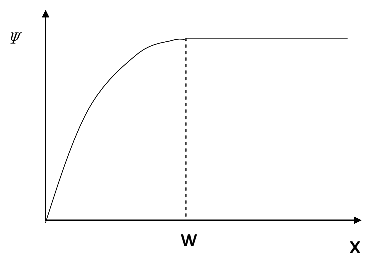
ECE/MAT 211A winter 07

HWK#2 solutions

#3•1-1: Spherical Potential Well

The lowest state must be an $l = 0$ state, hence the equivalent 1-D potential for the problem is of the shape of Fig. 2•2-7, with w = R, and part (a) reduces to problem #2•2-3.

First, we have to solve #2•2-3.



For x>w, the wave function of bound state with infinitesimally small binding energy must consist of an infinitely slowly decaying exponential, that is, a horizontal straight line. Inside the well, it must be a sine wave, with zero slope at x = w, in order to connect smoothly to the wave function on the outside. Hence, its wave number must be

$$k = \frac{2\pi}{\lambda} = \frac{\pi}{2w},$$

corresponding to the energy

$$\varepsilon = \frac{\hbar^2 k^2}{2M} = \frac{\hbar^2 \pi^2}{8Mw^2}.$$

And truly bound state must have a shorter wavelength and hence a higher kinetic energy. But since a bound state must have an energy less than the depth of the well, this means that bound states can exist only if $\varepsilon < V_0$, or

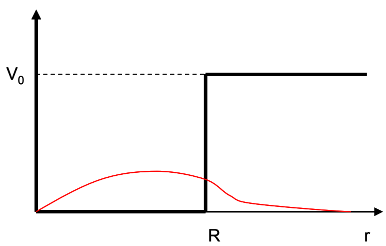
$$V_0 w^2 > \frac{\hbar^2 \pi^2}{8M}$$

(a)

Inserting w = R and M = m_e into the solution above yields

$$\boxed{V_0 > \frac{\hbar^2 \pi^2}{8m_e R^2}}. \qquad (1)$$

To set up the mathematical formalism for determine the energy of the lowest bound state, we can consider the wave function as shown below:



$$\psi_1(r) = A \sin kr$$
$$\psi_2(r) = Be^{-\alpha r}$$

Solving boundary conditions yields:

$k\cot kR = -\alpha$.

Since $\alpha = \sqrt{\dfrac{2m_e(V_0-\varepsilon)}{\hbar^2}}$ and $k = \sqrt{\dfrac{2m_e\varepsilon}{\hbar^2}}$,

$$\cot kR = \frac{-\alpha}{k} = -\sqrt{\frac{V_0-\varepsilon}{\varepsilon}}$$

$$\cot^2 kR = \csc^2 kR - 1 = \frac{1}{\sin^2 kR} - 1 = \frac{V_0-\varepsilon}{\varepsilon} = \frac{V_0}{\varepsilon} - 1$$

So $\sin^2 kR = \dfrac{\varepsilon}{V_0}$

As a result, the energy of the lowest bound state should satisfy

$$\boxed{\sin\sqrt{\frac{2m_e\varepsilon}{\hbar^2}}R = \sqrt{\frac{\varepsilon}{V_0}}}$$

or in terms of k,

$$\boxed{\sin kR = \sqrt{\frac{\hbar^2k^2}{2m_eV_0}} = \frac{k}{k_0}} \quad \text{where} \quad k_0^2 \equiv \frac{2m_eV_o}{\hbar^2}$$

(b)

Because the wave function has a null at $r = 0$, its energy is the same as that of the odd-parity *second* energy level in a 1-D well of twice the width, w = 2a = 2R, and the same depth – see Sec. 2.2.3 and Fig. 2•2-6. Hence (2•2-28b) applies here,

$$\sin kR = \pm kR / k_0R \quad , \tag{2}$$

where k_0 obeys (2•2-25) with $M = m_e$,

$$V_0 = \frac{\hbar^2k_0^2}{2m_e} = R_\infty \cdot k_0^2a_0^2 , \tag{3}$$

using (2•2-9). Setting $V_0 = R_\infty$ and $R = 2a_0$ implies $k_0R = 2$, and (2) becomes

$$x \equiv kR = 2\sin x \quad . \tag{4}$$

Solve (4) numerically yields kR = 1.896, with an associated energy

$$\boxed{\varepsilon = -V_0 + \frac{\hbar^2k^2}{2m_e} = \left[-1 + (ka_0)^2\right] = \left(-1 + \frac{1}{4}x^2\right)\cdot R_\infty = -0.102R_\infty}$$

Exercise: Derive (3•2-21), (3•2-23), and (3•2-24)

(a) Derivation of (3•2-21)

From (3•2-20), we get

$$\chi = A \cdot L(s) \cdot s^{l+1} \cdot e^{-\frac{s}{2}}$$

$$\frac{d\chi}{ds} = A \cdot \frac{dL}{ds} \cdot s^{l+1} \cdot e^{-\frac{s}{2}} + A \cdot L \cdot (l+1)s^{l} \cdot e^{-\frac{s}{2}} + A \cdot L \cdot s^{l+1} \cdot (-\frac{1}{2})e^{-\frac{s}{2}}$$

$$\frac{d^2\chi}{ds^2} =$$

$$A \cdot \frac{d^2L}{ds^2} \cdot s^{l+1} \cdot e^{-\frac{s}{2}} + A \cdot \frac{dL}{ds} \cdot (l+1)s^{l} \cdot e^{-\frac{s}{2}} + A \cdot \frac{dL}{ds} \cdot s^{l+1} \cdot (-\frac{1}{2})e^{-\frac{s}{2}} + A \cdot \frac{dL}{ds} \cdot (l+1)s^{l} \cdot e^{-\frac{s}{2}} +$$
$$A \cdot L \cdot l(l+1)s^{l-1} \cdot e^{-\frac{s}{2}} + A \cdot L \cdot (l+1)s^{l} \cdot (-\frac{1}{2})e^{-\frac{s}{2}} + A \cdot \frac{dL}{ds} \cdot s^{l+1} \cdot (-\frac{1}{2})e^{-\frac{s}{2}} +$$
$$A \cdot L \cdot (l+1)s^{l} \cdot (-\frac{1}{2})e^{-\frac{s}{2}} + A \cdot L \cdot s^{l+1} \cdot (\frac{1}{4})e^{-\frac{s}{2}}$$
$$= l(l+1)A \cdot L \cdot s^{l-1} \cdot e^{-\frac{s}{2}} - n \cdot A \cdot L \cdot s^{l} \cdot e^{-\frac{s}{2}} + (\frac{1}{4})A \cdot L \cdot s^{l+1} \cdot e^{-\frac{s}{2}}$$

For last equity we use (3•2-18). Eliminating identical terms and factoring will yield

$$\frac{d^2L}{ds^2} \cdot s^{l+1} + \frac{dL}{ds} \cdot (l+1)s^{l} + \frac{dL}{ds} \cdot s^{l+1} \cdot (-\frac{1}{2}) + \frac{dL}{ds} \cdot (l+1)s^{l} + L \cdot (l+1)s^{l} \cdot (-\frac{1}{2}) +$$
$$\frac{dL}{ds} \cdot s^{l+1} \cdot (-\frac{1}{2}) + L \cdot (l+1)s^{l} \cdot (-\frac{1}{2}) + n \cdot L \cdot s^{l} = 0$$

After re-arranging the equation and dividing both sides with s^l, we will get

$$\boxed{s\frac{d^2L}{ds^2} - [s - 2(l+1)]\frac{dL}{ds} + [n - (l+1)]L = 0} \qquad \text{QED}$$

(b) Derivation of (3•2-23)

From (3•2-22), we get

$$L = \sum_{v=0}^{\infty} c_v s^v \tag{1}$$

$$\frac{dL}{ds} = \sum_{v=0}^{\infty} v c_v s^{v-1} \tag{2}$$

$$\frac{d^2L}{ds^2} = \sum_{v=0}^{\infty} v(v-1)c_v s^{v-2} \tag{3}$$

Inserting (1)(2)(3) into (3·2-21) yields

$$\left(\sum_{v=0}^{\infty} v(v-1)c_v s^{v-1}\right) - [s-2(l+1)]\cdot\left(\sum_{v=0}^{\infty} vc_v s^{v-1}\right) + [n-(l+1)]\cdot\left(\sum_{v=0}^{\infty} c_v s^{v}\right) = 0 \tag{4}$$

We can re-write (4) as

$$\left(\sum_{v=0}^{\infty} v(v-1)c_v s^{v-1} + 2(l+1)\cdot vc_v s^{v-1}\right) + \left(\sum_{v=0}^{\infty} [n-(l+1)]\cdot c_v s^{v} - vc_v s^{v}\right) = 0 \tag{5}$$

$$\rightarrow \quad \left(\sum_{v=0}^{\infty} [v(v-1)+2v(l+1)]c_v s^{v-1}\right) + \left(\sum_{v=0}^{\infty} [n-(l+1)-v]\cdot c_v s^{v}\right) = 0 \tag{6}$$

Changing the indices of both terms in (6) yields

$$\left(\sum_{v=1}^{\infty} [v(v-1)+2v(l+1)]c_v s^{v-1}\right) + \left(\sum_{v=1}^{\infty} [n-(l+1)-(v-1)]\cdot c_{v-1} s^{v-1}\right) = 0 \tag{7}$$

Re-arranging (7) and multiplying both sides by s yields

$$\boxed{\sum_{v=1}^{\infty} \{[v(v-1)+2v(l+1)]c_v - [(v-1)+(l+1)-n]c_{v-1}\} s^{v} = 0} \qquad \text{QED}$$

Note that the summation index starts from v = 1, not v = 0.

(c) Derivation of (3•2-24)

From (3•2-23), we know that each term of the summation *must* be zero, so

$$\frac{c_v}{c_{v-1}} = \frac{(v-1)+(l+1)-n}{v(v-1)+2v(l+1)} = \frac{v+l-n}{v(v+2l+1)}.$$

Thus,

$$\boxed{c_v = \frac{v+l-n}{v(v+2l+1)}c_{v-1}} \qquad \text{QED}$$

#4·2-1: Spreading of a Moving Wave Packet

The key to keeping the math of this problem simple is to know what to expect *physically*, namely, a wave packet that moves with a velocity

$$v_0 = \frac{\hbar k_0}{M}, \tag{1}$$

and to formulate the math in terms adapted to the physics.

The term $-i\hbar k^2 t/2M$ referred to just above (4•2-15) must now be added to the exponent in (4•2-13) rather than that of (4•2-7). We re-arrange this term in such a way that *k* occurs only in the combination $k - k_0$, and that any k_0 terms not occurring as $k - k_0$ are expressed as velocity terms via (1):

$$-\frac{i\hbar t}{2M}k^2 = -\frac{iht}{2M}\left[(k-k_0)^2 + 2(k-k_0)\cdot k_0 + k_0^2\right] = -\frac{iht}{2M}(k-k_0)^2 - i(k-k_0)v_0 t - \frac{it}{\hbar}\frac{1}{2}Mv_0^2 \tag{2}$$

The $(k - k_0)^2$-term in the last expression gets again combined with the other $(k - k_0)^2$-term in the exponent in (4•2-13), leading to a term of the same form as (4•2-15), except that k^2 has been replaced by $(k - k_0)^2$:

$$-\left[(k-k_0)/2\Delta k\right]^2 \cdot (1 + it/t_0) \quad , \tag{3}$$

where Δk and t_0 have the same meanings as before.

The v_0t-term may be combined with the x-term in the exponent, yielding

$$i(k-k_0)(x - v_0 t) \quad . \tag{4}$$

This is the term that describes the propagation through space of the wave packet, with the velocity v_0: Wherever x showed up inside the integral in (4•2-13), we now find $x - v_0t$.

Finally, the last term in (2) simply reflects the increase in kinetic energy of the moving wave packet relative to the same wave packet at rest. We bring it into a more usefulform by defining a frequency w_0 such that $\hbar w_0$ is the kinetic energy of the translational relation,

$$\hbar w_0 = \frac{1}{2}Mv_0^2 . \tag{5}$$

Putting everything together:

$$\boxed{\Psi(x,t) = \frac{c_0}{\sqrt{1 + it/t_0}} \cdot \exp\left[i(k_0 x - w_0 t)\right] \cdot \exp\left[-\frac{(x - v_0 t)^2}{(2\Delta x')^2} \cdot (1 - it/t_0)\right]}$$

We evidently have a plane wave corresponding to the center-of-mass motion of the object, modulated with a Gaussian that travels with the speed v_0 and spreads out with time.

#4·3-1: Uncertainty Product for the Hydrogen Atom

We need

$$\langle \Delta x \rangle^2 = \langle x^2 \rangle - \langle x \rangle^2 \quad \text{and} \quad \langle \Delta p_x \rangle^2 = \langle p_x^2 \rangle - \langle p_x \rangle^2 \quad ,$$

with the various expectation values calculated from the ground state wave function given in (3•2-43):

$$\psi(r) = \frac{1}{\sqrt{\pi} \cdot a_0^{3/2}} e^{-\frac{r}{a_0}} .$$

From symmetry:

$$\langle x \rangle = 0 , \ \langle p_x \rangle = 0 ,$$

$$\langle x^2 \rangle = \langle y^2 \rangle = \langle z^2 \rangle = \frac{1}{3} \langle r^2 \rangle , \ \langle p_x^2 \rangle = \langle p_y^2 \rangle = \langle p_z^2 \rangle = \frac{1}{3} \langle p^2 \rangle .$$

Hence, for Δx:

$$\langle \Delta x \rangle^2 = \frac{1}{3} \langle r^2 \rangle = \frac{1}{3} \int_0^\infty \psi^2 r^2 \cdot 4\pi r^2 dr = \frac{4\pi}{3} \cdot \frac{a_0^2}{32\pi} \int_0^\infty e^{-s} \cdot s^4 ds = a_0^2 .$$

For Δp_x we can simplify the problem by utilizing the relation (4•3-5) between $\langle p^2 \rangle$ and the expectation value $\langle \varepsilon_{kin} \rangle$ of the kinetic energy. Drawing on (3•2-5),

$$\langle \Delta p_x \rangle^2 = \frac{1}{3} \langle p^2 \rangle = \frac{2m_e}{3} \langle \varepsilon_{kin} \rangle = \frac{\hbar^2}{3a_0^2}$$

Putting it all together:

$$\boxed{\begin{array}{l} \Delta x \cdot \Delta p_x = \dfrac{\hbar}{\sqrt{3}} > \dfrac{\hbar}{2} \\ \langle \Delta p_x \rangle^2 = \dfrac{1}{3} \langle p^2 \rangle \end{array}}$$