Lec 26: 10/28/2009

WKB Approximation and Connection with Path Integrals:

To show this connection, we consider two cases:

1- $E > V(x)$ everywhere.

We have:

$$\psi(x,t) = \int U(x,t;x')\,\psi(x')\,dx'$$

$$U(x,t;x') = A \sum_{\text{all paths}} e^{iS/\hbar}$$

Lets focus on the classical path (that exists for $E>V$).

Then:

$$S_{cl} = \int_0^t (T-V)\,dt' = \int_0^t (\underbrace{-T-V}_{-E} + 2T)\,dt' = -\int_0^t E\,dt'$$

$$+ \int_0^t 2T\,dt'$$

$$\int_0^t E\,dt' = Et$$

$$\int_0^t 2T\,dt' = \int_0^t p\,v\,dt' = \int_{x_1}^{x} p(x'')\,dx''$$

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

Thus:

$$\Psi(x,t) \simeq A\, e^{-\frac{iEt}{\hbar}} \int e^{\frac{i}{\hbar}\int_{x_1}^{x} p(x'')\,dx''} \Psi(x')\,dx'$$

Since $\Psi(x,t)$ is an energy eigenstate with eigenvalue E, we know that:

$$\Psi(x,t) = \Psi(x)\, e^{-\frac{iEt}{\hbar}}$$

Implying that:

$$\Psi(x) \simeq A \int e^{\frac{i}{\hbar}\int_{x_1}^{x} p(x'')\,dx''} \Psi(x')\,dx'$$

Taking the derivative of both sides with respect to x, we find:

$$\frac{d\Psi(x)}{dx} = \frac{i}{\hbar} p(x)\Psi(x) \Rightarrow \frac{d\Psi(x)}{\Psi(x)} = \frac{i}{\hbar} p(x)\,dx$$

$$\Rightarrow \Psi(x) \propto e^{\frac{i}{\hbar}\int p(x')\,dx'} \Rightarrow \Psi(x) \simeq \Psi(x_0)\, e^{\frac{i}{\hbar}\int_{x_0}^{x} p(x')\,dx'}$$

Therefore, we can find the leading order term in the WKB approximation just by considering the classical trajectory in the path integral formalism.

To find the $\frac{1}{\sqrt{p(x)}}$ piece, we need to sum over all paths that are sufficiently close to the classical trajectory and make the significant contribution. This can be done in the so called "saddle point approximation", which involves Gaussian integrals, but it is beyond the scope of this course.

An important point to mention is that the expression $\psi(x) = \psi(x_0)\, e^{\frac{i}{\hbar}\int_{x_0}^{x} p(x')\,dx'}$ is exact for a particle in constant potential (p is constant in this case). This can be understood from path integrals since for $V = \text{const}$, we know that:

$$\sum_{\text{all path}} e^{iS/\hbar} = A\, e^{iS_{cl}/\hbar}$$

A some constant

Therefore S_{cl} is the only thing that we need in this case.

2. $E < V(x)$ everywhere. In this case there exists no classical trajectory. However, we can use the imaginary time method:

$\tau = it \Rightarrow t = -i\tau$

$$U(x, \tau; x') = \sum_{\text{all paths}} e^{-S/\hbar}$$

$$S = \int_0^{\tau} (T + V)\, d\tau' \qquad T = \frac{1}{2} m \left(\frac{dx}{d\tau}\right)^2$$

$E < V \Rightarrow -E > -V$ (imaginary time energy $>$ imaginary time potential)

Therefore in the imaginary time the energy is greater than the potential and a classical path exists.

We can now repeat all the steps as in case 1 above. However, $p = \pm\sqrt{2m(V-E)}$ in the imaginary time. Therefore we find:

$$\psi(x) \simeq \psi(x_0)\, e^{-\frac{1}{\hbar}\int_{x_0}^{x} p(x')\,dx'} = \psi(x_0)\, e^{\frac{i}{\hbar}\int_{x_0}^{x} p(x')\,dx'}$$

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

Since $E<V$, the $\sqrt{2m(E-V)}$ is an imaginary number.

We can also write it in the following form:

$$\psi(x) \approx \psi(x_0)\, e^{\pm \frac{1}{\hbar}\int_{x_0}^{x} \sqrt{2m(V-E)}\, dx'}$$

If we also consider paths that are sufficiently closed to the classical trajectory (in imaginary time), then we find:

$$\psi(x) \approx \frac{A}{\sqrt{p(x)}}\, e^{\pm \frac{1}{\hbar}\int_{x_0}^{x} \sqrt{2m(V-E)}\, dx'}$$

In short, for $E>V$ the solutions are (in the WKB approximation):

$$\psi(x) \approx \frac{A}{\sqrt{p(x)}}\, e^{\pm \frac{i}{\hbar}\int_{x_0}^{x} \sqrt{2m(E-V)}\, dx'}$$

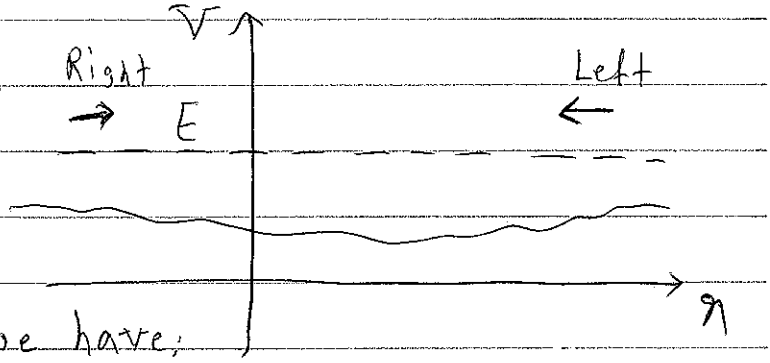
And for $E<V$:

$$\psi(x) \approx \frac{A}{\sqrt{p(x)}}\, e^{\pm \frac{1}{\hbar}\int_{x_0}^{x} \sqrt{2m(V-E)}\, dx'}$$

Which of the signs are chosen will depend on the

case at hand. For a right-moving particle with $E>V$, we have:

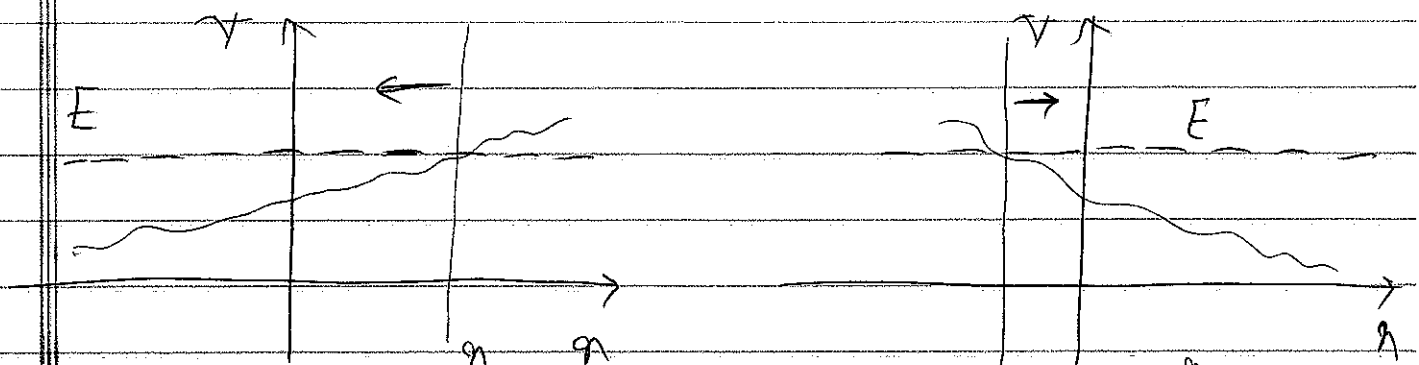
$$\psi(x) = \frac{A}{\sqrt{p(x)}} e^{\frac{i}{\hbar}\int_{x_0}^{x}\sqrt{2m(E-V)}\,dx'}$$



While for a left-moving one we have:

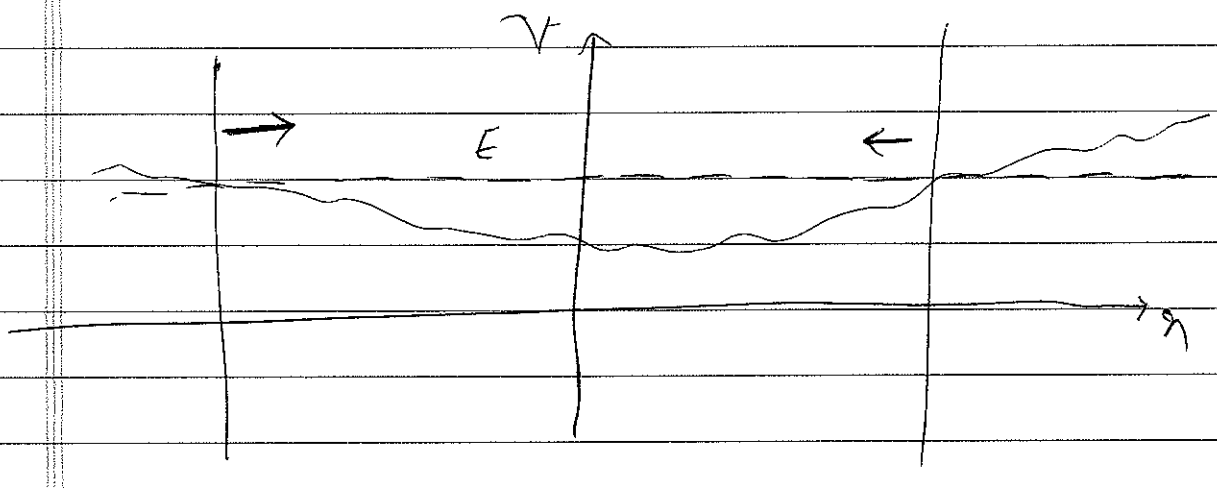
$$\psi(x) = \frac{A}{\sqrt{p(x)}} e^{-\frac{i}{\hbar}\int_{x_0}^{x}\sqrt{2m(E-V)}\,dx'}$$

For the following potentials, in the region where $E>V$, we have a superposition of the two solutions (due to reflection at the point $E=V$ changes sign):



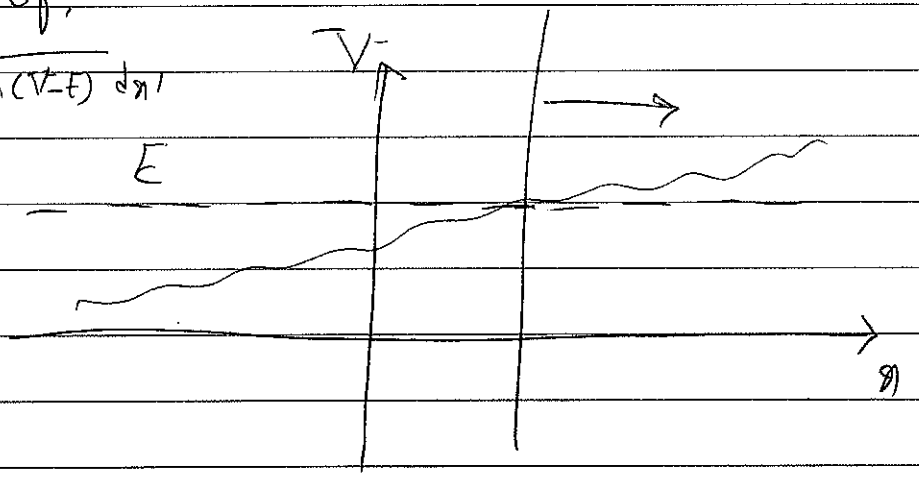
$$\psi = \frac{A}{\sqrt{p(x)}} e^{\frac{i}{\hbar}\int_{x_0}^{x}\sqrt{2m(E-V)}\,dx'} + \frac{B}{\sqrt{p(x)}} e^{-\frac{i}{\hbar}\int_{x_0}^{x}\sqrt{2m(E-V)}\,dx'}$$

And similarly for a bound state:

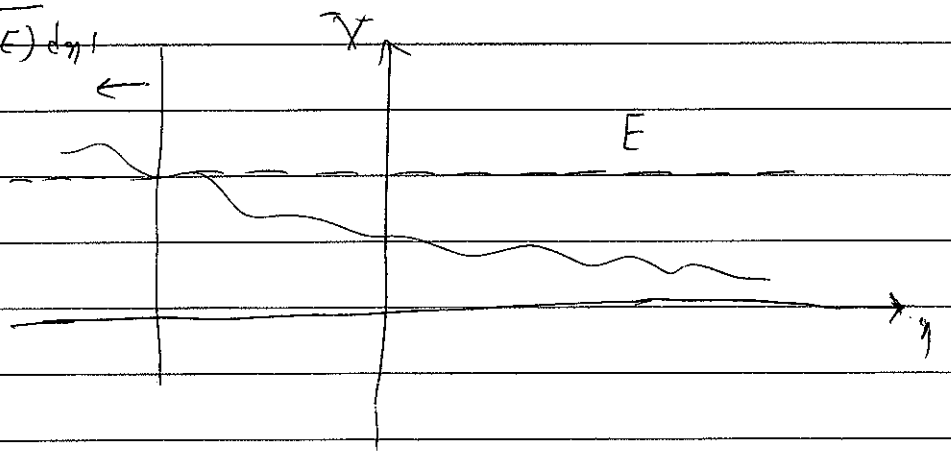


In the case $E < V_0$ if that regions extends to ∞, only one of the signs are chosen so that the solution will not blow up:

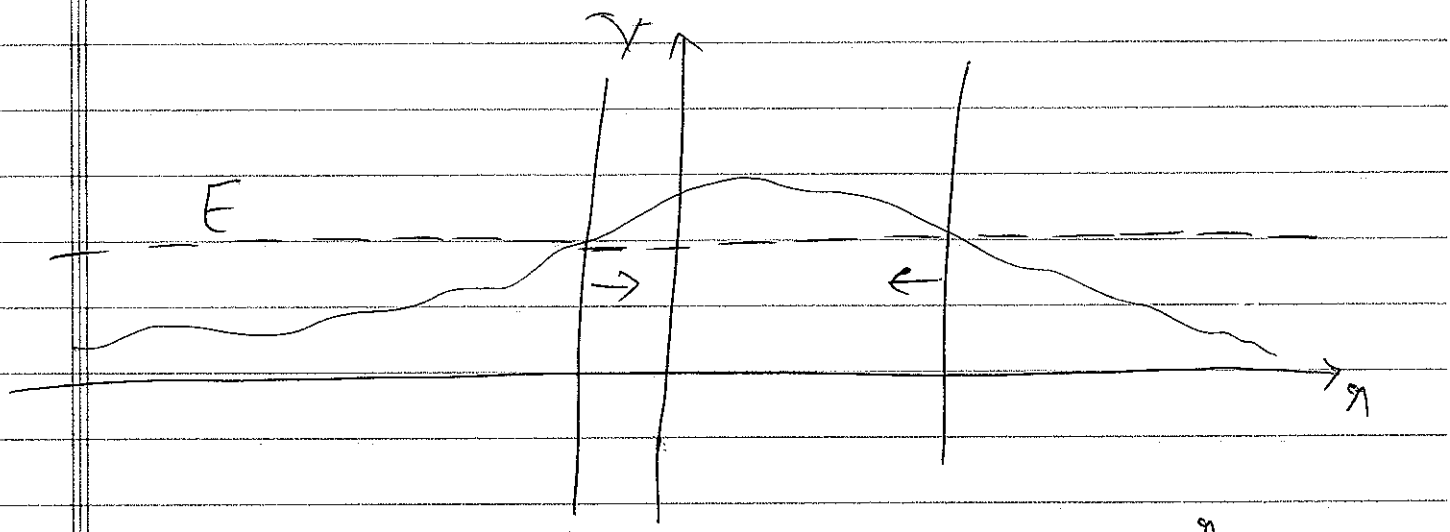
$$\psi(x) \approx \frac{A}{\sqrt{p(x)}} e^{-\frac{1}{\hbar}\int_{x_0}^{x} \sqrt{2m(V-E)}\, dx'}$$



$$\psi(x) \approx \frac{A}{\sqrt{p(x)}} e^{\frac{1}{\hbar}\int_{x_0}^{x} \sqrt{2m(V-E)}\, dx'}$$



In a finite region where $E<V$, we have a superposition of the two solutions:



$$\psi(x) \simeq \frac{A}{\sqrt{p(x)}} e^{\frac{1}{\hbar}\int_{x_0}^{x}\sqrt{2m(V-E)}\,dx'} + \frac{B}{\sqrt{p(x)}} e^{-\frac{1}{\hbar}\int_{x_0}^{x}\sqrt{2m(V-E)}\,dx'}$$

We reiterate that the WKB approximation is not valid near the classical turning points (where $E=V$). We need to use a different approximation around the turning points, and then glue the solution there to those far away obtained using the WKB method. That we will do later on.