Solution to HW#12

1. Reed Chapter 9

Problem 9-4

In Example 9.2 it was shown that the WKB method predicts the energy levels of the hydrogen atom exactly. Following the approach of Example 9.1, investigate the application of the classical approximation to this system at the point \( r_{\text{turn}}/2 \) for a general energy level \( E_n \).

Setting \( k = \frac{e^2}{4\pi \varepsilon_0} \) and \( \beta = \frac{m e^4}{8\varepsilon_0^2 \hbar^2} \), the potential and energy levels are \( V(r) = -\frac{k}{r} \) and \( E_n = -\frac{\beta}{n^2} \). The turning points are given by \( E_n = V(r) \), or \( r_{\text{turn}} = kn^2/\beta \), hence \( r_{\text{turn}}/2 = kn^2/2\beta \). With \( \frac{dV}{dr} = +\frac{k}{r^2} \), evaluating the classical approximation at \( r_{\text{turn}}/2 \) gives

\[
\frac{m h}{\left(2m[E - V(r)]\right)^{3/2}} \left(\frac{dV}{dr}\right) = \frac{h}{2^{5/2}} \sqrt{m (\beta/ n^2)^{3/2}} \frac{4\beta^2}{kn^4} = \frac{4h\sqrt{\beta}}{2^{5/2} \sqrt{mkn}^2}.
\]

Substituting for \( k \) and \( \beta \) reduces this to \( 2\pi/n \). The classical approximation is then \( n \gg 2\pi \); it is surprising that the WKB approximation works so well in this case.
2. Reed Chapter 9

Problem 9-5

Show that application of the WKB method to the harmonic-oscillator potential \( V(x) = kx^2/2 \) leads to \( E_n \sim n\hbar\omega \). Investigate the application of the classical approximation to this system at the point \( x_{\text{turn}}/2 \) for a general energy level \( E_n \).

The WKB approximation gives

\[
2\sqrt{2m} \int_{-a}^{a} \sqrt{E - kx^2/2} \, dx = n\hbar,
\]

where the limits of integration \( \pm a \) are given by \( E = ka^2/2 \), or \( a = \pm \sqrt{2E/k} = \sqrt{2E/m\omega^2} \) where \( \omega = \sqrt{k/m} \). Eliminating \( E \) in favor of \( ka^2/2 \) and accounting for symmetry about \( x = 0 \), the integral can be written as

\[
4\sqrt{mk} \int_{0}^{a} \sqrt{a^2 - x^2} \, dx = n\hbar,
\]

which solves as

\[
2\sqrt{mk} \left[ x \sqrt{a^2 - x^2} + a^2 \sin^{-1}(x/a) \right]_{0}^{a} = n\hbar,
\]

or

\[
2\sqrt{mk} \left[ a^2 (\pi/2) \right] = n\hbar,
\]

or, with \( a^2 = 2E/k \),

\[
E = n\hbar \sqrt{k/m} = n\hbar\omega.
\]
Application of the WKB approximation to the harmonic-oscillator potential fails to predict the zero-point energy, but does predict the important physical result that the energy levels are equally spaced.

We now examine the classical approximation for this solution. With \( E_n \sim n \hbar \omega \) the turning points are given by \( E_n = kx^2/2 \), or \( x_{\text{turn}} = \sqrt{2n\hbar \omega / k} \), hence \( x_{\text{turn}}/2 = \sqrt{n\hbar \omega / 2k} \). At \( x_{\text{turn}}/2 \), then,

\[
V(x) = \frac{k}{2} \left( \frac{x_{\text{turn}}}{2} \right)^2 = \frac{k}{2} \left( \frac{n \hbar \omega}{2k} \right) = \frac{n \hbar \omega}{4}.
\]

With \( dV/dx = kx \), evaluating the classical approximation at \( x_{\text{turn}}/2 \) gives

\[
\frac{m \hbar}{\{2m(E - V(x))\}^{3/2}} \left( \frac{dV}{dx} \right) = \frac{h}{2^{3/2}\sqrt{m(3n\hbar \omega / 4)^{3/2}}} \left( k \sqrt{\frac{n \hbar \omega}{2k}} \right).
\]

This expression reduces to \( 4\pi/3^{3/2}n \). The classical approximation then corresponds to

\[
n \gg \frac{4\pi}{3^{3/2}} \quad \Rightarrow \quad n \gg 2.418.
\]
Problem 9-6

Use the WKB method to derive an expression for the energy levels of a potential given by

\[ V(x) = \begin{cases} 
\infty & x \leq 0 \\
A \sin^2 \left( \frac{x}{\alpha} \right) & 0 \leq \left( \frac{x}{\alpha} \right) \leq \pi/2 \\
0 & \text{otherwise.} 
\end{cases} \]

If an electron were trapped in such a potential with \( A = 24 \text{ eV} \) and \( \alpha = 6 \text{ Å} \) at an energy of 12 eV, approximately what quantum state would it be in?

NOTE: \[ \int_0^{\pi/4} \sqrt{1-2\sin^2 y} \, dy = 0.5991. \]

This potential is sketched below:
The WKB approximation for this potential takes the form

\[2 \sqrt{2m} \int_0^\infty \sqrt{E - A \sin^2 \left(\frac{x}{\alpha}\right)} \, dx \approx n \hbar.\]

Upon extracting a factor of \(E\), changing variables to \(y = x/\alpha\) and setting \(A/E = 2\), we have

\[2\alpha \sqrt{2mE} \int_0^{\pi/4} \sqrt{1 - 2 \sin^2 y} \, dy \approx n \hbar.\]

The integral must be evaluated numerically, and comes to 0.5991. Hence we have

\[n \approx \frac{2 \alpha (0.5991) \sqrt{2mE}}{\hbar}.\]

Upon substituting \(\alpha = 6 \text{ Å}, \ E = 12 \text{ eV}, \text{ and } m = m_e = 9.109 \times 10^{-31} \text{ kg},\) we find

\[n \approx \frac{2 \left(6 \times 10^{-10} \text{ m}\right) (0.5991) \sqrt{2(9.109 \times 10^{-31} \text{ kg}) [12 \times (1.602 \times 10^{-19} \text{ J})]}}{6.626 \times 10^{-34} (\text{ J} - \text{ sec})} \approx 2.03,\]

or, say, \(n \approx 2.\)
4. 

Unperturbed wave function:

\[ \psi_n^0 = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \]

Perturbation to the potential:

\[ \Delta V = \frac{1}{2} k x^2 \]

The first-order energy correction:

\[
\varepsilon_n = \int \psi_n^{0*} \Delta V \psi_n^0 \, dx
\]

\[
= \int_0^L \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \cdot \left( \frac{1}{2} k x^2 \right) \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \, dx
\]

\[
= \frac{k}{L} \int_0^L x^2 \sin^2 \frac{n\pi x}{L} \, dx
\]

\[
= \frac{k}{L} \cdot \frac{1}{2} \int_0^L x^2 \left( 1 - \cos \frac{2n\pi x}{L} \right) \, dx
\]

\[
\text{Use: } \int x^2 \cos(ax) \, dx = \frac{a^2 x \cos(ax)}{a^2} + \frac{a^2 x^2 - 2}{a^3} \sin(ax)
\]

\[
\Rightarrow \varepsilon_n = \frac{kL^2}{2} \left( \frac{\pi^2}{3} - \frac{1}{2n^2\pi^2} \right) = \frac{kL^2}{2} \left( \frac{1}{3} - \frac{1}{2n^2\pi^2} \right)
\]

For the ground state, we would set \( n=1 \).
5.

Unperturbed wave function:

\[ \psi_0 = \frac{\sqrt{\alpha}}{\pi^{\nu_1}} e^{-\frac{x^2}{2\alpha}} \]

\[ \alpha = \left( \frac{m_0^2}{\hbar^2} \right)^{\frac{\gamma_1}{2}} \]

The first-order energy correction/perturbation:

\[ \varepsilon_n = \int \psi_0^* \Delta V \psi_0 dx = \int_{-\infty}^{\infty} \psi_0^* e^{\gamma_1} \psi_0 dx \]

\[ = \int_{-\infty}^{\infty} \beta x^\gamma \frac{\alpha}{\sqrt{\pi}} e^{-\frac{x^2}{2\alpha}} dx \]

\[ = \frac{2\alpha\beta}{\sqrt{\pi}} \left[ \frac{3}{8} \gamma_1 \sqrt{\frac{\pi}{\alpha^2}} \right] \]

\[ \Rightarrow \varepsilon_n = \frac{3 \beta}{4 \alpha^\gamma} \]

Use the last of the given integrals
Problem 9-21

Consider the following potential, a one-dimensional analog of the hydrogen atom

\[ V(x) = \begin{cases} \frac{\kappa}{x}, & x \geq 0 \\ \infty, & x \leq 0 \end{cases} \]

Carry out a variational analysis for a particle of mass \( m \) moving in this potential, taking as the trial wavefunction

\[ \phi(x) = C x e^{-\beta x} \quad (x \geq 0; \phi = 0 \text{ otherwise}), \]

where \( C \) is the normalization constant and \( \beta \) is the variational parameter. If \( \kappa = e^2/4\pi\epsilon_0 \) as in the Coulomb potential, how does your estimate of the ground-state energy (for an electron) compare with that for the usual Coulomb potential?

We begin by normalizing the trial wavefunction:

\[ C^2 \int_0^\infty x^2 e^{-2\beta x} \, dx = 1 \implies C^2 = 4\beta^3. \]

The second derivative of the trial wavefunction is

\[ \frac{d^2\phi}{dx^2} = C(-2\beta + \beta^2 x) e^{-\beta x}. \]

The variational energy estimate is

\[ E \leq \langle \phi \mid H \mid \phi \rangle = \int \phi(x) \left[ \frac{-\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \phi(x) \, dx, \]

which evaluates as

\[ E \leq -\epsilon C^2 \left\{ -2\beta \int_0^\infty x e^{-2\beta x} \, dx + \beta^2 \int_0^\infty x^2 e^{-2\beta x} \, dx \right\} - \kappa C^2 \int_0^\infty x e^{-2\beta x} \, dx = \epsilon \beta^2 - \kappa \beta, \]
where $\epsilon = h^2/2m$. Setting the derivative equal to zero gives $\beta = \kappa/2\epsilon$, and

$$E \leq -\frac{1}{4} \frac{\kappa^2}{\epsilon}.$$ 

For an electron and with $\kappa = e^2/4\pi\epsilon_0$, this gives

$$E \leq -\frac{m_e e^4}{32\pi^2 \epsilon_0^2 h^3},$$

exactly the hydrogen ground-state energy.