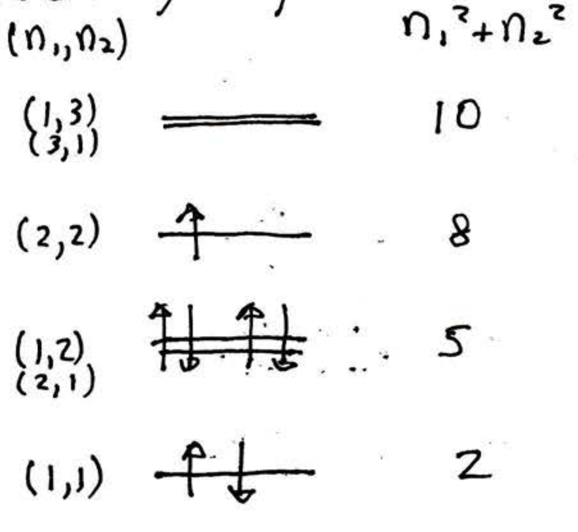
Physics 4E <u>Quiz 4 Solutions</u> Spring 2017

energies for electrons in 2D square box of length L:

$$E_{n_1,n_2} = \frac{\hbar^2 \pi^2}{2 m_e L^2}\left(n_1^2 + n_2^2\right)$$



Lowest energy states are:

(1,1) (1,2) (2,1) (2,2) (3,1) (1,3) (3,2) (2,3)

According to the Pauli exclusion principle, we can have 2 electrons of opposite spin in each energy state. See diagram, for 7 electrons

The lowest excitation energy is for the electron in (2,2) to go to (3,1) or (1,3), with energy change

$$\Delta E = E_{3,1} - E_{2,2} = \frac{\hbar^2\pi^2}{2m_eL^2}(10-8) = \frac{\hbar^2\pi^2}{2m_eL^2}\cdot 2 \Rightarrow$$

$$\Delta E = \frac{7.62\,\pi^2}{L^2} = \frac{hc}{\lambda} \Rightarrow L^2 = \frac{7.62\,\pi^2\lambda}{hc} = 25\,\text{Å}^2 \Rightarrow$$

$$\Rightarrow \boxed{L = 5\,\text{Å}} \quad (a)$$

(b) The next lowest excitation energy is for an electron in (1,2) or (2,1) to go to (2,2), with energy change

$$\Delta E = E_{2,2} - E_{1,2} = \frac{\hbar^2\pi^2}{2m_eL^2}\cdot 3 = \frac{hc}{\lambda} \Rightarrow \lambda = \frac{2}{3}\times 4122\,\text{Å}$$

$$\Rightarrow \boxed{\lambda = 2748\,\text{Å}}$$

Problem 2

$$\psi(r,\theta,\phi) = C r^2 e^{-r/a_0} \sin\theta \cos\theta \, e^{-i\phi}$$

From $e^{-i\phi} \Rightarrow m_l = -1$

From r^2 factn $\Rightarrow n = 3$ and $l = 2$

From $e^{-Zr/na_0} = e^{-r/a_0} \Rightarrow Z = 3$

(b) $P(r) = r^2 R(r)^2 \propto r^6 e^{-2r/a_0}$

$$P'(r_m) = 0 = 6 r_m^5 - \frac{2 r_m^6}{a_0} \Rightarrow \boxed{r_m = 3 a_0}$$

According to Bohr atom, $r_n = \frac{a_0}{Z} n^2 = \frac{a_0}{3} \cdot 3^2 = 3a_0 = r_m$

$\Rightarrow$ they agree.

(c) Electrons have spin $S = 1/2$, the total angular momentum quantum number j satisfies

$$|l - s| \le j \le l + s$$

$\Rightarrow j = 3/2$ or $j = 5/2$

Possible values of m_j: $-j$ to j in integer steps $\Rightarrow$

$$-\frac{5}{2}, -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}$$

Problem 3

The average energy of a 1D harmonic oscillator is

$$E = \frac{\hbar\omega}{2} + \frac{\hbar\omega}{e^{\hbar\omega/k_BT}-1}$$

Ground state energy is $E_0 = \frac{\hbar\omega}{2} = 0.01\,eV \Rightarrow \boxed{\hbar\omega = 0.02\,eV}$

For $E = 0.02\,eV = \hbar\omega \Rightarrow$

$$\frac{\hbar\omega}{2} + \frac{\hbar\omega}{e^{\hbar\omega/k_BT}-1} = \hbar\omega \Rightarrow \frac{1}{e^{\hbar\omega/k_BT}-1} = \frac{1}{2} \Rightarrow$$

$$\Rightarrow e^{\hbar\omega/k_BT} = 3 \Rightarrow T = \frac{\hbar\omega}{k_B \ln 3} = \boxed{211.2\,K} \text{ (a)}$$

Note: the "Einstein temperature" is $T_E = \frac{\hbar\omega}{k_B} = 232K$

(b) According to equipartition,

$$E = k_BT = \frac{211.2}{11{,}600}\,eV = \boxed{0.0182\,eV}$$

it is lower because it does not take into account zero-point energy

(c) The heat capacity for 1 oscillator is

$$C = \frac{dE}{dT} = \left(\frac{\hbar\omega}{k_BT}\right)^2 \frac{e^{\hbar\omega/k_BT}}{(e^{\hbar\omega/k_BT}-1)^2} k_B = \frac{(\ln 3)^2 e^{\ln 3}}{(e^{\ln 3}-1)^2} k_B =$$

$$= \frac{3}{4}(\ln 3)^2 k_B = \boxed{0.905\,k_B}$$

equipartition predicts $C = k_B$, so it differs by $\boxed{\sim 10\%}$

(9.5% more precisely)

Exact answer is lower than predicted by equipartition at all T.