Quantum Mechanics and Atomic Physics 750:361

Prof. Sean Oh, Fall 2011

HW #13

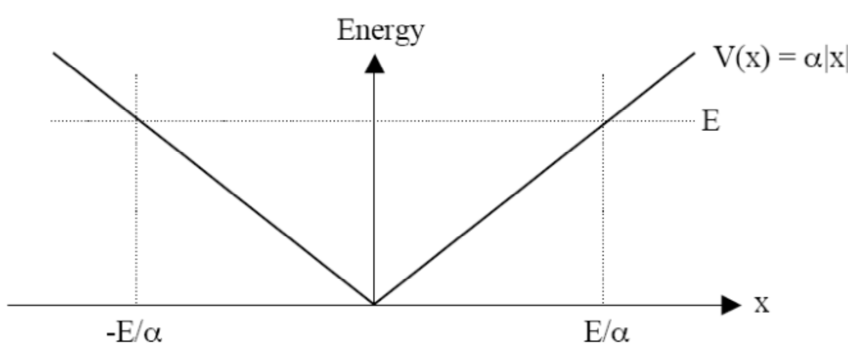
Due date: Monday, Dec. 12, 2011, at the beginning of class: no late HW will be accepted.

1. Reed, Prob. 9-3

Problem 9-3

Using the WKB approximation, determine the energy eigenvalues for a particle of mass m moving in a potential given by $V(x) = \alpha|x|$, $(-\infty \le x \le \infty)$.

This potential is sketched below, and is symmetric around x = 0. An energy level E cuts the potential at $E = \alpha|x|$, or $x = \pm E/\alpha = \pm\beta$, say. Utilizing this symmetry, the WKB approximation gives



$$4\sqrt{2m}\int_0^\beta \sqrt{E-\alpha x}\,dx \approx nh.$$

Extracting a factor of α from under the radical gives

$$4\sqrt{2m\alpha}\int_0^\beta \sqrt{\beta - x}\,dx \approx nh,$$

which on solving reduces to

$$\frac{8}{3}\beta^{3/2}\sqrt{2m\alpha} \approx nh.$$

On substituting for β and solving for E, we find

$$E \approx \left(\frac{3\alpha h}{8\sqrt{2m}}\right)^{2/3} n^{2/3}.$$

Energy levels for this potential increase in proportion to the two-thirds power of n.

2. Reed, Prob. 9-5

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

$$2\sqrt{2m}\int_{-a}^{a}\sqrt{E - kx^2/2}\,dx \approx nh,$$

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

$$4\sqrt{mk}\int_0^a \sqrt{a^2 - x^2}\,dx \approx nh,$$

which solves as

$$2\sqrt{mk}\left[x\sqrt{a^2 - x^2} + a^2\,\mathrm{Sin}^{-1}(x/a)\right]_0^a \approx nh,$$

or

$$2\sqrt{mk}\left[a^2(\pi/2)\right] \approx nh,$$

or, with $a^2 = 2E/k$,

$$E \approx n\hbar\sqrt{k/m} \approx n\hbar\omega.$$

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 $x_{turn} = \sqrt{2n\hbar\omega/k}$, hence $x_{turn}/2 = \sqrt{n\hbar\omega/2k}$. At $x_{turn}/2$, then,

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

With $dV/dx = kx$, evaluating the classical approximation at $x_{turn}/2$ gives

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

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

$$n >> \frac{4\pi}{3^{3/2}} \quad\Rightarrow\quad n >> 2.418.$$

4. Reed, Prob. 9-12

Problem 9-12

As the previous problem but with $V(r) = Ar^2 \sin\theta$. Derive an expression for the first order correction to the energy for state n.

The unperturbed n-th level wavefunction for a particle with $\ell = 0$ in an infinite spherical well of radius a is given by

$$\psi_{n00} = \frac{1}{\sqrt{2\pi a}} \frac{\sin(n\pi r/a)}{r}.$$

With a perturbing potential

$$V(r) = A r^2 \sin\theta,$$

the perturbation to energy level n is given by

$$\langle \psi_n^0 | V' | \psi_n^0 \rangle = \iiint \psi_{n00} \, V(r) \, \psi_{n00} \, dV$$

$$= \frac{A}{2\pi a} \int_0^a \int_0^\pi \int_0^{2\pi} \frac{\sin^2(n\pi r/a)}{r^2} (r^2 \sin\theta) \, r^2 \sin\theta \, d\phi \, d\theta \, dr$$

$$= \frac{A}{a} \left\{ \int_0^a r^2 \sin^2(n\pi r/a) \, dr \right\} \left\{ \int_0^\pi \sin^2\theta \, d\theta \right\}.$$

The integral over θ proceeds as

$$\int_0^\pi \sin^2\theta \, d\theta = \left[\frac{\theta}{2} - \frac{\sin(2\theta)}{4}\right]_0^\pi = \frac{\pi}{2}.$$

The integral over r is identical to that which appeared in the previous problem:

$$\int_0^a r^2 \sin^2\left(\frac{n\pi r}{a}\right) dr = \left[\frac{r^3}{6} - \left(\frac{r^2}{4\alpha} - \frac{1}{8\alpha^3}\right)\sin(2\alpha r) - \frac{r\cos(2\alpha r)}{4\alpha^2}\right]_0^a$$

$$= a^3\left[\frac{1}{6} - \frac{1}{4n^2\pi^2}\right].$$

Hence we have

$$\langle \psi_n^0 | V' | \psi_n^0 \rangle = \frac{A}{a}\left\{a^3\left[\frac{1}{6} - \frac{1}{4n^2\pi^2}\right]\right\}\left(\frac{\pi}{2}\right) = \frac{\pi A a^2}{4}\left[\frac{1}{3} - \frac{1}{2n^2\pi^2}\right].$$

To first order, all energy levels are perturbed upward; as $n \to \infty$, the energy perturbation approaches $Aa^2\pi/12$.

5. Reed, Prob. 9-16

Problem 9-16

I In Chapter 8 it was shown that an electron orbiting a nucleus with orbital angular momentum **L** gives rise to a (vector) magnetic dipole moment $\mu = (e/2m_e)\mathbf{L}$. A magnetic dipole moment placed in a magnetic field **B** acquires a potential energy given by $V = -\mu \bullet \mathbf{B}$. Consider hydrogen atoms in general (n, ℓ, m) states suddenly subjected to a magnetic field $\mathbf{B} = Bz$ where z denotes the usual Cartesian-coordinate unit vector in the z-direction. Use non-degenerate first-order perturbation theory to show that the hydrogenic states will be perturbed by an amount $\Delta E = -\mu_B mB$ where μ_B is the Bohr magneton, $\mu_B = (e\hbar/2m_e)$. What does this result imply for the normally fourfold-degenerate n = 2 states? Within sunspots, magnetic fields can be as strong as B = 0.3 T. In the unperturbed Bohr model, 3→2 transitions usually give rise to photons of wavelength 6564Å. What alteration in the photon wavelength would you expect to observe for hydrogen in the vicinity of such a sunspot?

The perturbing potential is

$$V' = -\mu \bullet \mathbf{B} = -\left(\frac{e}{2m_e}\right)\mathbf{L} \bullet \mathbf{B} = -\left(\frac{e}{2m_e}\right)L_z B$$

where L_z denotes the z-component of **L**. But $L_z = m\hbar$, so

$$V' = -\left(\frac{e\hbar}{2m_e}\right)mB = -\mu_B mB.$$

Non-degenerate first-order perturbation theory gives

$$\Delta E \sim \langle \psi_{n\ell m} | V' | \psi_{n\ell m} \rangle \sim \langle \psi_{n\ell m} | -\mu_B mB | \psi_{n\ell m} \rangle = -\mu_B mB \langle \psi_{n\ell m} | \psi_{n\ell m} \rangle = -\mu_B mB$$

where $\psi_{n\ell m}$ denotes a hydrogenic state. For the four n = 2 states, those with m = 0 (for both ℓ = 0 and ℓ = 1) will be unperturbed. Those with m = ±1 will be displaced by $\Delta E \sim \mp\mu_B mB$. The four states then split into three distinct states. From chapter 1, if both λ and dλ are measured in Å and ΔE in eV,

$$d\lambda = -\frac{\lambda^2 \Delta E}{12398} \sim \pm\frac{\lambda^2 \mu_B mB}{12398\,e},$$

where the factor of the electron charge (e) arises from converting Joules to eV. For λ = 6564Å, $\mu_B = 9.274 \times 10^{-24}$ amp-m^2, B = 0.3T, and m = 1, dλ ~ ± 0.06Å.

6. Reed, Prob. 9-21

Problem 9-21

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

$$V(x) = \begin{cases} -\dfrac{\kappa}{x}, & x \geq 0 \\ \infty, & x \leq 0 \end{cases}$$

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

$$\phi(x) = C x e^{-\beta x} \qquad (x \geq 0;\ \phi = 0 \text{ otherwise}),$$

where C is the normalization constant and β is the variational parameter. If $\kappa = e^2/4\pi\varepsilon_o$ 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

$$\frac{d^2\phi}{dx^2} = C\left(-2\beta + \beta^2 x\right)e^{-\beta x}.$$

The variational energy estimate is

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

which evaluates as

$$E \leq -\varepsilon C^2\left\{-2\beta\int_0^\infty xe^{-2\beta x}dx + \beta^2\int_0^\infty x^2e^{-2\beta x}dx\right\} - \kappa C^2\int_0^\infty xe^{-2\beta x}dx = \varepsilon\beta^2 - \kappa\beta,$$

where $\varepsilon = \hbar^2/2m$. Setting the derivative equal to zero gives $\beta = \kappa/2\varepsilon$, and

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

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

$$E \leq -\frac{m_e e^4}{32\pi^2\varepsilon_o^2\hbar^2},$$

exactly the hydrogen ground-state energy.

3. For an infinite potential well defined over [0, L], the wavefunction of a particle is prepared at t=0 as $\varphi(x) = \begin{cases} Ax, & for\ 0 < x < L/2 \\ -A(x-L), & for \frac{L}{2} < x < L \end{cases}$. Each of the following parts is worth a full HW problem.

(a) Find the normalization constant A

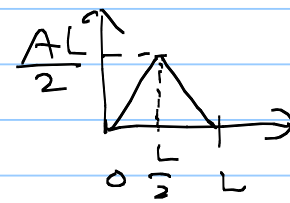
(b) When you do the energy measurement, find the probability of getting energy of E_1, which represents the lowest energy value of the infinite potential well problem.

(b) When you do the energy measurement, find the probability of getting energy of E_2, which represents the second lowest energy value of the infinite potential well problem.

3. For the infinite potential well problem, $\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right)$, $0 < x < L$

$$E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2$$

(a)



$$1 = \int_0^L |\varphi(x)|^2 dx$$

$$= 2\int_0^{\frac{L}{2}} A^2 x^2 dx$$

$$= 2A^2 \frac{1}{3}\left(\frac{L}{2}\right)^3 = \frac{A^2 L^3}{12}$$

$$\Rightarrow A = \left(\frac{12}{L^3}\right)^{\frac{1}{2}} = \frac{2\sqrt{3}}{L^{3/2}}$$

(b) $a_n = \langle \psi_n | \varphi \rangle = \int_0^L \psi_n^*(x)\varphi(x) dx$

$$= A\sqrt{\frac{2}{L}}\left[\int_0^{\frac{L}{2}} \sin\left(\frac{n\pi}{L}x\right) x\, dx - \int_{\frac{L}{2}}^{L} \sin\left(\frac{n\pi}{L}x\right)(x-L)\, dx\right]$$

$$= A\sqrt{\frac{2}{L}}\left[\int_0^{\frac{n\pi}{2}} \sin(y)\left(\frac{L}{n\pi}\right)^2 y \cdot dy - \int_{\frac{n\pi}{2}}^{n\pi} \sin(y)\left(\frac{Ly}{n\pi} - L\right)\frac{L\,dy}{n\pi}\right]$$

$\frac{n\pi}{L}x \equiv y$

$\Rightarrow \frac{n\pi}{L}dx = dy$

$$= A\sqrt{\frac{2}{L}}\left\{ \left(\frac{L}{n\pi}\right)^2 \left[\int_0^{\frac{n\pi}{2}} \sin(y)\, y\, dy - \int_{\frac{n\pi}{2}}^{n\pi} \sin(y)\, y\, dy \right] + \frac{L^2}{n\pi} \int_{\frac{n\pi}{2}}^{n\pi} \sin(y)\, dy \right\}$$

For a_1,

$$\int_0^{\frac{\pi}{2}} \sin y\, y\, dy = \left[\sin y - y\cos y\right]_0^{\frac{\pi}{2}}$$

$$= 1$$

$$\int_{\frac{\pi}{2}}^{\pi} \sin y\, y\, dy = \left[\sin y - y\cos y\right]_{\frac{\pi}{2}}^{\pi}$$

$$= \cancel{\sin\pi} - \pi\cos(\pi) - \sin\frac{\pi}{2} + \frac{\pi}{2}\cos\frac{\pi}{2}$$

$$= \pi - 1$$

$$\int_{\frac{\pi}{2}}^{\pi} \sin y\, dy = -\cos y \Big|_{\frac{\pi}{2}}^{\pi} = 1$$

So

$$a_1 = A\sqrt{\frac{2}{L}}\left[\left(\frac{L}{\pi}\right)^2 \cdot (1 - \pi + 1) + \frac{L^2}{\pi} \right]$$

$$= A\,\frac{\sqrt{2}\,L^{\frac{3}{2}}}{\pi^2}\left[1 - \pi + 1 + \pi \right]$$

$$= \frac{2\sqrt{3}}{L^{\frac{3}{2}}}\;\frac{\sqrt{2}\,L^{\frac{3}{2}}}{\pi^2}\cdot 2 = \frac{4\sqrt{6}}{\pi^2}$$

$$P(E_1) = |a_1|^2 = \frac{96}{\pi^4} \approx 0.986$$

(c) For a_2

$$\int_0^{\pi} y \cdot \sin y \, dy = [\sin y - y\cos y]_0^{\pi}$$

$$= -\pi \cos(\pi) = \pi$$

$$\int_{\pi}^{2\pi} \sin y \cdot y \, dy = [\sin y - y\cos y]_{\pi}^{2\pi}$$

$$= -2\pi \cos 2\pi + \pi \cos\pi$$

$$= -2\pi - \pi = -3\pi$$

$$\int_{\pi}^{2\pi} \sin y \, dy = -\cos y \Big|_{\pi}^{2\pi}$$

$$= -[\cos 2\pi - \cos\pi]$$

$$= -2$$

So

$$a_2 = A\sqrt{\frac{2}{L}}\left[\left(\frac{L}{2\pi}\right)^2(\pi - (-3\pi)) + \frac{L^2}{2\pi}\cdot(-2)\right]$$

$$= \frac{2\sqrt{3}}{L^{\frac{3}{2}}} \frac{\sqrt{2}\,L^{\frac{3}{2}}}{4\pi^2}[4\pi - 4\pi]$$

$$= 0$$

$$P(E_2) = |a_2|^2 = 0$$