WKB APPROXIMATION AND THE RADIAL EQUATION

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 8.13.

So far, we've applied the WKB approximation to one-dimensional potential problems. It might seem that that's all we can manage since WKB is essentially a way of approximating the solution of a one-dimensional ODE. However, we can use it on 3-d problems in those cases where the solution is separable, such as spherically symmetric potentials. For such potentials, the general wave function can be written as the product of a radial function $R(r)$ and a spherical harmonic $Y(\theta,\phi)$.

With the substitution $u(r) \equiv rR(r)$ we found that the radial equation can be written as

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2}+\left(V(r)+\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right)u=Eu \tag{0.1}$$

For the simplest case, we take $l=0$ so the equation becomes

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2}+V(r)u=Eu \tag{0.2}$$

which has exactly the same form as the one-dimensional Schrödinger equation, so we should be able to use WKB to get approximate solutions.

There is one detail we need to work out first, though. In applying WKB to a true 1-d situation, the x coordinate extended to infinity in both directions which allowed us to discard exponential terms that blow up as we approach one extreme or the other. In this equation, the r coordinate starts at 0. One way of handling this is to assume that there is an infinite wall at $r=0$ so that $u(0)=0$. Since $u(r)=rR(r)$, this is a reasonable assumption, since it requires only that $R(0)$ is finite.

We can therefore consider a spherically symmetric potential well with an infinite barrier at $r=0$ and then some potential that increases from $r=0$ out to $r=\infty$. For a given energy E, there will be one turning point r_2 where $E=V(r_2)$.

For a turning point where V is increasing, we've seen that the WKB functions on either side of the turning point are

$$u(r)=\begin{cases}\frac{2D}{\sqrt{p(r)}}\sin\left[\int_r^{r_2}p(r')\ dr'/\hbar+\pi/4\right] & r<r_2\\ \frac{D}{\sqrt{|p(r)|}}\exp\left[-\int_{r_2}^{r}|p(r')|\ dr'/\hbar\right] & r>r_2\end{cases}\tag{0.3}$$

The requirement $u(0)=0$ means that the sine must be zero at $r=0$, so

$$\int_0^{r_2}p(r)\ dr/\hbar+\frac{\pi}{4}=n\pi\tag{0.4}$$

$$\int_0^{r_2}p(r)\ dr=\left(n-\frac{1}{4}\right)\pi\hbar\tag{0.5}$$

Example. We can apply this formula to the potential

$$V(r)=V_0\ln\frac{r}{a}\tag{0.6}$$

The turning point is defined by

$$E=V_0\ln\frac{r_2}{a}\tag{0.7}$$

so the integral 0.5 is

$$\sqrt{2m}\int_0^{r_2}\sqrt{E-V_0\ln\frac{r}{a}}dr=\sqrt{2m}\int_0^{r_2}\sqrt{V_0\ln\frac{r_2}{a}-V_0\ln\frac{r}{a}}dr\tag{0.8}$$

$$=\sqrt{2mV_0}\int_0^{r_2}\sqrt{\ln\frac{r_2}{r}}dr\tag{0.9}$$

We can use the substitution

$$v=\ln\frac{r_2}{r}\tag{0.10}$$

$$dv=\frac{r}{r_0}\left(-\frac{r_0}{r^2}\right)dr\tag{0.11}$$

$$=-\frac{1}{r}dr\tag{0.12}$$

$$=-\frac{e^v}{r_0}dr\tag{0.13}$$

The limits on the integral in terms of v are

$$r = 0 \rightarrow u = \infty \tag{0.14}$$
$$r = r_2 \rightarrow u = 0 \tag{0.15}$$

so the integral transforms as

$$\sqrt{2mV_0}\int_0^{r_2}\sqrt{\ln\frac{r_2}{r}}dr = r_2\sqrt{2mV_0}\int_0^{\infty}\sqrt{v}e^{-v}dv \tag{0.16}$$
$$= r_2\sqrt{2mV_0}\Gamma\left(\frac{3}{2}\right) \tag{0.17}$$
$$= \frac{\sqrt{2\pi mV_0}r_2}{2} \tag{0.18}$$
$$= \left(n-\frac{1}{4}\right)\pi\hbar \tag{0.19}$$

where we used 0.5 in the last line.

To get the allowed energies we can substitute for r_2 using 0.7:

$$r_2 = ae^{E/V_0} \tag{0.20}$$
$$= \sqrt{\frac{2\pi}{mV_0}}\left(n-\frac{1}{4}\right)\hbar \tag{0.21}$$
$$E_n = V_0\ln\left(\sqrt{\frac{2\pi}{mV_0}}\left(n-\frac{1}{4}\right)\frac{\hbar}{a}\right) \tag{0.22}$$

The spacing between successive energy levels is

$$E_{n+1}-E_n = V_0\left[\ln\left(\sqrt{\frac{2\pi}{mV_0}}\left(n+\frac{3}{4}\right)\frac{\hbar}{a}\right)-\ln\left(\sqrt{\frac{2\pi}{mV_0}}\left(n-\frac{1}{4}\right)\frac{\hbar}{a}\right)\right] \tag{0.23}$$
$$= V_0\ln\left(\frac{n+3/4}{n-1/4}\right) \tag{0.24}$$

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