LULEÅ UNIVERSITY OF TECHNOLOGY
Division of Physics

Solution to written exam in QUANTUM PHYSICS AND STATISTICAL PHYSICS MTF131

Examination date: 2006-12-19

1. (a) $i\hbar\frac{\partial}{\partial t}\sin\omega t = i\hbar\omega\cos\omega t$ **NO**

   (b) $-i\hbar\frac{\partial}{\partial z}C(1+z^2) = -i\hbar C(0+2z)$ **NO**

   (c) $-i\hbar\frac{\partial}{\partial z}(C_1 e^{ikz} + C_2 e^{-ikz}) = -i\hbar(C_1 ike^{ikz} + C_2 - ike^{-ikz})$ **NO**

   (d) $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}Ce^{-3z} = -\frac{\hbar^2}{2m}C(-3)^2 e^{-3z} \propto \psi(z)$ **YES**

   (e) $\frac{C}{2}(z^2 - \frac{\partial^2}{\partial z^2})e^{-\frac{1}{2}z^2} = \frac{C}{2}(z^2 e^{-\frac{1}{2}z^2} - \frac{\partial}{\partial z}(-ze^{-\frac{1}{2}z^2})) =$
   $\frac{C}{2}(z^2 e^{-\frac{1}{2}z^2} - (-e^{-\frac{1}{2}z^2} + z^2 e^{-\frac{1}{2}z^2})) = \frac{C}{2}e^{-\frac{1}{2}z^2} \propto \psi(z)$ **YES**

   (f) $\frac{C}{2}(z^2 - \frac{\partial^2}{\partial z^2})ze^{-\frac{1}{2}z^2} = ?$ Do this derivative first: $-\frac{\partial^2}{\partial z^2}ze^{-\frac{1}{2}z^2} = -\frac{\partial}{\partial z}(e^{-\frac{1}{2}z^2} - z^2 e^{-\frac{1}{2}z^2}) =$
   $-(-ze^{-\frac{1}{2}z^2} - 2ze^{-\frac{1}{2}z^2} + z^3 e^{-\frac{1}{2}z^2}) = 3ze^{-\frac{1}{2}z^2} - z^3 e^{-\frac{1}{2}z^2}$ Go back to the start:
   $\frac{C}{2}(z^2 - \frac{\partial^2}{\partial z^2})ze^{-\frac{1}{2}z^2} = \frac{C}{2}(z^3 e^{-\frac{1}{2}z^2} + 3ze^{-\frac{1}{2}z^2} - z^3 e^{-\frac{1}{2}z^2}) = \frac{C}{2}(+3ze^{-\frac{1}{2}z^2}) = \propto \psi(z)$ **YES**

2. (a) $\langle H \rangle = \frac{1}{2}0.27 + \frac{1}{4}1.08 + \frac{3}{16}3.65 + \frac{1}{16}4.06 = 1.343125 \approx 1.34\text{eV}$.

   Uncertainty is defined by: $\langle \Delta H \rangle = \sqrt{\langle H^2 \rangle - \langle H \rangle^2}$

   $\langle H^2 \rangle = \frac{1}{2}(0.27)^2 + \frac{1}{4}(1.08)^2 + \frac{3}{16}(3.65)^2 + \frac{1}{16}(4.06)^2 = 3.85624375 \; (\text{eV})^2$.

   $\langle \Delta H \rangle = \sqrt{3.85624375 - 1.343125^2} = 1.432571 \approx 1.43\text{eV}$

   (b) The expression is not unique as we only know the probabillities which are the squares of the coefficients. In the evaluation of $\langle H \rangle$ and $\langle H^2 \rangle$ only the probabillities are important thats why a different sign $\pm$ is of no importance in this calculation.

   One is: $\Psi(z) = \frac{1}{\sqrt{2}}\psi_1(z) + \frac{1}{2}\psi_2(z) + \frac{\sqrt{3}}{4}\psi_3(z) + \frac{1}{4}\psi_4(z)$.

   Another is: $\Psi(z) = \frac{1}{\sqrt{2}}\psi_1(z) - \frac{1}{2}\psi_2(z) + \frac{\sqrt{3}}{4}\psi_3(z) - \frac{1}{4}\psi_4(z)$.

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 $T_F = k_B\tau_F = 5.0\text{K}$ 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 $C_v = \frac{1}{2}\pi^2 Nk_B T/T_F$ is reached. Evaluating the fermi contribution gives $C_v = 0.49 Nk_B = 4.10$ J/mole/K at $T = 0.5\text{K}$.

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

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

   The five lowest one particle energies are: $\frac{1^2\pi^2\hbar^2}{2mL^2}$, $\frac{2^2\pi^2\hbar^2}{2mL^2}$, $\frac{3^2\pi^2\hbar^2}{2mL^2}$, $\frac{4^2\pi^2\hbar^2}{2mL^2}$ and $\frac{5^2\pi^2\hbar^2}{2mL^2}$.

   b) The eigenfunctions inside the well for two noninteracting and spinless particles (=bosons)

   $$\psi_{n,m}(x_1, x_2) = \sqrt{\frac{2}{L}}\sin\frac{n\pi x_1}{L} \cdot \sqrt{\frac{2}{L}}\sin\frac{m\pi x_2}{L} \quad \text{where} \quad n = 1, 2, 3, .. \text{ and } m = 1, 2, 3, ..$$

where index n and x_1 is for one particle and m and x_2 for the other.

$$\Psi_{n,m}(x_1, x_2) = \frac{1}{\sqrt{2}}(\psi_{n,m}(x_1, x_2) + \psi_{n,m}(x_2, x_1))$$

The five lowest eigenenergies are

$$E_{n,m} = \frac{\pi^2 \hbar^2}{2mL^2}(n^2 + m^2), \quad \text{where the 5 lowest are} \quad (n^2 + m^2) = 2, 5, 8, 10 \text{ and } 13.$$

c) To form the partition sum we must take the degeneracy into consideration. The states are non degenerate as an exchange of particles does not change the state, they are the same. Note how this condition enters into the limits of the second sum.

$$Z = \sum_{n=1}^{\infty}\sum_{m=n}^{\infty} e^{-\frac{\pi^2 \hbar^2}{2mL^2}(n^2+m^2)/\tau} = \sum_{n=1}^{\infty} e^{-\frac{\pi^2 \hbar^2}{2mL^2}n^2/\tau} \cdot \sum_{m=1}^{\infty} e^{-\frac{\pi^2 \hbar^2}{2mL^2}m^2/\tau}$$

There are two ways we can make an approximation. In the low temperature limit we keep the two first terms in the sum and in the high temperature limit more excited states become important and we can change the sum to an gaussian integral. In the high temperature limit we get:

$$Z = \sum_{n=1}^{\infty} e^{-\frac{\pi^2 \hbar^2}{2mL^2}n^2/\tau} \cdot \sum_{m=1}^{\infty} e^{-\frac{\pi^2 \hbar^2}{2mL^2}m^2/\tau} = \int_0^{\infty} dn\ e^{-\frac{\pi^2 \hbar^2}{2mL^2}n^2/\tau} \cdot \int_0^{\infty} dm\ e^{-\frac{\pi^2 \hbar^2}{2mL^2}m^2/\tau} = (\frac{1}{2})^2 \frac{2mL^2\tau}{\pi\hbar^2}$$

In the low temperature limit we get:

$$Z = \sum_{n=1}^{\infty} e^{-\frac{\pi^2 \hbar^2}{2mL^2}n^2/\tau} \cdot \sum_{m=1}^{\infty} e^{-\frac{\pi^2 \hbar^2}{2mL^2}m^2/\tau} = \left(e^{-\frac{\pi^2 \hbar^2}{2mL^2}1/\tau} + e^{-\frac{\pi^2 \hbar^2}{2mL^2}4/\tau}\right)^2$$

5. 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 $x = \frac{\hbar^2}{I\tau} >> 1$ in the high temperature limit. For N identical molecules $Z_{\text{rot}}^{(N)} = \frac{1}{N!}Z_{\text{rot}}^N$, and hence $F_{\text{rot}} = -N\tau \ln Z_{\text{rot}} + \tau \ln N! = -N\tau \ln(1 + 3e^{-x}) + \tau \ln N! \approx -3N\tau e^{-x} + \tau \ln N! = -3N\tau e^{-\frac{\hbar^2}{I\tau}} + \tau \ln N!$. The entropy is: $\sigma_{\text{rot}} = -(\frac{\partial F}{\partial \tau})_v \approx$ $3N(1+x)e^{-x} + \ln N! = 3N(1 + \frac{\hbar^2}{I\tau})e^{-\frac{\hbar^2}{I\tau}} + \ln N!$ and the specific heat in the low temperature limit is: $(C_v)_{\text{rot}} = \tau(\frac{\partial \sigma}{\partial \tau})_v \approx 3Nx^2 e^{-x} = 3N\left(\frac{\hbar^2}{I\tau}\right)^2 e^{-\frac{\hbar^2}{I\tau}}$. You can also calculate the inner energy $U = -\tau^2(\frac{\partial}{\partial \tau}\frac{F}{\tau})_{v,N} = 3N\left(\frac{\hbar^2}{I\tau}\right)e^{-\frac{\hbar^2}{I\tau}}$.