

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

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

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

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

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

$$(3) \quad u(r) = \begin{cases} \frac{2D}{\sqrt{p(r)}} \sin \left[\int_r^{r_2} p(r') dr' / \hbar + \pi/4 \right] & r < r_2 \\ \frac{D}{\sqrt{|p(r)|}} \exp \left[- \int_{r_2}^r |p(r')| dr' / \hbar \right] & r > r_2 \end{cases}$$

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

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

$$(5) \quad \int_0^{r_2} p(r) dr = \left(n - \frac{1}{4} \right) \pi \hbar$$

Example. We can apply this formula to the potential

$$(6) \quad V(r) = V_0 \ln \frac{r}{a}$$

The turning point is defined by

$$(7) \quad E = V_0 \ln \frac{r_2}{a}$$

so the integral 5 is

$$(8) \quad \sqrt{2m} \int_0^{r_2} \sqrt{E - V_0 \ln \frac{r}{a}} dr = \sqrt{2m} \int_0^{r_2} \sqrt{V_0 \ln \frac{r_2}{a} - V_0 \ln \frac{r}{a}} dr$$

$$(9) \quad = \sqrt{2mV_0} \int_0^{r_2} \sqrt{\ln \frac{r_2}{r}} dr$$

We can use the substitution

$$(10) \quad v = \ln \frac{r_2}{r}$$

$$(11) \quad dv = \frac{r}{r_0} \left(-\frac{r_0}{r^2} \right) dr$$

$$(12) \quad = -\frac{1}{r} dr$$

$$(13) \quad = -\frac{e^v}{r_0} dr$$

The limits on the integral in terms of v are

$$(14) \quad r = 0 \rightarrow u = \infty$$

$$(15) \quad r = r_2 \rightarrow u = 0$$

so the integral transforms as

$$(16) \quad \sqrt{2mV_0} \int_0^{r_2} \sqrt{\ln \frac{r_2}{r}} dr = r_2 \sqrt{2mV_0} \int_0^\infty \sqrt{v} e^{-v} dv$$

$$(17) \quad = r_2 \sqrt{2mV_0} \Gamma\left(\frac{3}{2}\right)$$

$$(18) \quad = \frac{\sqrt{2\pi mV_0} r_2}{2}$$

$$(19) \quad = \left(n - \frac{1}{4}\right) \pi \hbar$$

where we used 5 in the last line.

To get the allowed energies we can substitute for r_2 using 7:

$$(20) \quad r_2 = ae^{E/V_0}$$

$$(21) \quad = \sqrt{\frac{2\pi}{mV_0}} \left(n - \frac{1}{4}\right) \hbar$$

$$(22) \quad E_n = V_0 \ln \left(\sqrt{\frac{2\pi}{mV_0}} \left(n - \frac{1}{4}\right) \frac{\hbar}{a} \right)$$

The spacing between successive energy levels is

$$(23) \quad E_{n+1} - E_n = V_0 \left[\ln \left(\sqrt{\frac{2\pi}{mV_0}} \left(n + \frac{3}{4}\right) \frac{\hbar}{a} \right) - \ln \left(\sqrt{\frac{2\pi}{mV_0}} \left(n - \frac{1}{4}\right) \frac{\hbar}{a} \right) \right]$$

$$(24) \quad = V_0 \ln \left(\frac{n + 3/4}{n - 1/4} \right)$$

PINGBACKS

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