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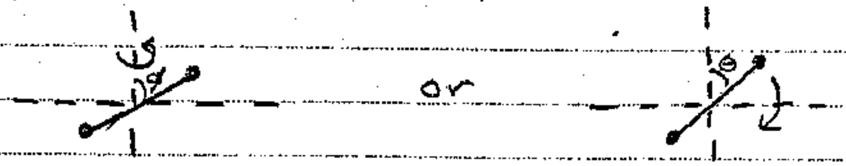
The rotational motion of a diatomic molecule is by two angular variables, ϕ and Θ, and by the canonical conjugate momenta p_ϕ and p_Θ, as well the moment of inertia I.

a) What is the kinetic energy of the rotational motion?

→ The kinetic energy of a rotating system is given by $E = \frac{p^2}{2I}$ where is the angular momentum. However, the diatomic molecule has two rotational degrees of freedom, about the ϕ and Θ directions, which must be considered separately:



for rotation in the Θ direction, the energy is just $E_1 = \frac{p_\Theta^2}{2I}$ but for the ϕ rotation, we must 1st find the moment of inertia which corresponds to the axis of rotation. Ordinarily $I = \sum m_i r_i^2$, so we must take the projection $r' = r\sin\Theta$. So the new I' value is $I' = I\sin^2\Theta$. Thus, the total energy is:

$$\boxed{E_{rot} = \frac{p_\Theta^2}{2I} + \frac{p_\phi^2}{2I\sin^2\Theta}}$$

b) Using classical statistics, obtain the rotational partition function in terms of I and T.

$$Z_r(T) = \int_0^{\pi} d\Theta \int_0^{2\pi} d\phi \int_{-\infty}^{\infty} dp_\Theta \int_{-\infty}^{\infty} dp_\phi \exp\left[-\frac{1}{kT}\left(\frac{p_\Theta^2}{2I} + \frac{p_\phi^2}{2I\sin^2\Theta}\right)\right]$$

$$\int_{-\infty}^{+\infty} \exp\left(\frac{-p_\phi^2}{2IkT\sin^2\Theta}\right) dp_\phi = \sqrt{2IkT\pi}\,\sin\Theta$$

$$\int_{-\infty}^{\infty} \exp\left(\frac{-p_\Theta^2}{2IkT}\right) dp_\Theta = \sqrt{2IkT\pi}$$

$$\int_0^{\pi} d\Theta \int_0^{2\pi} d\phi \; 2IkT\pi \sin\Theta = 4\pi^2 IkT\left[-\cos\Theta\right]_0^{\pi}$$

$$= -[(-1) - 1] = 2$$

$$\boxed{Z_R(T) = 8\pi^2 IkT}$$ ← note that in classical statistics, phase space is infinitely divisible

d) Calculate the corresponding entropy and specific heat.

Start with relation $F = -kT \ln Z$ (Reif eq 6.6.9

$$F = -kT \ln(8\pi^2 IkT)$$

Next use $-\left(\frac{\partial F}{\partial T}\right)_V = S$ (Reif eq 5.5.14

$$-\frac{\partial F}{\partial T} = k \ln(8\pi^2 IkT) + \frac{kT\,(8\pi^2 Ik)}{8\pi^2 IkT}$$

$$\boxed{S = k\left(1 + \ln(8\pi^2 IkT)\right)}$$

$$C_V = T\left(\frac{\partial S}{\partial T}\right)_V$$

$$= T\left(\frac{k\, 8\pi^2 Ik}{8\pi^2 IkT}\right)$$

$\boxed{C_V = k}$ ← this is the same result one would get using the equipartition theorem