Review Question 4.1-4.3

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1 Problem

Consider a gas (initial density ρ_0) of N molecules each with mass m and moment of inertia I. Account for translational motion as well as rotational and vibrational excitations, and assume that the vibrational excitations are describable by a two-dimensional harmonic oscillator (two independent 1-D oscillators) with frequency ω. In addition, assume that $\hbar\omega \ll T$ and $\frac{\hbar^2}{2I} \ll T$.

1. Find the energy per particle.
2. Find the entropy per particle in terms of the density.
3. If the gas undergoes an adiabatic expansion from temperature T_0 to T_1, what is the final density?

2 Solution

1. Because we are in the classical limit, we can treat the vibrational excitations as classical harmonic oscillators and turn the rotational partition function into an integral, so the partition function is

$$Z = Z_{tr}Z_{HO}Z_{rot} = \frac{1}{\hbar^2}\frac{N}{\rho(2\pi\hbar)^3}\left(\int_{-\infty}^{\infty} e^{-\frac{p^2}{2mT}}\,dp\right)^5\left(\int_{-\infty}^{\infty} e^{-\frac{m\omega^2x^2}{2T}}\,dx\right)^2\int_0^{\infty}(2l+1)e^{-\frac{\hbar^2 l(l+1)}{2IT}}\,dl,$$

which evaluates to

$$Z = \frac{2ITN}{\rho\hbar^2}\left(\frac{T}{\hbar\omega}\right)^2\left(\frac{mT}{2\pi\hbar^2}\right)^{\frac{3}{2}}$$

for a single particle; for N particles it becomes $\frac{Z^N}{N!}$. The energy per particle is

$$\frac{\langle E\rangle}{N} = \frac{T^2}{N}\frac{\partial \ln Z}{\partial T} = \frac{\frac{9}{2}T^{2+\frac{7}{2}}}{NT^{\frac{9}{2}}} = \frac{9}{2}T,$$

consistent with the equipartition theorem.

2. Let $a = \frac{\rho Z}{N}$; then by Stirling's approximation

$$\ln\left(\frac{Z^N}{N!}\right) = N\ln\frac{Na}{\rho} - \ln N! = N\ln N + N\ln\frac{a}{\rho} - \ln N! \approx N\left(1+\ln\frac{a}{\rho}\right),$$

and the entropy per particle is

$$\frac{S}{N} = \frac{1}{N}\ln\left(\frac{Z^N}{N!}\right) + \frac{\langle E\rangle}{NT} = \frac{11}{2} + \ln\left(\frac{2IT}{\rho\hbar^2}\left(\frac{T}{\hbar\omega}\right)^2\left(\frac{mT}{2\pi\hbar^2}\right)^{\frac{3}{2}}\right).$$

3. If the expansion is adiabatic, the entropy is conserved, so requiring that the entropy at T_0 is the same as the entropy at T_1 gives

$$\frac{T_0^{\frac{9}{2}}}{\rho_0} = \frac{T_1^{\frac{9}{2}}}{\rho_1},$$

or

$$\rho_1 = \rho_0 \left(\frac{T_1}{T_0}\right)^{\frac{9}{2}}.$$