Homework 1

Chapters 12 and 13

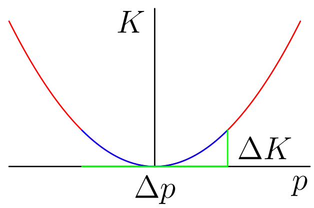
Problem 1. *It would take a huge potential energy barrier to confine an electron to the nucleus of an atom (diameter $d \approx 10$ fm). (a) Use the Heisenberg uncertainty principle to find the momentum uncertainty of such a bound electron. (b) Use the monemtum uncertainty from (a) to find the minimum binding energy U. Note that the total energy $E = K + U < 0$ for a bound particle. You may use the non-relativistic form of kinetic energy even though it's not particularly valid for this situation.*

(a) The uncertainty principle gives a lower bound on our momentum uncertainty Δp

$$\Delta x \Delta p \geq \frac{\hbar}{2} \tag{1}$$

$$\Delta p \geq \frac{\hbar}{2\Delta x} = \frac{\hbar}{2d} = 5.27 \cdot 10^{-21} \text{ kg·m/s} . \tag{2}$$

(b) The momentum uncertainty puts a lower bound on the kinetic energy uncertainty ΔK.



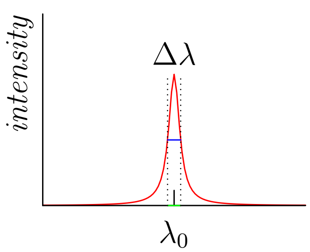
$$\Delta K = \frac{(\Delta p/2)^2}{2m} = \frac{\hbar^2}{32 d^2 m} \tag{3}$$

The binding potential must be at least this deep, or the electron would occasionally have enough kinetic energy to escape.

$$\Delta U < -\Delta K \approx -\frac{\hbar^2}{32 d^2 m} = -3.8 \text{ pJ} = -24 \text{ MeV} . \tag{4}$$

So the energy barrier is 24 MeV, which is much greater than the electron's rest mass energy of 511 keV, so the electron would be extremely relativistic. This is one reason why light particles such as electrons do not collapse into the nucleus of the atom, despite the electromagnetic attraction to the protons.

Problem 2. *The time/energy Heisenberg uncertainty principle is the source of an natural linewidth $\Delta\lambda$ in photons emitted from atoms when electrons change orbitals. (a) Calculate the frequency of light emitted in the $n_2 \to n_1$ transition for Hydrogen. (b) Assuming that transition has an average lifetime of $\tau = 1.6$ ns, estimate the relative uncertainty in the energy of the emitted photon.*



(a) From the Rydberg formula

$$\frac{1}{\lambda} = R_H \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \tag{5}$$

$$f = \frac{c}{\lambda} = c R_H \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) = 3 \cdot 10^8 \text{ m/s} \cdot 1.097 \cdot 10^7 \text{ 1/m} \left(1 - \frac{1}{4} \right) = 2.47 \cdot 10^{15} \text{ Hz} \tag{6}$$

(b) Using the energy/time uncertainty principle,

$$\Delta E \Delta t \geq \frac{\hbar}{2} \tag{7}$$

$$\Delta E \geq \frac{\hbar}{2\Delta t} \approx \frac{\hbar}{2\tau} = 3.3 \cdot 10^{-26} \text{ J} = 2.1 \cdot 10^{-7} \text{ eV} \tag{8}$$

$$\frac{\Delta E}{E} = \frac{\Delta E}{hf} \geq 2.0 \cdot 10^{-8} \tag{9}$$

(bonus) We can see find the natural linewidth $\Delta\lambda$ through a propagation-of-errors approach

$$\lambda = \frac{hc}{E} = \frac{c}{f} = 121 \text{ nm} \tag{10}$$

$$\partial\lambda = -\frac{hc}{E^2}\partial E = -\lambda\frac{\partial E}{E} \; . \tag{11}$$

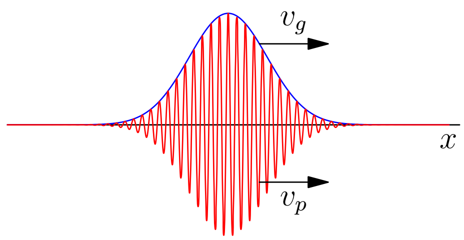
Since $\Delta E \ll E$, this relationship doesn't change much over the span of $E \pm \Delta E/2$, so

$$\Delta\lambda \approx -\lambda\frac{\Delta E}{E} \geq 2.4 \text{ fm} \; , \tag{12}$$

where we dropped the sign because we only care about the range $\Delta\lambda$, not whether increasing E increases or decreases λ. Note that the propagation-of-errors approach would *not* work for Problem 1, since $\partial K/\partial p(p=0) = 0$. Therefore, assuming the slope to be constant over the range Δp would give $\Delta K = 0$. Instead, we used a quasi-graphical approach that took advantage of our understanding of $K(p) = p^2/2m$.

Problem 3. *In the particle-wave duality, localized particles are modeled as wave packets, with both a group speed and a phase speed. Between Equations 28.13 and 28.16, the text shows that the group speed v_g of a wave function ψ is the same as the particle speed u. Treat the particle as a non-relativistic de Broglie wave, and use $v_p = \lambda f$ to show that the phase speed $v_p = u/2 \neq u = v_g$.*

Here's a picture of the wave packet, just as a reminder of what we're talking about.



We start with the given definition of the phase velocity

$$v_p = \lambda f \; . \tag{13}$$

DeBroglie tells us (Equations 28.10 and 28.11)

$$\lambda = \frac{h}{p} \tag{14}$$

$$E = hf \; , \tag{15}$$

so

$$v_p = \lambda f = \frac{hf}{p} = \frac{E}{p} \; . \tag{16}$$

Then we use the non-relativistic kinetic energy and momentum

$$E = \frac{p^2}{2m} \tag{17}$$

$$p = mu \tag{18}$$

$$v_p = \frac{E}{p} = \frac{\frac{p^2}{2m}}{p} = \frac{p}{2m} = \frac{mu}{2m} = \frac{u}{2} \; . \tag{19}$$

As a side note, I have no idea why the text uses u instead of v for Equation 28.16, but I though I should stick with it here to avoid adding to the confusion.

Problem 4. *An electron that has an energy of approximately 6 eV moves between rigid walls 1.00 nm apart. Find (a) the quantum number n for the energy state that the electron occupies and (b) the precise energy of the electron.*

(a) The allowed energy levels for a particle in a box are (Equation 28.30)

$$E_n = \frac{h^2 n^2}{8mL^2} \; . \tag{20}$$

For an electron ($m = 9.11 \cdot 10^{-31}$ kg) in a box of length $L = 1$ nm, this works out to

$$E_1 = 0.377 \text{ eV} \tag{21}$$
$$E_2 = 1.51 \text{ eV} \tag{22}$$
$$E_3 = 3.39 \text{ eV} \tag{23}$$
$$E_4 = 6.02 \text{ eV} \tag{24}$$
$$E_5 = 9.41 \text{ eV} \tag{25}$$

So the electron is in the $n = 4$ state.
(b) The precise energy is $E_4 = 6.02$ eV.

Problem 5. *The wave function for a particle confined to moving in a one-dimensional box is*

$$\psi(x) = A\sin\left(\frac{n\pi x}{L}\right) \tag{26}$$

Use the normalization condition to show that

$$A = \sqrt{\frac{2}{L}} \tag{27}$$

HINT*: Because the box length is L, the wave function is zero for $x < 0$ and for $x > L$.*

$$1 = \int_{-\infty}^{\infty} \psi dx \psi^* = \int_0^L \psi^2 dx \ , \tag{28}$$

where we used the fact that $\psi(x) = 0$ for $x < 0$ and $x > L$ to reduce the range of integration, and the fact that ψ is real to reduce $\psi\psi^2 = \psi^2$. So we must integrate

$$1 = \int_0^L \psi^2 dx = \int_0^L A^2 \sin^2\left(\frac{n\pi x}{L}\right) dx = A^2 \int_0^\pi \sin^2(nu)\frac{Ldu}{\pi} = \frac{LA^2}{\pi}\int_0^\pi \sin^2(nu)du \ , \tag{29}$$

where $u \equiv \pi x/L$, so $dx = Ldu/\pi$.
There are two possible approaches. The easiest way is to use symmetry. We're integrating over multiples of half wavelengths of sin ($\lambda = 2\pi/n$ so $\pi = n\lambda/2$), so we're integrating through full wavelengths of $\sin^2$. Over a full wavelength, the averages $< \sin^2 >=< \cos^2 >= 1/2$ since $\sin^2 + \cos^2 = 1$. so

$$1 = \frac{LA^2}{\pi}\int_0^\pi \sin^2(nu)du = \frac{LA^2}{\pi} \cdot \pi\frac{1}{2} = \frac{LA^2}{2} \tag{30}$$
$$A = \sqrt{\frac{2}{L}} \ . \tag{31}$$

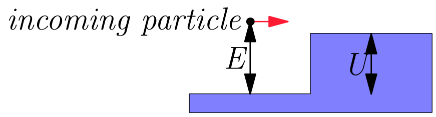
The slightly harder way is to use the double-angle identity $\sin^2(\theta) = [1 - \cos(2\theta)]/2$.

$$1 = \frac{LA^2}{\pi}\int_0^\pi \sin^2(nu)du = \frac{LA^2}{2\pi}\int_0^\pi [1-\cos(2nu)]du = \frac{LA^2}{2\pi}\cdot\left[\int_0^\pi du - \int_0^\pi \cos(2nu)du\right] \tag{32}$$
$$= \frac{LA^2}{2\pi}\cdot\left[u + \frac{1}{2n}\sin(2nu)\right]_0^\pi = \frac{LA^2}{2\pi}\cdot\pi = \frac{LA^2}{2} \tag{33}$$
$$A = \sqrt{\frac{2}{L}} \ . \tag{34}$$

Problem 6. BONUS PROBLEM. *Particles incident from the left are confronted with a step in potential energy. Located at $x = 0$, the step has a height U. The particles have energy $E > U$. Classically, we would expect all the particles to continue on, although with reduced speed. According to quantum mechanics, a fraction of the particles are reflected at the barrier. Prove that the reflection coefficient R for this case is*

$$R = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2} \ , \tag{35}$$

where $k_1 = 2\pi/\lambda_1$ and $k_2 = 2\pi/\lambda_2$ are the wave numbers for the incident and transmitted particles. Proceed as follows. Impose the boundary conditions $\psi_1 = \psi_2$ and $d\psi_1/dx = d\psi_2/dx$ at $x = 0$ to find the relationships between B and A. Then evaluate $R = B^2/A^2$.
Assume the wave function $\psi_1 = Ae^{ik_1x} + Be^{-ik_1x}$ satisfies the Schrödinger equation in region 1, for $x < 0$. Also assume that $\psi_2 = Ce^{ik_2x}$ satisfies the Schrödinger equation in region 2, for $x > 0$. These assumptions will be derived in the posted solutions in case you are interested, but they are pretty straightforward.



Show that ψ_1 satisfies the Schrödinger equation

$$-\frac{\hbar}{2m}\frac{d^2\psi}{dx^2} = (E-U)\psi \tag{36}$$

in region 1.

$$\frac{d\psi_1}{dx} = ik_1Ae^{ik_1x} - ik_1Be^{-ik_1x} \tag{37}$$

$$\frac{d\psi_1^2}{dx^2} = i^2k_1^2Ae^{ik_1x} + i^2k_1^2Be^{-ik_1x} = -k_1^2\psi\ . \tag{38}$$

So the Schrödinger equation is satisfied if

$$k_1^2\frac{\hbar}{2m} = E - U_1 = E \tag{39}$$

$$k_1 = \frac{\sqrt{2mE}}{\hbar} \tag{40}$$

Show that ψ_2 satisfies the Schrödinger equation in region 2.

$$\frac{d\psi_2}{dx} = ik_2Ce^{ik_2x} \tag{41}$$

$$\frac{d\psi_2^2}{dx^2} = i^2k_2^2Ce^{ik_2x} = -k_2^2\psi\ . \tag{42}$$

So the Schrödinger equation is satisfied if

$$k_2^2\frac{\hbar}{2m} = E - U_2 = E - U \tag{43}$$

$$k_2 = \frac{\sqrt{2m(E-U)}}{\hbar} \tag{44}$$

Imposing the continuous ψ boundary condition

$$\psi_1(x=0) = \psi_2(x=0) \qquad \to \qquad A + B = C \tag{45}$$

Imposing the smooth ψ boundary condition

$$\frac{d\psi_1}{dx}(x=0) = \frac{d\psi_2}{dx}(x=0) \qquad \to \qquad ik_1A - ik_1B = ik_2C \qquad \to \qquad \frac{k_1}{k_2}(A-B) = C \tag{46}$$

Putting this together to find the reflection coefficient

$$A + B = C = \frac{k_1}{k_2}(A-B) \tag{47}$$

$$k_2B + k_1B = k_1A - k_2A \tag{48}$$

$$B = \frac{k_1-k_2}{k_1+k_2}A \tag{49}$$

$$\frac{B}{A} = \frac{k_1-k_2}{k_1+k_2} \tag{50}$$

$$R = \frac{B^2}{A^2} = \left(\frac{B}{A}\right)^2 = \frac{(k_1-k_2)^2}{(k_1+k_2)^2}\ , \tag{51}$$

which is what we set out to show.