LULEÅ UNIVERSITY OF TECHNOLOGY
Division of Physics

Solution to written exam in QUANTUM PHYSICS AND STATISTICAL PHYSICS MTF131

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1. The eigenfunctions of the infinite square well in one dimension are (Here a solution of the S.E. in one dimesion is adequate)

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} \quad \text{and the eigenenergys are } E_n = \frac{n^2\pi^2\hbar^2}{2Ma^2} \quad \text{where} \quad n = 1, 2, 3, ...$$

$$\psi_m(x) = \sqrt{\frac{2}{\sqrt{2}a}} \sin \frac{m\pi y}{\sqrt{2}a} \quad \text{and the eigenenergys are } E_n = \frac{n^2\pi^2\hbar^2}{2M2a^2} \quad \text{where} \quad m = 1, 2, 3, ...$$

In two dimensions the eigenfunctions and eigenenergys for the rectangular well are (Here an argument about separation of variables is needed)

$\Psi_{n,m}(x, y) = \psi_n(x) \cdot \psi_m(y)$ and eigenenergys $E_{n,m} = E_n + E_m$ where $n = 1, 2, 3, ..$ and $m = 1, 2, 3, ..$

a) The eigenfunctions inside the rectangle

$$\Psi_{n,m}(x, y) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} \cdot \sqrt{\frac{2}{\sqrt{2}a}} \sin \frac{m\pi y}{\sqrt{2}a} \quad \text{where} \quad n = 1, 2, 3, .. \text{ and } m = 1, 2, 3, ..$$

The eigenfunctions outside the rectangle $\Psi_{n,m}(x, y) = 0$
b) The five lowest eigenenergies are

$$E_{n,m} = \frac{\pi^2\hbar^2}{2Ma^2}(n^2 + \frac{m^2}{2}), \quad \text{where the 5 lowest are} \quad (n^2 + \frac{m^2}{2}) = 1.5, 3, 4.5, 5.5, 6, \ \mathit{8.5} \text{ and } \mathit{9}.$$

c) The five lowest eigenenergys have degeneracys (not degenerate !) as follows:

$$E_{1,1} = \text{ one state } \ (n^2 + \frac{m^2}{2} = 1.5)$$

$$E_{1,2} = \text{ one state } \ (n^2 + \frac{m^2}{2} = 3)$$

$$E_{2,1} = \text{ one state } \ (n^2 + \frac{m^2}{2} = 4.5)$$

$$E_{1,3} = \text{ one state } \ (n^2 + \frac{m^2}{2} = 5.5)$$

$$E_{2,2} = \text{ one state } \ (n^2 + \frac{m^2}{2} = 6)$$

$$E_{2,3} = \text{ one state } \ (n^2 + \frac{m^2}{2} = 8.5)$$

$$E_{1,4} = \text{ one state } \ (n^2 + \frac{m^2}{2} = 9)$$

2. The pressure is given by $P = k_B T \left(\frac{\partial \ln Z}{\partial V}\right)_T = \frac{N k_B T}{V - bN} - \frac{aN^2}{V^2}$ which can be rewritten as $\left(P + \frac{aN^2}{V^2}\right)(V - bN) = N k_B T$. The internal energy is given by $U = k_B T^2 \left(\frac{\partial \ln Z}{\partial T}\right)_V = N\left(\frac{3k_B T}{2} - \frac{aN}{V}\right)$

3. Count the states in a box of size L. After some steps one reaches at (eq 7 page 185 KK) $\tau_F = (3\pi^2 n)^{2/3} \frac{\hbar^2}{2m}$ this gives $T_F = k_B \tau_F = 5.0$K which much less than $T = 0.5K$ so the approximation of the Fermi-Dirac distribution function as a step function will be fairly good. Calculate U (along lines according to eq 27 page 189 KK) after some steps $C_v = \frac{1}{2}\pi^2 N k_B T/T_F$ is reached. Evaluating the fermi contribution gives $C_v = 0.49 N k_B = 4.10$ J/mole/K at $T = 0.5$K.

4. The partition function is $Z_{\text{rot}} = \sum_{j=0}^{\infty}(2j+1)e^{-j(j+1)\frac{\hbar^2}{2I\tau}} \approx 1 + 3e^{-\frac{\hbar^2}{I\tau}} = 1 + 3e^{-x}$ where only the two first terms are kept and where $x = \frac{\hbar^2}{I\tau} >> 1$. For N identical molecules $Z_{\text{rot}}^{(N)} = \frac{1}{N!} Z_{\text{rot}}^N$.
And hence we get the free energy for the rotational degrees of freedom as
$F_{\text{rot}} = -N\tau \ln Z_{\text{rot}} + \tau \ln N! = -N\tau \ln(1 + 3e^{-x}) + \tau \ln N! \approx -3N\tau e^{-x} + \tau \ln N! = -3N\tau e^{-\frac{\hbar^2}{I\tau}} + \tau \ln N!$. The entropy of the system is given by the following derivative $\sigma_{\text{rot}} = -\frac{\partial F}{\partial \tau}_V = 3N(1 + \frac{\hbar^2}{I\tau})e^{-\frac{\hbar^2}{I\tau}} - \ln N! = 3N(1+x)e^{-x} + \ln N!$.
The specific heat we get from
$(C_v)_{\text{rot}} = \tau \frac{\partial \sigma}{\partial \tau}_V = 3N\frac{\hbar^2}{I}[\frac{\hbar^2}{I\tau^2} - \frac{1}{\tau}]e^{-\frac{\hbar^2}{I\tau}} 3N[(\frac{\hbar^2}{I\tau})^2 - \frac{\hbar^2}{I\tau}]e^{-\frac{\hbar^2}{I\tau}} \approx 3N[(\frac{\hbar^2}{I\tau})^2]e^{-\frac{\hbar^2}{I\tau}} (= 3Nx^2 e^{-x})$

5. Rewrite the wave function in terms of spherical harmonics:

$$\psi(\boldsymbol{r}) = \psi(x, y, z) = N(xy + zy)e^{-\alpha r} = Nr^2 e^{-\alpha r}\left(\frac{1}{i}\sqrt{\frac{2\pi}{15}}(Y_{2,2} - Y_{2,-2}) + \frac{1}{i}\sqrt{\frac{2\pi}{15}}(-Y_{2,1} - Y_{2,-1})\right)$$

As all the $Y_{l,m}$ have $l = 2$ the probability to get $\mathbf{L}^2 = 2(2+1)\hbar^2 = 6\hbar^2$ is one. For L_z we must first normalize the coefficients in front of the $Y_{l,m}$. The sum of the squares is $\frac{8\pi}{15}$ and hence we get the following expression:

$$\psi(\boldsymbol{r}) = Nr^2 e^{-\alpha r}\sqrt{\frac{8\pi}{15}}\left(\frac{1}{i}\sqrt{\frac{1}{4}}(Y_{2,2} - Y_{2,-2}) + \frac{1}{i}\sqrt{\frac{1}{4}}(-Y_{2,1} - Y_{2,-1})\right)$$

The probability to get $m = 2$ is $|\sqrt{\frac{1}{4}}|^2 = \frac{1}{4}$, for $m = 1$ is $|\sqrt{\frac{1}{4}}|^2 = \frac{1}{4}$, for $m = 0$ is $= 0$ for $m = -1$ is $|\sqrt{\frac{1}{4}}|^2 = \frac{1}{4}$, and for $m = -2$ is $|\sqrt{\frac{1}{4}}|^2 = \frac{1}{4}$
The expectation value $\langle L^2 \rangle = 6\hbar^2$ and for $\langle L_z \rangle = 2\frac{1}{4} + 1\frac{1}{4} + 0 - 1\frac{1}{4} - 2\frac{1}{4} = 0\hbar$.