

Solution to written exam in QUANTUM PHYSICS AND STATISTICAL PHYSICS
MTF131

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1. The energy eigenvalues for a particle in a box are given by

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 \pi^2 n^2}{2ma^2}, \text{ where } n = 1, 2, 3, \dots$$

- (a) There is no limit on the number of bosons in one state. Therefore, the ground state energy of five bosons is $5E_1 = \frac{5\hbar^2 \pi^2}{2ma^2}$.

The first excited state for the system we get by putting taking one particle from level 1 to level 2 and it will have the energy: $4E_1 + E_2 = \frac{4\hbar^2 \pi^2}{2ma^2} + \frac{\hbar^2 \pi^2 2^2}{2ma^2} = \frac{8\hbar^2 \pi^2}{2ma^2}$.

- (b) Fermions obey the Pauli principle. (only one fermion in a state taking spin into account). Thus, the ground state energy of five fermions is given by

$$E = 2E_1 + 2E_2 + E_3 = 2 \frac{\hbar^2 \pi^2 1^2}{2ma^2} + 2 \frac{\hbar^2 \pi^2 2^2}{2ma^2} + 1 \frac{\hbar^2 \pi^2 3^2}{2ma^2} = \frac{19\hbar^2 \pi^2}{2ma^2}.$$

Note in each 'particle in the box state' we can put two fermions one with spin up and one with spin down. The first excited state will have the energy:

$$E = 2E_1 + E_2 + 2E_3 = 2 \frac{\hbar^2 \pi^2 1^2}{2ma^2} + 1 \frac{\hbar^2 \pi^2 2^2}{2ma^2} + 2 \frac{\hbar^2 \pi^2 3^2}{2ma^2} = \frac{24\hbar^2 \pi^2}{2ma^2}.$$

2.

$$\langle S_x \rangle = \frac{1}{9} (2 + 2i, 1) \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 2 - 2i \\ 1 \end{pmatrix} = \frac{2}{9} \hbar$$

$$\langle S_y \rangle = \frac{1}{9} (2 + 2i, 1) \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 2 - 2i \\ 1 \end{pmatrix} = \frac{2}{9} \hbar$$

$$\langle S_z \rangle = \frac{1}{9} (2 + 2i, 1) \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 2 - 2i \\ 1 \end{pmatrix} = \frac{7}{18} \hbar$$

The square of the spin matrix σ_i^2 equals the unit matrix for i equal to x, y or z . This gives :

$$\langle S_x^2 \rangle = \langle S_y^2 \rangle = \langle S_z^2 \rangle = \hbar^2 \frac{1}{36} (2 + 2i, 1) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 2 - 2i \\ 1 \end{pmatrix} = \frac{1}{4} \hbar^2$$

3. (a) Let the commutator act on a wave function $\Psi(x)$ and $p_x = -i\hbar \frac{d}{dx}$

$$\begin{aligned} [x^2, p_x^2] \Psi(x) &= -\hbar^2 \left(x^2 \frac{d^2 \Psi(x)}{dx^2} - \frac{d^2 (x^2 \Psi(x))}{dx^2} \right) = \\ &= -\hbar^2 \left(x^2 \frac{d^2 \Psi(x)}{dx^2} - x^2 \frac{d^2 \Psi(x)}{dx^2} - 4x \frac{d\Psi(x)}{dx} - 2\Psi(x) \right) = +\hbar^2 2\Psi(x) + 4x\hbar^2 \frac{d\Psi(x)}{dx} = \\ &= \left(+\hbar^2 2 + i4\hbar x p_x \right) \Psi(x) \text{ concluding for the commutator: } [x^2, p_x^2] = +2\hbar^2 + 4i\hbar x p_x . \end{aligned}$$

- (b) The energy levels for a hydrogen like system are given by: $E_n = -13.6 \frac{Z^2}{n^2}$ [eV], here we have $Z = +3$:

$$\Delta E = E(2s) - E(1s) = E_2 - E_1 = -13.54 \cdot \left(\frac{9}{2^2} - \frac{9}{1^2} \right) = 13.54 \cdot \frac{27}{4} = 91, 53 \text{ eV}$$

(c) The angular part of the wave function can be written as a spherical harmonic:

$$3 \cos^2 \theta - 1 \propto Y_{20}$$

Which gives $l = 2$ och $m = 0$. The part depending on r (r^2/a_μ^2) $e^{-r/3a_\mu}$ corresponding to the principal quantum number $n = 3$ och $l = 2$ consistent with Y_{20} .

4. The Carbon ion has $Z = 6$ and hence energys $E_n = -\frac{488.16}{n^2}$ eV. Try to find a start of the series. The energy of $\lambda = 207.80$ nm is $E = h\nu = \frac{hc}{\lambda} = \frac{6.626 \cdot 10^{-34} \cdot 2.9979 \cdot 10^8}{207.80 \cdot 10^{-9} \cdot 1.6022 \cdot 10^{-19}} = 5.9663$ eV A similar calculation gives for the other lines in the series: 9.56395, 11.8989, 13.4997 eV.

As the Balmer series in Hydrogen is for transitions down to level $n=2$ we have to go higher up for the Carbon ion as the energys for the level $n =$ would be far to large.

Using the fact that can assume levels are adjacent we let n be the quantum number for the lower level and m for a level above, we have no knowledge of how n and m relate. We know however that for the next level we have n and $m + 1$. One can form the following two equations 5.9663 eV= $488.16(\frac{1}{n^2} - \frac{1}{m^2})$ eV and 9.56395 eV= $488.16(\frac{1}{n^2} - \frac{1}{(m+1)^2})$ eV ie we only need two of the lines to form an appropriate set of equations. (You can use the other lines as well to form two equations.) Subtracting one equation from the other to eliminat n you get $3.59765=488.16(\frac{1}{m^2} - \frac{1}{(m+1)^2})$ and $\frac{1}{m^2} - \frac{1}{(m+1)^2} = 0.007369817273025237627$ solving for m you arrive at $m = 6$.

Then there is the tour of brute force ie just trial and error: If we try $n=5$ we have transitions from $m=6, 7, 8, 9,$ etc. The corresponding energys will be: $488.16(\frac{1}{5^2} - \frac{1}{6^2})=5.97$ eV, the next one will be: $488.16(\frac{1}{5^2} - \frac{1}{7^2})=9.56$ eV, $488.16(\frac{1}{5^2} - \frac{1}{8^2})=11.899$ eV and so on. So these are down to $n=5$ from level $m=6, 7, 8$ and 9 .

5. There are two ways one can solve this problem. One can separate the two dimensional oscillator into two one dimensionall oscillators or one can define a degeneracy $g(n)$. Here the later solution is presented. As the energy is given by $\epsilon_n = (n_x + n_y + \frac{2}{2})\hbar\omega$ the number of states with the same energy is given by $g(n) = n + 1$ where $n = n_x + n_y$ and we now have a single index n .

The form for $g(n)$ can easily be seen by counting the number of pairs (n_x, n_y) that will give the same result for the sum $n_x + n_y$.

$$\text{The partition function is } Z = \sum_{n=0}^{\infty} g(n)e^{-(n+1)\hbar\omega/\tau} = e^{-\frac{\hbar\omega}{\tau}} \sum_{n=0}^{\infty} [ne^{-n\hbar\omega/\tau} + e^{-n\hbar\omega/\tau}] = e^{-\frac{\hbar\omega}{\tau}} \left[\frac{e^{-\frac{\hbar\omega}{\tau}}}{(1-e^{-\hbar\omega/\tau})^2} + \frac{1}{1-e^{-\hbar\omega/\tau}} \right] = \frac{e^{-\frac{\hbar\omega}{\tau}}}{(e^{\hbar\omega/\tau}-1)^2} = \frac{1}{2(\cosh(\hbar\omega/\tau)-1)}$$

$$\text{The free energy becomes } F = -\tau \ln Z = -\hbar\omega + 2\tau \ln \left(e^{\frac{\hbar\omega}{\tau}} - 1 \right) = \hbar\omega + 2\tau \ln \left(1 - e^{-\frac{\hbar\omega}{\tau}} \right)$$

$$\text{and the entropy } \sigma = - \left(\frac{\partial F}{\partial \tau} \right)_{V,N} = -2 \ln \left(e^{\frac{\hbar\omega}{\tau}} - 1 \right) + \frac{2\hbar\omega/\tau}{1 - e^{-\frac{\hbar\omega}{\tau}}}$$

$$\text{and the specific heat is } C_v = \tau \frac{\partial \sigma}{\partial \tau} = 2 \left(\frac{\hbar\omega}{\tau} \right)^2 \frac{e^{-\frac{\hbar\omega}{\tau}}}{\left(e^{\frac{\hbar\omega}{\tau}} - 1 \right)^2}$$

the low temperature limit $\tau \rightarrow 0$ evaluates to $C_v \rightarrow 2 \left(\frac{\hbar\omega}{\tau} \right)^2 e^{-\frac{\hbar\omega}{\tau}}$ and as $\tau \rightarrow \infty$ this gives $C_v \rightarrow 2$

See figure next page!

C_V for two dimensional harmonic osc.

