PHY456H1F: Quantum Mechanics II. Lecture 12 (Taught by Mr. Federico Duque Gomez). WKB Method

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Contents

1. Disclaimer.

Peeter's lecture notes from class. May not be entirely coherent.

2. WKB (Wentzel-Kramers-Brillouin) Method.

This is covered in §24 in the text [1]. Also §8 of [2].
We start with the 1D time independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2U}{dx^2} + V(x)U(x) = EU(x) \tag{1}$$

which we can write as

$$\frac{d^2U}{dx^2} + \frac{2m}{\hbar^2}(E - V(x))U(x) = 0 \tag{2}$$

Consider a finite well potential as in figure (1)
With

$$k = \frac{2m(E-V)}{\hbar}, \qquad E > V \tag{3}$$

$$\kappa = \frac{2m(V-E)}{\hbar}, \qquad V > E, \tag{4}$$

we have for a bound state within the well

$$U \propto e^{\pm ikx} \tag{5}$$

and for that state outside the well

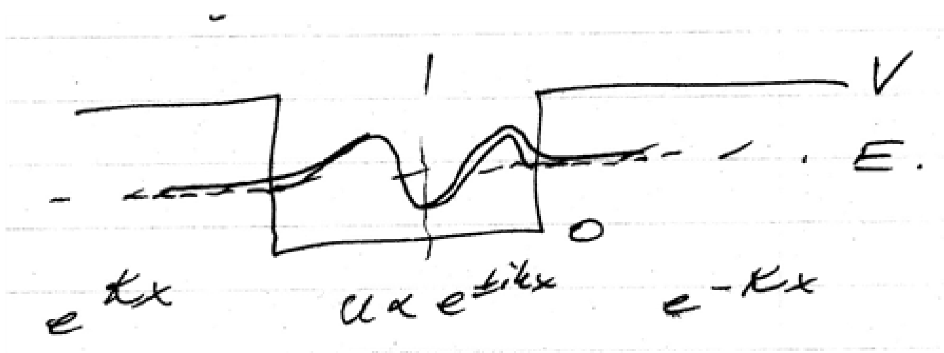

Figure 1: Finite well potential

$$U \propto e^{\pm\kappa x} \tag{6}$$

In general we can hope for something similar. Let's look for that something, but allow the constants k and κ to be functions of position

$$k^2(x) = \frac{2m(E - V(x))}{\hbar}, \qquad E > V \tag{7}$$

$$\kappa^2(x) = \frac{2m(V(x) - E)}{\hbar}, \qquad V > E. \tag{8}$$

In terms of k Schrödinger's equation is just

$$\frac{d^2U(x)}{dx^2} + k^2(x)U(x) = 0. \tag{9}$$

We use the trial solution

$$U(x) = Ae^{i\phi(x)}, \tag{10}$$

allowing $\phi(x)$ to be complex

$$\phi(x) = \phi_R(x) + i\phi_I(x). \tag{11}$$

We need second derivatives

$$\begin{aligned}
(e^{i\phi})'' &= (i\phi' e^{i\phi})' \\
&= (i\phi')^2 e^{i\phi} + i\phi'' e^{i\phi},
\end{aligned}$$

and plug back into our Schrödinger equation to obtain

$$-(\phi'(x))^2 + i\phi''(x) + k^2(x) = 0. \tag{12}$$

For the first round of approximation we assume

$$\phi''(x) \approx 0, \tag{13}$$

and obtain

$$(\phi'(x))^2 = k^2(x), \tag{14}$$

or

$$\phi'(x) = \pm k(x). \tag{15}$$

A second round of approximation we use 15 and obtain

$$\phi''(x) = \pm k'(x) \tag{16}$$

Plugging back into 12 we have

$$-(\phi'(x))^2 \pm ik'(x) + k^2(x) = 0, \tag{17}$$

or

$$\begin{aligned} \phi'(x) &= \pm\sqrt{\pm ik'(x) + k^2(x)} \\ &= \pm k(x)\sqrt{1 \pm i\frac{k'(x)}{k^2(x)}}. \end{aligned} \tag{18}$$

If k' is small compared to k^2

$$\frac{k'(x)}{k^2(x)} \ll 1, \tag{19}$$

we have

$$\phi'(x) = \pm k(x) \pm i\frac{k'(x)}{2k(x)} \tag{20}$$

Integrating

$$\begin{aligned} \phi(x) &= \pm\int dx k(x) \pm i\int dx \frac{k'(x)}{2k(x)} + \text{const} \\ &= \pm\int dx k(x) \pm i\frac{1}{2}\ln k(x) + \text{const} \end{aligned}$$

Going back to our wavefunction, if $E > V(x)$ we have

$$\begin{aligned} U(x) &\sim Ae^{i\phi(x)} \\ &= \exp\left(i\left(\pm\int dx k(x) \pm i\frac{1}{2}\ln k(x) + \text{const}\right)\right) \\ &\sim \exp\left(i\left(\pm\int dx k(x) \pm i\frac{1}{2}\ln k(x)\right)\right) \\ &= e^{\pm i\int dx k(x)} e^{\mp\frac{1}{2}\ln k(x)} \end{aligned}$$

or

$$U(x) \propto \frac{1}{\sqrt{k(x)}} e^{\pm i \int dx k(x)} \tag{21}$$

FIXME: Question: the $\pm$ on the real exponential got absorbed here, but would not $U(x) \propto \sqrt{k(x)} e^{\pm i \int dx k(x)}$ also be a solution? If so, why is that one excluded?

Similarly for the $E < V(x)$ case we can find

$$U(x) \propto \frac{1}{\sqrt{\kappa(x)}} e^{\pm i \int dx \kappa(x)}. \tag{22}$$

Validity

1. V(x) changes very slowly $\implies$ $k'(x)$ small, and $k(x) = \sqrt{2m(E - V(x))}/\hbar$.
2. E very far away from the potential $|(E - V(x))/V(x)| \gg 1$.

3. **Examples**

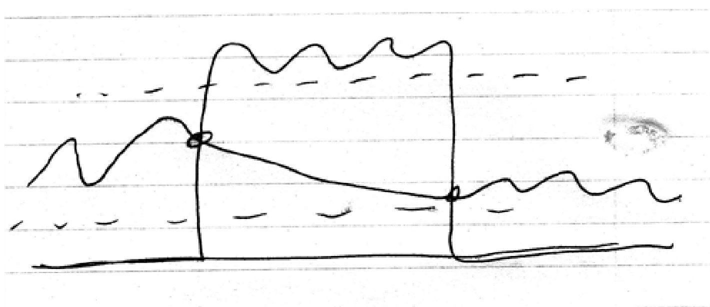

Figure 2: Example of a general potential

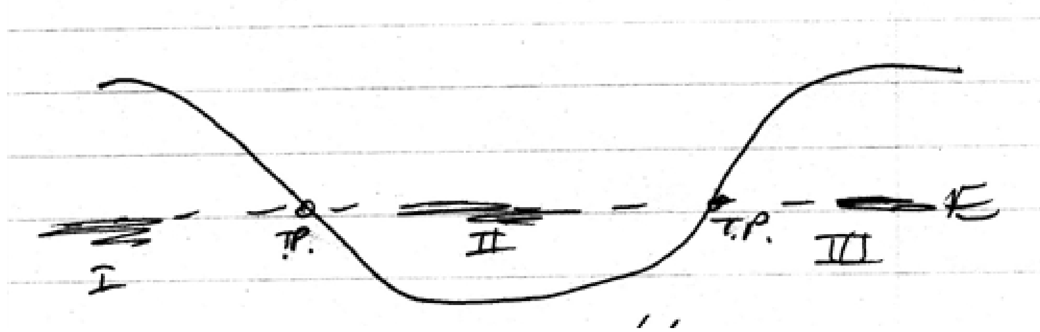

Figure 3: Turning points where WKB won't work

WKB won't work at the turning points in this figure since our main assumption was that

$$\left| \frac{k'(x)}{k^2(x)} \right| \ll 1 \tag{23}$$

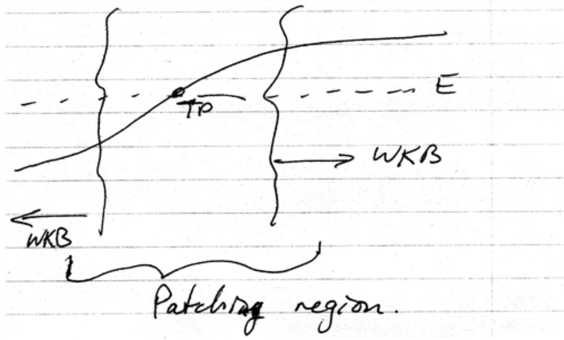

Figure 4: Diagram for patching method discussion

so we get into trouble where $k(x) \sim 0$. There are some methods for dealing with this. Our text as well as Griffiths give some examples, but they require Bessel functions and more complex mathematics.

The idea is that one finds the WKB solution in the regions of validity, and then looks for a polynomial solution in the patching region where we are closer to the turning point, probably requiring lookup of various special functions.

This power series method is also outlined in [3], where solutions to connect the regions are expressed in terms of Airy functions.

References

[1] BR Desai. *Quantum mechanics with basic field theory*. Cambridge University Press, 2009. 2

[2] D.J. Griffiths. *Introduction to quantum mechanics*, volume 1. Pearson Prentice Hall, 2005. 2

[3] Wikipedia. Wkb approximation — wikipedia, the free encyclopedia, 2011. [Online; accessed 19-October-2011]. Available from: http://en.wikipedia.org/w/index.php?title=WKB_approximation&oldid=453833635. 3