Chapter 3.7: Quantized rotation

Possible internal degrees of freedom of gases

1.) Rotations

2.) Vibrations

3.) Spin

Quantum description of angular momentum

$$\varepsilon_\ell = \frac{\widehat{L}^2}{2I} \quad \to \quad \frac{\hbar^2 \ell(\ell+1)}{2I}$$

$$Z_{rot} = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} e^{-\beta\varepsilon_\ell}$$

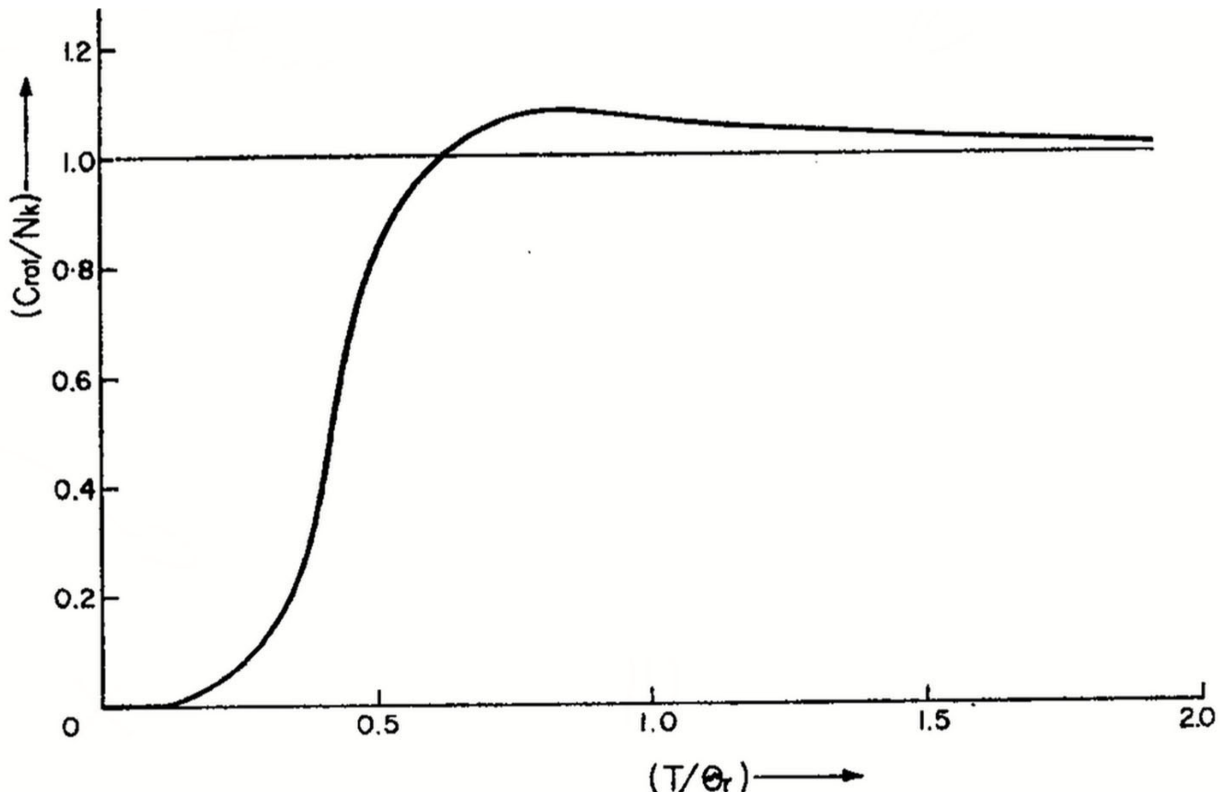
Euler-Maclaurin Formula

$$\sum_{l=0}^{\infty} f(l) = \int_0^{\infty} f(l)\,dl + \frac{f(0)}{2} - \frac{f'(0)}{12} + \frac{f'''(0)}{720} - \dots$$

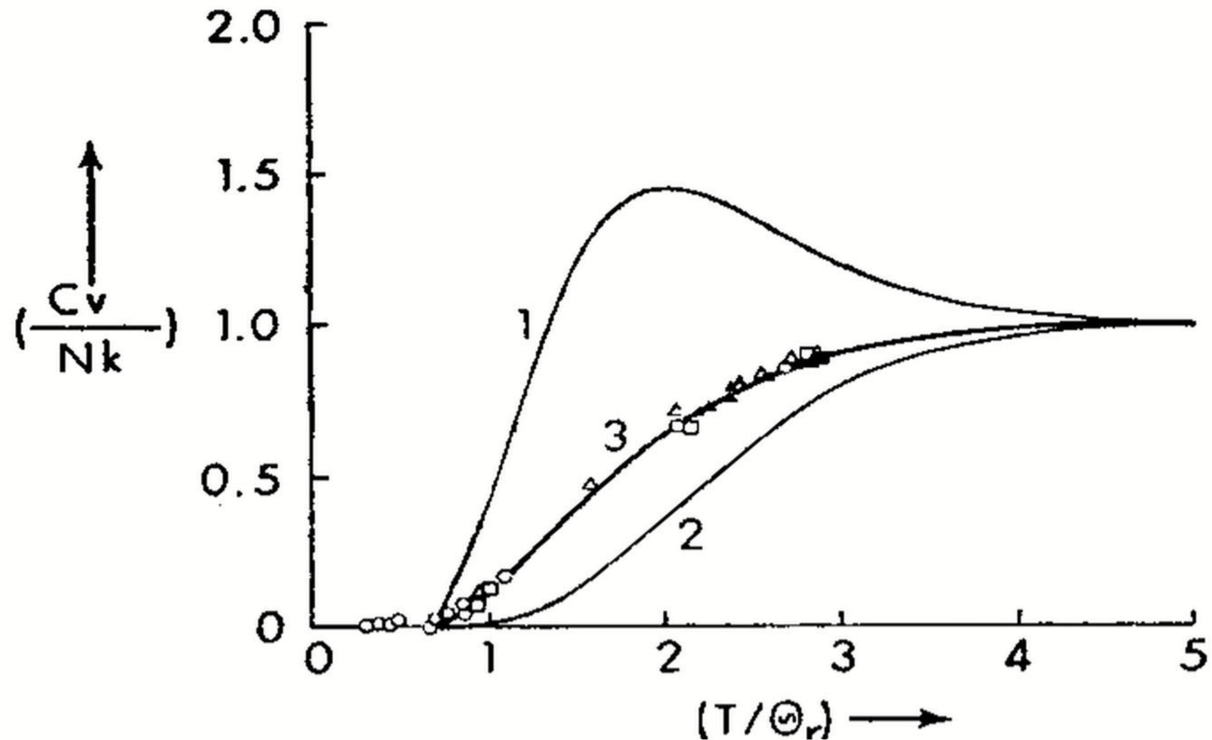
$$\varepsilon_\ell = \frac{\widehat{L}^2}{2I} \quad \rightarrow \quad \frac{\hbar^2 \ell(\ell+1)}{2I}$$

Low temperature expansion:

$$Z_{rot} = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} e^{-\beta\varepsilon_\ell}$$



Molecules of identical atoms



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e = -D[Log[Sum[(2 n + 1) Exp[- b n (n + 1)], {n, 0, Infinity}]], b]
cv  =  - b b D[e, b]
Plot[cv, {b, .1, 5}]
Plot[{cv, 1 + b^2 / 45}, {b, .01, .051}]
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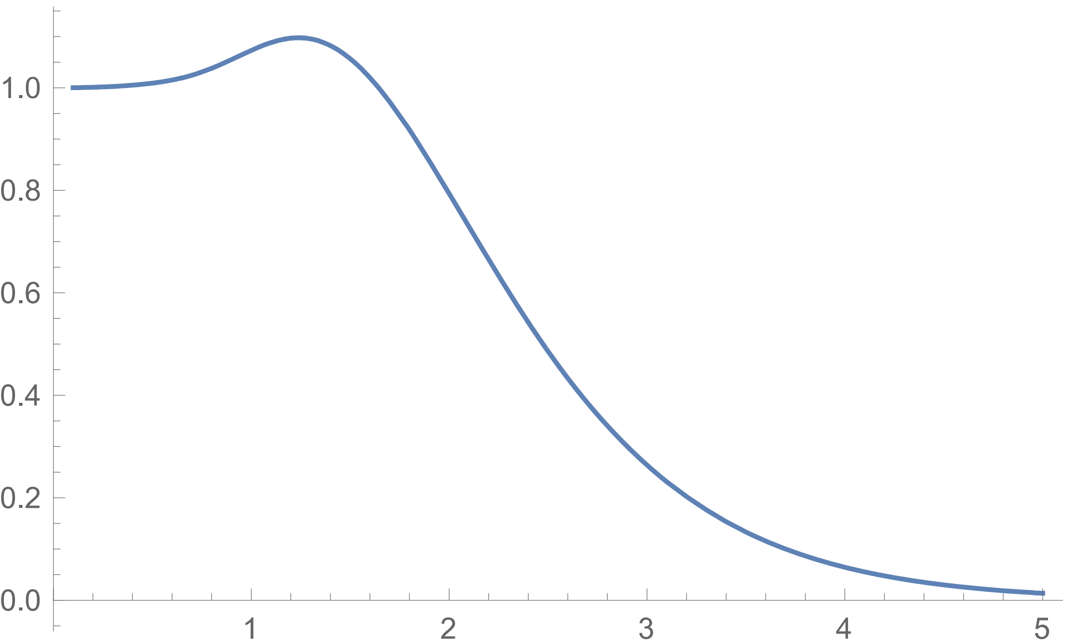
$$-\frac{\sum_{n=0}^{\infty} -e^{-b\,n\,(1+n)}\; n\,(1+n)\,(1+2\,n)}{\sum_{n=0}^{\infty} e^{-b\,n\,(1+n)}\,(1+2\,n)}$$

$$-b^2\left(\frac{\left(\sum_{n=0}^{\infty} -e^{-b\,n\,(1+n)}\; n\,(1+n)\,(1+2\,n)\right)^2}{\left(\sum_{n=0}^{\infty} e^{-b\,n\,(1+n)}\,(1+2\,n)\right)^2}-\frac{\sum_{n=0}^{\infty} e^{-b\,n\,(1+n)}\; n^2\,(1+n)^2\,(1+2\,n)}{\sum_{n=0}^{\infty} e^{-b\,n\,(1+n)}\,(1+2\,n)}\right)$$



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General ::stop : Further output of FactorSquareFree ::lrgexp will be suppressed during this calculation . >>