Physics 251 exam 2, November 9, 2006.

1. A He^+ ion has its electron undergo a transition from the $2p$ to the $1s$ state. What is the mean wavelength of the emitted photon? If the $2p$ state were to have a lifetime of 2×10^{-14} seconds or 20 fsec, what would be the wavelength spread about the mean?
Answer: We have $E = -E_0 Z^2/n^2$ so in this case the photon energy is

$$\Delta E = E_2 - E_1 = (-13.6)\frac{2^2}{2^2} - (-13.6)\frac{2^2}{1^2} = 13.6(4-1) = 40.8 \text{ eV}$$

and the photon wavelength is $\lambda = hc/E = 1240/40.8 = 30.4$ nm. The energy width is given by the uncertainty principle $(\Delta E)(\Delta t) = \hbar/2$ or

$$\Delta E = \frac{\hbar}{2\Delta t} = \frac{6.582 \times 10^{-16} \text{ eV} \cdot \text{sec}}{2 \cdot (2 \times 10^{-14} \text{ sec})} = 0.016 \text{ eV}$$

and since $\Delta E/E = \Delta\lambda/\lambda$ we have

$$\Delta\lambda = \lambda\frac{\Delta E}{E} = \frac{hc}{E}\frac{\Delta E}{E} = \frac{(1240 \text{ eV} \cdot \text{nm})(0.016 \text{ eV})}{(40.8 \text{ eV})^2} = 0.012 \text{ nm}$$

as the 1σ spread in wavelength.

Many people calculated ΔE from the uncertainty principle but then calculated the wavelength spread with

$$\Delta\lambda = \frac{hc}{\Delta E} = \frac{1240 \text{ eV} \cdot \text{nm}}{0.016 \text{ eV}} = 77,000 \text{ nm}.$$

This is incorrect! Getting a wavelength spread of 77,000 nm when the mean wavelength is only 30.4 nm should have made you stop and think. Because the wavelength decreases as the energy is increased, let's consider a small difference in energy ΔE from a mean energy E, and a correspondingly small decrease in wavelength $\Delta\lambda$:

$$\begin{aligned}
\lambda - \Delta\lambda &= \frac{hc}{E + \Delta E} = \frac{hc}{E(1 + \Delta E/E)} = \lambda(1 + \Delta E/E)^{-1} \simeq \lambda(1 - \Delta E/E) \\
\lambda - \Delta\lambda &= \lambda - \lambda\frac{\Delta E}{E} \\
-\frac{\Delta\lambda}{\lambda} &= \frac{\Delta E}{E}
\end{aligned}$$

or in other words $\lambda \mp \Delta\lambda = hc/(E \pm \Delta E)$.

2. Boron (B; $Z = 5$) has its electrons arranged as follows: $1s^2\, 2s^2\, 2p^1$. What's the electronic configuration of Scandium (Sc; $Z = 21$)?
Answer: From the equation sheet we have the following energy order for states:
$1s < 2s < 2p < 3s < 3p < 4s \lesssim 3d < 4p < 5s \ldots$ We need to come up with 21 electrons. Let's make a table:

State	n	ℓ	m_ℓ	Number of electrons	Running total
$1s$	1	0	0	2	2
$2s$	2	0	0	2	4
$2p$	2	1	[-1,0,1]	6	10
$3s$	3	0	0	2	12
$3p$	3	1	[-1,0,1]	6	18
$4s$	4	0	0	2	20
$3d$	3	2	[-2,-1,0,1,2]	1 of 10	21

So it looks like the ground state electronic configuration of Scandium is
$1s^2\,2s^2\,2p^6\,3s^2\,3p^6\,4s^2\,3d^1$

3. For box of width L and potential $U = 0$ inside the box and $U \to \infty$ outside, we guessed at a ground state wavefunction solution of $\psi(x) = A\sin(\pi x/L)$. Do the calculations to show that this satisfies the Schrödinger equation, solve for the coefficient A (that is, show how you calculate it and do the calculation), and derive the expression for the energy of the state.
Answer: We will need the second derivative of $\psi(x)$:

$$\frac{d^2}{dx^2}\psi(x) = \frac{d}{dx}\frac{\pi}{L}A\cos(\pi\frac{x}{L}) = -\frac{\pi^2}{L^2}A\sin(\pi\frac{x}{L}) = -\frac{\pi^2}{L^2}\psi(x).$$

The wavefunction is zero outside the box. The 1D, time-independent Schrödinger equation inside the box is then

$$\begin{aligned}
-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + U\psi(x) &= E\psi(x) \\
-\frac{\hbar^2}{2m}(-\frac{\pi^2}{L^2})\psi(x) + (0)\psi(x) &= E\psi(x) \\
\text{giving} \qquad E &= \frac{h^2}{8mL^2}
\end{aligned}$$

for the energy (and yes, it satisfies the Schrödinger equation). The normalization condition is

$$\int_{-\infty}^{\infty} |\psi(x)|^2\,dx = 1 \;\; \Rightarrow \;\; \int_0^L A^2\sin^2(\frac{\pi}{L}x)\,dx = A\int_0^L \sin^2(ax)\,dx \qquad \text{with} \qquad a \equiv \frac{\pi}{L}$$

$$\begin{aligned}
1 &= A^2\left(\frac{x}{2} - \frac{\sin(2ax)}{4a}\right)\Big|_{x=0}^{L} \\
&= A^2\left(\frac{L}{2} - \frac{\sin(2\pi L/L)}{4\pi/L}\right) - A^2\left(\frac{0}{2} - \frac{\sin(0)}{4\pi/L}\right) \\
&= A^2\frac{L}{2}
\end{aligned}$$

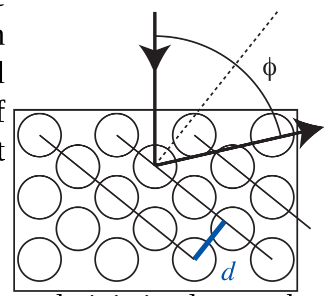
or $A = \sqrt{2/L}$.

4. What is the $1/e$ distance over which an electron's wavefunction tunnels outside a finite potential square well? The electron's kinetic energy is 3 eV and the depth of the potential well is 5 eV.
Answer: When $E < U$ the wavefunction takes the form $\psi(x) = C \exp[-kx]$ with $k = \sqrt{2m(U-E)}/\hbar$. As a result, the $1/e$ tunneling distance is $\delta = 1/k$ or

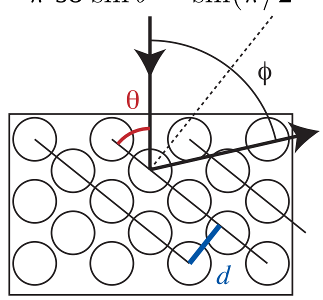
$$\begin{aligned} \delta &= \frac{1}{k} = \frac{\hbar}{\sqrt{2m(U-E)}} = \frac{hc}{2\pi\sqrt{2\,mc^2\,(U-E)}} \\ &= \frac{1240 \text{ eV} \cdot \text{nm}}{2\pi\sqrt{2 \cdot (511 \times 10^3 \text{ eV}) \cdot (5-3 \text{ eV})}} = 0.14 \text{ nm} \end{aligned}$$

as the $1/e$ distance over which $\psi(x)$ tunnels outside the box.

5. An electron beam with kinetic energy K is at normal incidence to a crystal. The first diffraction peak appears at an angle ϕ from the incident beam direction, due to a periodicity d in the crystal (a periodicity of d means that atomic planes have a spacing of d). Find an analytical expression for ϕ. Find a numerical result for ϕ with $K = 10$ eV and $d = 0.2$ nm.



Answer: With a kinetic energy of only 10 eV, this is a very non-relativistic electron beam. From Bragg's law we know $2d\sin\theta = \lambda$ for the $n = 1$ diffraction order, and from the following diagram we see that $2\theta + \phi = \pi$ so $\sin\theta = \sin(\pi/2 - \phi/2) = \cos(\phi/2)$.



In addition, we have $K = p^2/(2m)$ or $p = \sqrt{2mK}$ and the de Broglie wavelength $\lambda = h/p$. If we put these things together we have

$$\begin{aligned} 2d\sin\theta &= \lambda \\ 2d\cos(\frac{\phi}{2}) &= \frac{h}{\sqrt{2mK}} \\ \phi &= 2\arccos\left(\frac{h}{2d\sqrt{2mK}}\right) = 2\arccos\left(\frac{hc}{2d\sqrt{2mc^2K}}\right) \\ &= 2\arccos\left(\frac{1240 \text{ eV} \cdot \text{nm}}{2(0.3 \text{ nm})\sqrt{2 \cdot (511 \times 10^3 \text{ eV}) \cdot (20 \text{ eV})}}\right) = 28.3^\circ \end{aligned}$$