The WKB Approximation

Griffiths problem 8.2: Alternative derivation of WKB

(a)

$$\begin{aligned} \psi(x) &= e^{if(x)/\hbar} \\ \frac{d\psi}{dx} &= \frac{i}{\hbar} f' e^{if/\hbar} \\ \frac{d^2\psi}{dx^2} &= \frac{i}{\hbar} f'' e^{if/\hbar} - \frac{1}{\hbar^2} f'^2 e^{if/\hbar} \end{aligned}$$

So the Schrödinger equation is

$$\frac{i}{\hbar} f'' e^{if/\hbar} - \frac{1}{\hbar^2} f'^2 e^{if/\hbar} = -\frac{p^2(x)}{\hbar^2} e^{if/\hbar}$$

or

$$i\hbar f'' - f'^2 + p^2(x) = 0. \tag{1}$$

(b)

$$\begin{aligned} f(x) &= f_0(x) + \hbar f_1(x) + \hbar^2 f_2(x) + \cdots \\ f' &= f_0' + \hbar f_1' + \hbar^2 f_2' + \cdots \\ (f')^2 &= f_0'^2 + \hbar(2f_0'f_1') + \hbar^2(f_1'^2 + 2f_0'f_2') + \cdots \end{aligned}$$

Plug these into equation (1) to find

$$i\hbar[f_0'' + \hbar f_1'' + \cdots] - [f_0'^2 + \hbar(2f_0'f_1') + \hbar^2(f_1'^2 + 2f_0'f_2') + \cdots] + p^2(x) = 0.$$

Whence, collecting like powers of $\hbar$ (dimensional analysis!)

$$f_0'^2 = p^2(x) \tag{2}$$

$$i f_0'' = 2f_0'f_1' \tag{3}$$

$$i f_1'' = f_1'^2 + 2f_0'f_2' \tag{4}$$

(c) From eqn. (2), we obtain

$$f_0'(x) = \pm p(x) \tag{5}$$

$$f_0(x) = \pm \int p(x)\, dx. \tag{6}$$

Meanwhile, take the derivative of (5) to find $f_0'' = \pm p'(x)$. Plug this into the left-hand side of (3) to obtain

$$\begin{aligned} \pm i p'(x) &= 2(\pm p(x)) f_1' \\ f_1'(x) &= \frac{i p'(x)}{2p(x)} \\ f_1(x) &= \frac{i}{2}\int \frac{p'(x)}{p(x)} dx = \frac{i}{2}\int \frac{dp}{p} = \frac{i}{2}\log p(x) \end{aligned} \tag{7}$$

Meanwhile, Griffiths [8.10] is

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

Take the log of each side

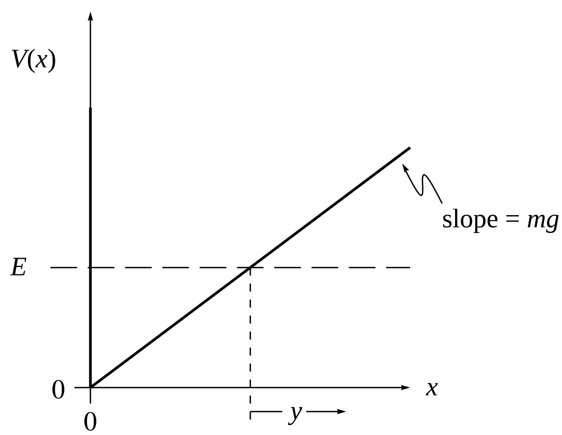
$$\frac{i}{\hbar} f(x) = \pm \frac{i}{\hbar} \int p(x)\,dx + \log C - \frac{1}{2}\log p(x)$$

and incorporate the constant "$\log C$" into the constant of integration to find

$$f(x) = \underbrace{\pm \int p(x)\,dx}_{\text{same as (6)}} + \underbrace{i\frac{\hbar}{2}\log p(x)}_{\text{same as (7)}}$$

Griffiths problem 8.5: The quantum bouncer

(a)



(b) Apply the Schrödinger equation

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

to the quantum bouncer to find that

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = (E - mgx)\psi(x) \qquad \text{for } x > 0$$

with the boundary condition $\psi(0) = 0$.

Rewrite as

$$\frac{d^2\psi}{dx^2} = \frac{2m^2 g}{\hbar^2}\left(x - \frac{E}{mg}\right)\psi(x),$$

change variable (shift of origin) to $y = x - E/mg$,

$$\frac{d^2\psi}{dy^2} = \frac{2m^2g}{\hbar^2} y\psi(y),$$

and then change to the dimensionless variable

$$z = \left(\frac{2m^2g}{\hbar^2}\right)^{1/3} y$$

to find

$$\frac{d^2\psi}{dz^2} = z\psi(z).$$

This O.D.E. has the solution

$$\psi(z) = a\text{Ai}(z).$$

[It also has the solution $\text{Bi}(z)$, but that solution is obviously unnormalizable.]

(c) In addition, the solution must satisfy the boundary condition

$$\psi = 0 \text{ at } x = 0, \text{ i.e. at } y = -E/mg, \text{ i.e. at } z = \left(\frac{2m^2g}{\hbar^2}\right)^{1/3}\left(-\frac{E}{mg}\right).$$

In other words, the eigenenergies are related to the zeros z_0 of $\text{Ai}(z)$ through

$$\begin{aligned} E &= -mg\left(\frac{\hbar^2}{2m^2g}\right)^{1/3} z_0 \\ &= -(\tfrac{1}{2}\hbar^2 mg^2)^{1/3} z_0 \\ &= -(3.766 \times 10^{-23} \text{ Joule})\, z_0 \end{aligned}$$

The zeros of $\text{Ai}(z)$ are tabulated in Abramowitz and Stegun, *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables.* (And also in the Digital Library of Mathematical Functions, release date 2011-08-29, National Institute of Standards and Technology, `http://dlmf.nist.gov/9.9#T1`, table 9.9.1.)

zero	energy (Joules)
−2.338	8.805×10^{-23}
−4.088	15.395×10^{-23}
−5.521	20.791×10^{-23}
−6.787	25.559×10^{-23}
−7.944	29.916×10^{-23}
⋮	⋮

Griffiths problem 8.6: The quantum bouncer in the WKB approximation

This all hinges on Griffiths [8.47]:

$$
\begin{aligned}
(n-\tfrac{1}{4})\pi\hbar &= \int_0^{x_2} p(x)\,dx \\
&= \int_0^{x_2} \sqrt{2m(E-V(x))}\,dx \\
&= \int_0^{E/mg} \sqrt{2m(E-mgx)}\,dx \qquad [\![\text{use } u=(mg/E)x]\!] \\
&= \frac{E}{mg}\int_0^1 \sqrt{2mE}\,\sqrt{1-u}\,du \\
&= \sqrt{\frac{2E^3}{mg^2}}\int_0^1 \sqrt{1-u}\,du \qquad [\![\text{use } y=1-u]\!] \\
&= \sqrt{\frac{2E^3}{mg^2}}\int_0^1 \sqrt{y}\,dy \\
&= \sqrt{\frac{2E^3}{mg^2}}\left[\frac{1}{3/2}y^{3/2}\right]_0^1 \\
&= \sqrt{\frac{2E^3}{mg^2}}\left[\frac{2}{3}\right]
\end{aligned}
$$

Solve for E:

$$E = (\tfrac{9}{8}\pi^2\hbar^2 mg^2)^{1/3}(n-\tfrac{1}{4})^{2/3}$$

Plug in to build the table of values:

n	energy (Joules)
1	8.738×10^{-23}
2	15.371×10^{-23}
3	20.777×10^{-23}
4	25.549×10^{-23}
5	29.910×10^{-23}
⋮	⋮

The last value is accurate to 2 parts in 10,000!

Griffiths problem 8.14: WKB for the Coulomb problem

The effective potential is

$$V_{\text{eff}}(r) = \left[-\frac{e^2}{4\pi\epsilon_0}\frac{1}{r} + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\right]$$

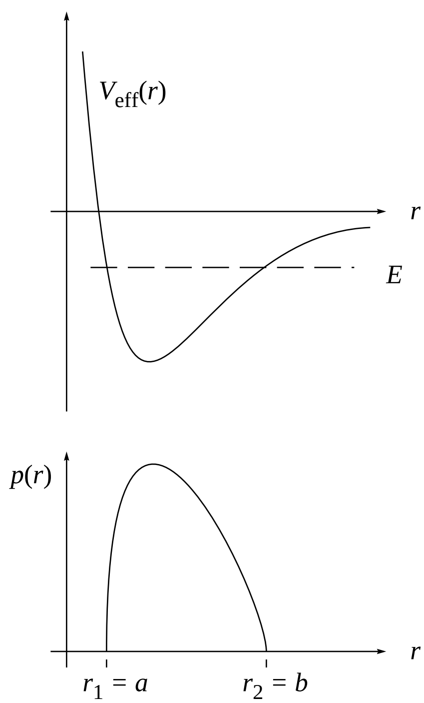
or, in atomic units,

$$V_{\rm eff}(r) = \left[-\frac{1}{r} + \frac{1}{2}\frac{\ell(\ell+1)}{r^2}\right].$$

Thus

$$\begin{aligned} p(r) &= \sqrt{2[E - V_{\rm eff}(r)]} \\ &= \sqrt{2\left[E + \frac{1}{r} - \frac{\ell(\ell+1)}{2r^2}\right]} \\ &= \frac{\sqrt{2(-E)}}{r}\sqrt{-r^2 + \frac{r}{(-E)} - \frac{\ell(\ell+1)}{2(-E)}}. \end{aligned}$$

I prefer to use the constant $(-E)$, which is positive, rather than E.



The turning points are when $p(r) = 0$, that is,

$$-r_{tp}^2 + \frac{r_{tp}}{(-E)} - \frac{\ell(\ell+1)}{2(-E)} = 0,$$

with solutions

$$\begin{aligned} r_{tp} &= \frac{1/(-E) \pm \sqrt{1/(-E)^2 - 4\ell(\ell+1)/2(-E)}}{2} \\ &= \frac{1 \pm \sqrt{1 - 2\ell(\ell+1)(-E)}}{2(-E)} \end{aligned}$$

or

$$
\begin{aligned}
r_1 = a &= \frac{1 - \sqrt{1 - 2\ell(\ell+1)(-E)}}{2(-E)} \\
r_2 = b &= \frac{1 + \sqrt{1 - 2\ell(\ell+1)(-E)}}{2(-E)}.
\end{aligned}
$$

This means that

$$
p(r) = \frac{\sqrt{2(-E)}}{r}\sqrt{(r-a)(b-r)}.
$$

Note that for $a < r < b$, the quantity under the square root sign is positive, namely

$$
(r-a)(b-r) = -r^2 + (a+b)r - ab = -r^2 + \frac{r}{(-E)} - \frac{\ell(\ell+1)}{2(-E)}.
$$

Now we're ready to invoke the WKB condition (in atomic units with $\hbar = 1$)

$$
\begin{aligned}
(n - \tfrac{1}{2})\pi &= \int_a^b p(r)\,dr \\
&= \sqrt{2(-E)} \int_a^b \frac{1}{r}\sqrt{(r-a)(b-r)}\,dr \\
&= \sqrt{2(-E)}\frac{\pi}{2}(\sqrt{b} - \sqrt{a})^2 \\
&= \sqrt{2(-E)}\frac{\pi}{2}[(a+b) - 2\sqrt{ab}] \\
&= \sqrt{2(-E)}\frac{\pi}{2}\left[\frac{1}{(-E)} - 2\sqrt{\frac{\ell(\ell+1)}{2(-E)}}\right] \\
&= \frac{\pi}{2}\left[\sqrt{\frac{2}{(-E)}} - 2\sqrt{\ell(\ell+1)}\right].
\end{aligned}
$$

Thus

$$
\begin{aligned}
2(n - \tfrac{1}{2}) + 2\sqrt{\ell(\ell+1)} &= \sqrt{\frac{2}{(-E)}} \\
4[(n - \tfrac{1}{2}) + \sqrt{\ell(\ell+1)}]^2 &= \frac{2}{(-E)} \\
(-E) &= \frac{1}{2[(n - \frac{1}{2}) + \sqrt{\ell(\ell+1)}]^2}.
\end{aligned}
$$

To convert from atomic units back to regular units, remember that the symbol E is shorthand for $\tilde{E} = E/(2\,\mathrm{Ry})$ so

$$
E = -\frac{\mathrm{Ry}}{[n - \frac{1}{2} + \sqrt{\ell(\ell+1)}]^2}.
$$