# Exam 1 with Answers

1. For each part below write one or two sentences IN YOUR OWN WORDS.

(i) Briefly discuss an experiment which implies that light behaves as a wave phenomenon.

(ii) Briefly discuss an experiment which implies that light is made of particles.

(iii), (iv) Repeat (i) and (ii) for electrons.

(i) Young's double slit diffraction experiment.

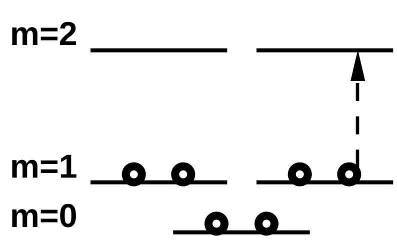
(ii) Photoelectric effect, blackbody radiation, Compton effect, Young experiment with filters.

(iii) Electron diffraction, quantum mechanics!

(iv) television

2. A free-electron model for cyclic conjugated molecules can be based on solutions of the particle in a ring problem. Apply this model to benzene, assuming 6 mobile electrons moving on a ring of radius of 1.39 Å. Calculate the wavelength (in nm) of the lowest-energy electronic transition in benzene. In what region of the electromagnetic spectrum is this transition?

Recall the energy level diagram for ring:



The longest wavelength absorption in the benzene spectrum can be estimated according to this model as

$$\frac{hc}{\lambda} = E_2 - E_1 = \frac{2}{2mR^2}(2^2 - 1^2)$$

The ring radius $R$ can be approximated by the C–C distance in benzene, 1.39 Å. We predict $\lambda \approx 210$ nm, whereas the experimental absorption has $\lambda_{\max} \approx 268$ nm. These are in the ultraviolet.

3. A particle of mass $m$ moves in three dimensions with the potential energy

$$V(x, y, z) = \frac{k}{2}(x^2 + y^2 + z^2)$$

Write down the Schrödinger equation and solve it for the ground state. Determine the energy eigenvalue and normalized eigenfunction for the ground state.

Schrödinger equation in cartesian coordinates, $\psi = \psi(x, y, z)$

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right] + \frac{k}{2}(x^2 + y^2 + z^2)\psi = E\psi$$

Separate variables in cartesian coordinates

$$\psi(x, y, z) = X(x)Y(y)Z(z)$$

Equation for $X(x)$:

$$-\frac{\hbar^2}{2m}X''(x) + \frac{k}{2}x^2X(x) = E_X X(x)$$

and analogously for $Y$ and $Z$, so that

$$E_X + E_Y + E_Z = E$$

But above differential equation already solved for harmonic oscillator! Normalized ground state solution is

$$X_0(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2}$$

with the corresponding eigenvalue $E_X = \frac{1}{2}\hbar\,\omega$. Therefore

$$\psi(x, y, z) = \left(\frac{\alpha}{\pi}\right)^{3/4} e^{-\alpha(x^2+y^2+z^2)/2}$$

with ground state energy

$$E_0 = E_X + E_Y + E_Z = \tfrac{3}{2}\hbar\,\omega$$

4. The following reaction might occur in the interior of a star:

$$\mathrm{He}^{++} + \mathrm{H} \rightarrow \mathrm{He}^{+} + \mathrm{H}^{+}$$

Calculate the electronic energy change in eV assuming all species in their ground states.

$He^{++}$ and $H^{+}$ are bare nuclei so their electronic energies equal zero. $He^{+}$ and H are hydrogenlike with $Z = 2$ and $Z = 1$, respectively. Their 1s energies equal $-Z^2/2$. Thus $\Delta E = -4/2 + 1/2 = -3/2$ hartrees $= -40.8$ eV.

5. Determine whether the function

$$\psi(r,\theta,\phi) = \text{const}\left[1 - r\,\sin^2(\theta/2)\right]e^{-r/2}$$

is a solution of the Schrödinger equation for the hydrogen atom. If it is, find the corresponding eigenvalue (in atomic units). You might need the trigonometric identity

$$\sin(\theta/2) = \sqrt{\frac{1-\cos\theta}{2}}$$

Lengthy computation gives

$$\left[-\frac{1}{2r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} - \frac{1}{2r^2\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} - \frac{1}{r}\right]\psi(r,\theta) = E\,\psi(r,\theta)$$

with

$$E = -\frac{1}{8}$$

Easier solution. After putting in formula for $\sin(\theta/2)$, note that

$$\psi(r,\theta) = \text{const}\left[\left(1-\frac{r}{2}\right) + \frac{1}{2}\,r\,cos\theta\right]e^{-r/2}$$

$$= \text{const}\,(\psi_{2s} + \psi_{2p_z})$$