We compute the heat capacity of a diatomic gas, where the molecules can translate, rotate, and vibrate.

The partition function of a single molecule can be separated into

$$Z_1 = Z_{trans} Z_{rot} Z_{vib}$$

We compute each in turn.

$$Z_{trans} = \frac{1}{(2\pi\hbar)^3} \int d^3p\, d^3x\, e^{-\beta p^2/2m} = \frac{1}{8\pi^3\hbar^3} \cdot V \cdot \sqrt{\frac{2m\pi}{\beta}}^{\,3} .$$

(I hope to understand this part of the derivation better in the future.)

To compute Z_{rot}, we wish to find the kinetic energy of a rod rotating about its center of mass. In our case, the moment of inertia along the long axis of the rod will vanish, as we assume that the object has no spatial extent perpendicular to this axis.

We know we can choose the principle axes of the rod such that the moment of inertia takes the form

$$I = \begin{pmatrix} I & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & 0 \end{pmatrix} \Rightarrow T = \frac{1}{2} I (\Omega_1^2 + \Omega_2^2), \text{ where}$$

Ω_1 and Ω_2 are the components of the angular velocity vector about the two remaining principle axes.

If we introduce Euler angles following Landau's convention on p.110-111, we can deduce

$$\Omega_1 = \dot{\phi}\sin\theta\sin\psi + \dot{\theta}\cos\psi$$
$$\Omega_2 = \dot{\phi}\sin\theta\cos\psi - \dot{\theta}\sin\psi \Rightarrow$$

$$\Omega_1^2 + \Omega_2^2 = \dot{\phi}^2\sin^2\theta + 2\dot{\phi}\sin\theta\sin\psi\dot{\theta}\cos\psi + \dot{\theta}^2\cos^2\psi$$
$$- 2\dot{\phi}\sin\theta\cos\psi\dot{\theta}\sin\psi + \dot{\theta}^2\sin^2\psi$$

$$= \dot{\theta}^2 + \dot{\phi}^2\sin^2\theta \Rightarrow T = L = \frac{1}{2}I\left(\dot{\theta}^2 + \dot{\phi}^2\sin^2\theta\right).$$

We now find the Hamiltonian:

$$\frac{\partial L}{\partial\dot{\theta}} = I\dot{\theta} \equiv p_\theta, \quad \frac{\partial L}{\partial\dot{\phi}} = I\dot{\phi}\sin^2\theta \equiv p_\phi \Rightarrow$$

$$H = \frac{p_\theta^2}{2I} + \frac{p_\phi^2}{2I\sin^2\theta} \Rightarrow Z = \frac{1}{(2\pi\hbar)^2}\int d\theta\, d\phi\, dp_\theta\, dp_\phi\, e^{-\beta\left(p_\theta^2/2I + p_\phi^2/2I\sin^2\theta\right)}$$

$$= \frac{1}{2\cancel{4}\pi^2\hbar^2}\cdot\cancel{2}\pi\cdot\sqrt{\frac{2I\pi}{\beta}}\int_0^\pi\int_{-\infty}^{\infty} dp_\phi\, d\theta\, e^{-\beta p_\phi^2/2I\sin^2\theta} =$$

$$\frac{1}{\cancel{4\pi}\hbar^2}\sqrt{\frac{2I\cancel{\pi}}{\beta}}\cdot\cancel{2}\sqrt{2\cancel{\pi}}\sqrt{\frac{I}{\beta}} = \frac{2I}{\beta\hbar^2}.$$

Finally, the vibrational degree of freedom is simply a simple harmonic oscillator, so its Hamiltonian is given by

$$H = \frac{p^2}{2m}+\frac{1}{2}m\omega^2x^2 \Rightarrow Z = \frac{1}{2\pi\hbar}\int d^3p\, e^{-\beta p^2/2m}\int d^3x\, e^{-\beta m\omega^2 x^2/2}$$

$$= \frac{1}{\cancel{2\pi}\hbar}\sqrt{\frac{\cancel{2\pi m}}{\beta}}\sqrt{\frac{\cancel{2\pi}}{\beta\cancel{m}\omega^2}} = \frac{1}{\beta\hbar\omega}.$$

Combining these, the partition function of the diatomic gas is given by

$$Z = \frac{1}{N!}\left(\frac{1}{8\pi^3\hbar^3}\cdot V\cdot\sqrt{\frac{2m\pi}{\beta}}^{\,3}\right)^N\left(\frac{2I}{\beta\hbar^2}\right)^N\left(\frac{1}{\beta\hbar\omega}\right)^N$$

It follows that

$$\langle E\rangle = -\frac{\partial}{\partial\beta}\log Z = -\frac{\partial}{\partial\beta}\left(-\frac{3N}{2}\log\beta - N\log\beta - N\log\beta + \_\right)$$

$$= \frac{3N}{2\beta}+\frac{N}{\beta}+\frac{N}{\beta} = \frac{7Nk_BT}{2} \Rightarrow \boxed{C_V = \frac{7Nk_B}{2}}$$