**Solution to HW#12**

1. 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 $x_{turn}/2$ 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

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

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

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

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

$$n \gg \frac{4\pi}{3^{3/2}} \Rightarrow n \gg 2.418.$$
2. Reed Chapter 9

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?

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

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

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

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

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

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

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

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

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

or, say, \( n \approx 2 \).
Problem 9-9

An infinite rectangular potential well is subject to a perturbing potential $V(x) = \alpha x^2$, $(0 \leq x \leq L)$. Determine a first order approximation for the energy for any state $\psi_n(x)$.

We treat this problem as a perturbed infinite square well. First we compute the perturbations to the energy levels via first-order perturbation theory,

$$ E \sim E_n^0 + \langle \psi_n^0 | V' | \psi_n^0 \rangle. $$

We have $V' = \alpha x^2$, $(0 \leq x \leq L)$ and

$$ E_n^0 = \frac{n^2 \hbar^2}{8mL^2}. $$

The perturbation integral gives

$$ \langle \psi_n^0 | V' | \psi_n^0 \rangle = \frac{2\alpha}{L} \int_0^L x^2 \sin^2 (c x) \, dx, $$

where $c = n\pi/L$. This evaluates as

$$ \langle \psi_n^0 | V' | \psi_n^0 \rangle = \frac{2\alpha}{L} \left[ \frac{x^3}{6} - \frac{x^2}{4c} - \frac{1}{8c^3} \right] \sin(2cx) - \frac{x \cos(2cx)}{4c^2} \right|_0^L $$

$$ = \frac{2\alpha}{L} \left[ \frac{L^3}{6} - \frac{L}{4c^2} \right] = \alpha L^2 \left( \frac{1}{3} - \frac{1}{2\pi^2 n^2} \right). $$

Hence

$$ E \sim \frac{n^2 \hbar^2}{8mL^2} + \alpha L^2 \left( \frac{1}{3} - \frac{1}{2\pi^2 n^2} \right). $$

As $n \to \infty$, each energy level is perturbed upward by $\alpha L^2/3$. 
Problem 9-13

A ground-state \((n = 0)\) harmonic oscillator is subject to a perturbing potential \(V' = \beta x^4\).

(a) Determine the first-order perturbation to the ground-state energy.

(b) Derive an expression for the perturbed ground-state wavefunction. Note that Hermite polynomials satisfy the identity

\[
\int_{-\infty}^{\infty} e^{-\xi^2} H_n(\xi) H_{n+p}(\xi) d\xi = \begin{cases} 
0, & (p > r) \\
2^n (n + r)! \sqrt{\pi}, & (p = r).
\end{cases}
\]

Hint: The parity properties of Hermite polynomials are useful in eliminating some of the integrals not covered by this identity. Leave your answer in terms of \(H_2(\xi)\) and \(H_4(\xi)\).

The \(n\)-th level harmonic-oscillator wavefunction is given in general by

\[
\psi_n(x) = A_n e^{-\alpha^2 x^2/2} H_n(\alpha x),
\]

with

\[
A_n = \sqrt{\frac{\alpha}{\sqrt{\pi} 2^n n!}}, \quad \text{where} \quad \alpha = (\text{km}/\text{h}^2)^{1/4}.
\]

The perturbing potential is \(\beta x^4\). The perturbation to the ground state energy is then

\[
\langle \psi_0 | \beta x^4 | \psi_0 \rangle = A_0^2 \beta \int_{-\infty}^{\infty} x^4 e^{-\alpha^2 x^2} dx = \frac{3\beta}{4\alpha^4}.
\]

where we have used \(H_0(x) = 1\). To first order, the perturbed ground-state \((n = 0)\) energy is then

\[
E \sim \frac{\hbar \omega}{2} + \frac{3\beta}{4\alpha^4}.
\]
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

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

where \( C \) is the normalization constant and \( \beta \) is the variational parameter. If \( \kappa = e^2/4\pi\varepsilon_0 \) 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:

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

The second derivative of the trial wavefunction is

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

The variational energy estimate is

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

which evaluates as

\[ E \leq -\varepsilon C^2 \left\{ -2\beta \int_0^\infty xe^{-2\beta x} \, dx + \beta^2 \int_0^\infty x^2 e^{-2\beta x} \, dx \right\} - \kappa C^2 \int_0^\infty xe^{-2\beta x} \, dx = \varepsilon \beta^2 - \kappa \beta, \]
where \( \epsilon = \frac{\hbar^2}{2m} \). Setting the derivative equal to zero gives \( \beta = \frac{\kappa}{2\epsilon} \), and

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

For an electron and with \( \kappa = \frac{e^2}{4\pi\epsilon_0} \), this gives

\[
E \leq -\frac{m_e e^4}{32\pi^2 \epsilon_0^2 \hbar^2},
\]

exactly the hydrogen ground-state energy.