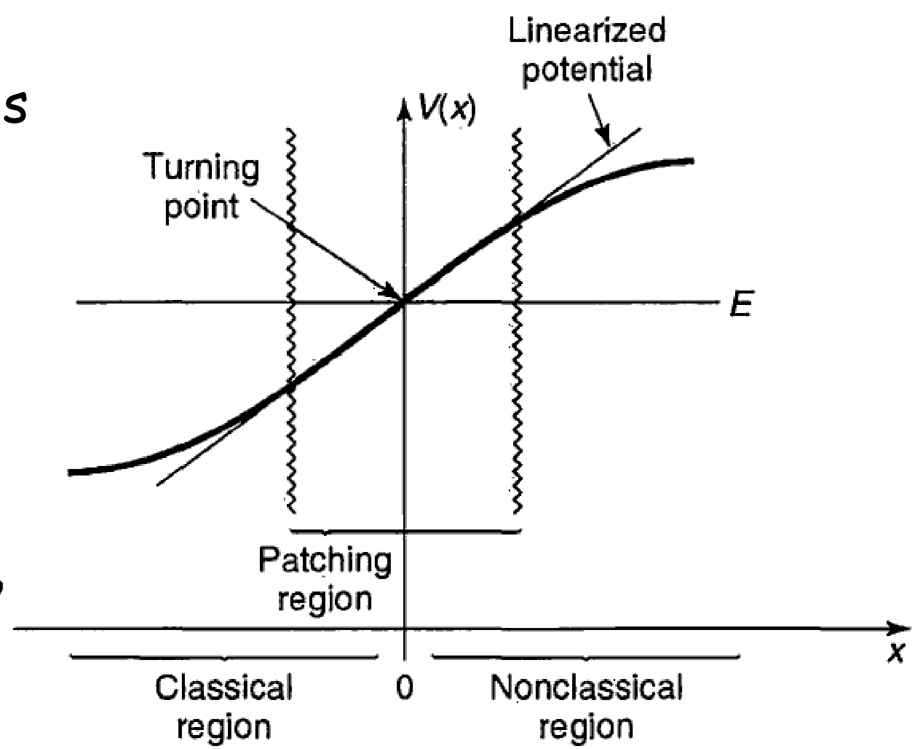
However, at exactly the "x" where we switch from classical to non-classical then p(x) = V(x)-E is zero. Then, WKB wave functions explode. Not realistic!

$$\psi(x) \cong \frac{C}{\sqrt{|p(x)|}} e^{\pm \frac{1}{\hbar}\int |p(x)|\, dx}$$

In practice a "patching procedure" is followed, where a "third region" is introduced where the potential is linearized

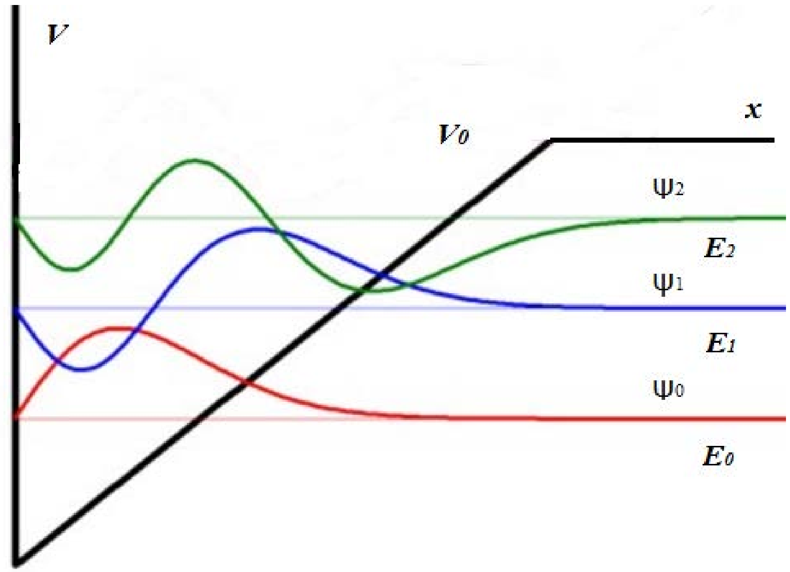
$$V(x) \cong E + V'(0)x$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_p}{dx^2} + [E + V'(0)x]\psi_p = E\psi_p$$



A problem with a linear potential is exactly solvable and leads to the Airy functions, complicated functions usually given in an integral form. They are oscillatory on one side and exponential on the other.

If we had a sharp wall on one side (not the actual problem at hand) the shape of the Airy functions is as shown (leading to bound states):



The WKB patching procedure would be too complicated to describe in detail, just be aware of its existence.