Chapter 3.8: Quantized vibrations

Quantum harmonic oscillator:

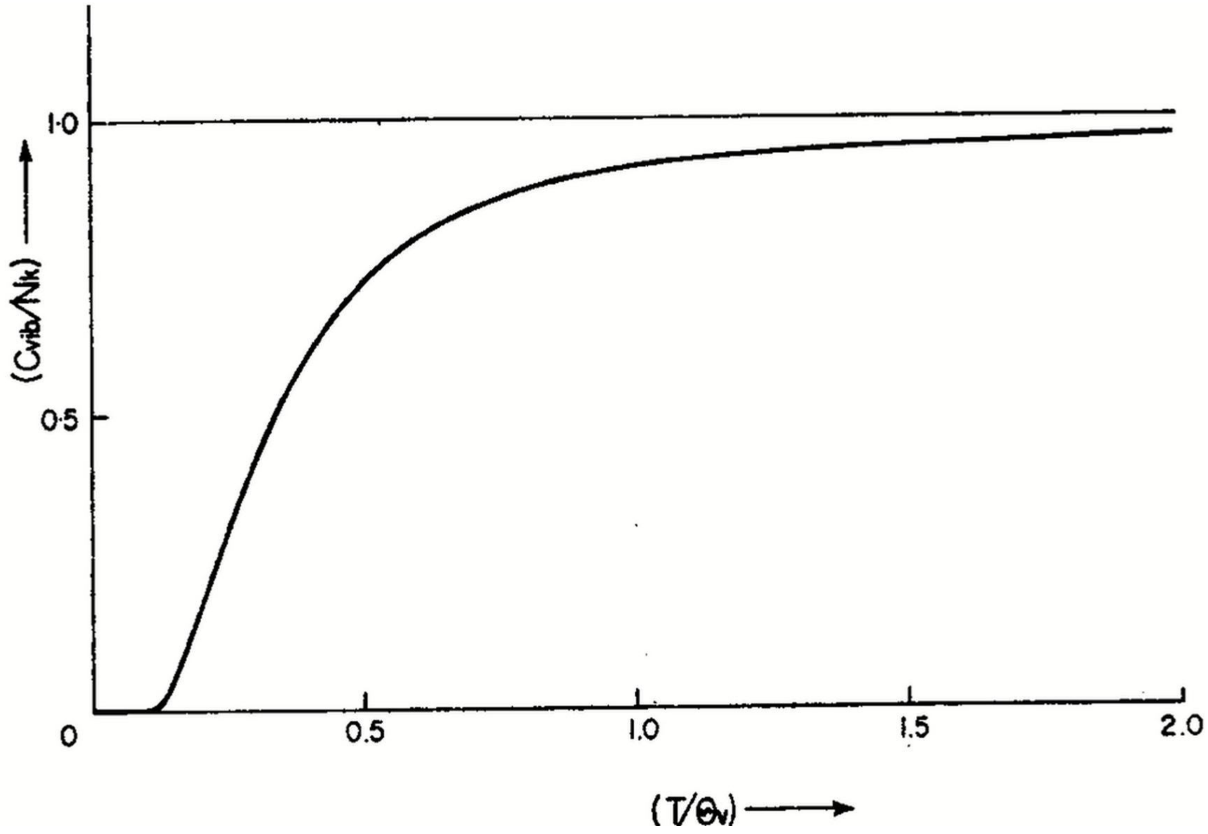
$$H = \frac{\hat{P}^2}{2m} + \frac{1}{2} m\omega^2 \hat{X}^2 = \hbar\omega(a^\dagger a + \frac{1}{2})$$

Quantization $\varepsilon_n = \hbar\omega(n + \frac{1}{2})$

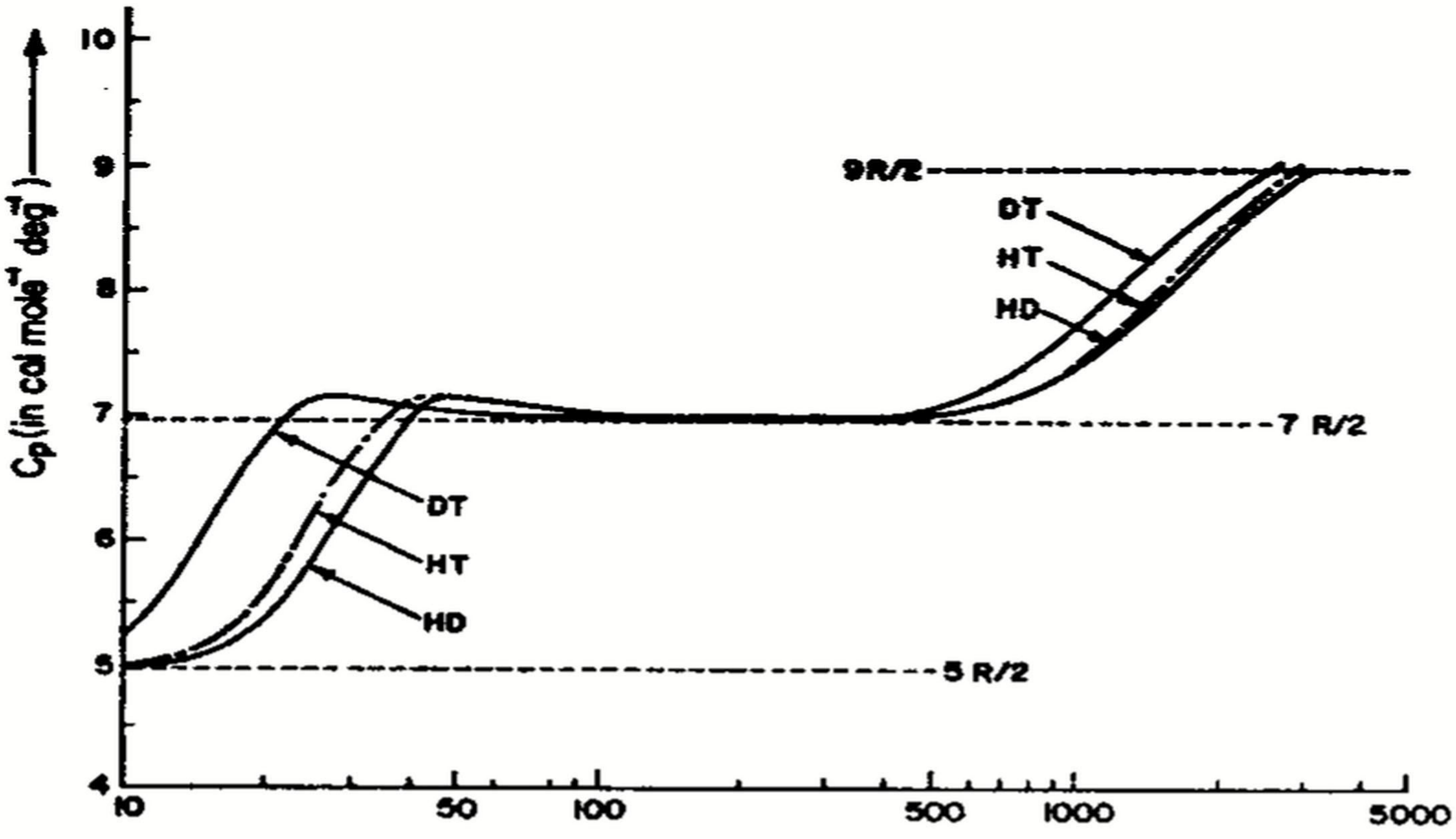
$$Z_{osc} = \sum_{n=0}^{\infty} e^{-\beta\hbar\omega(n+\frac{1}{2})}$$

Specific heat

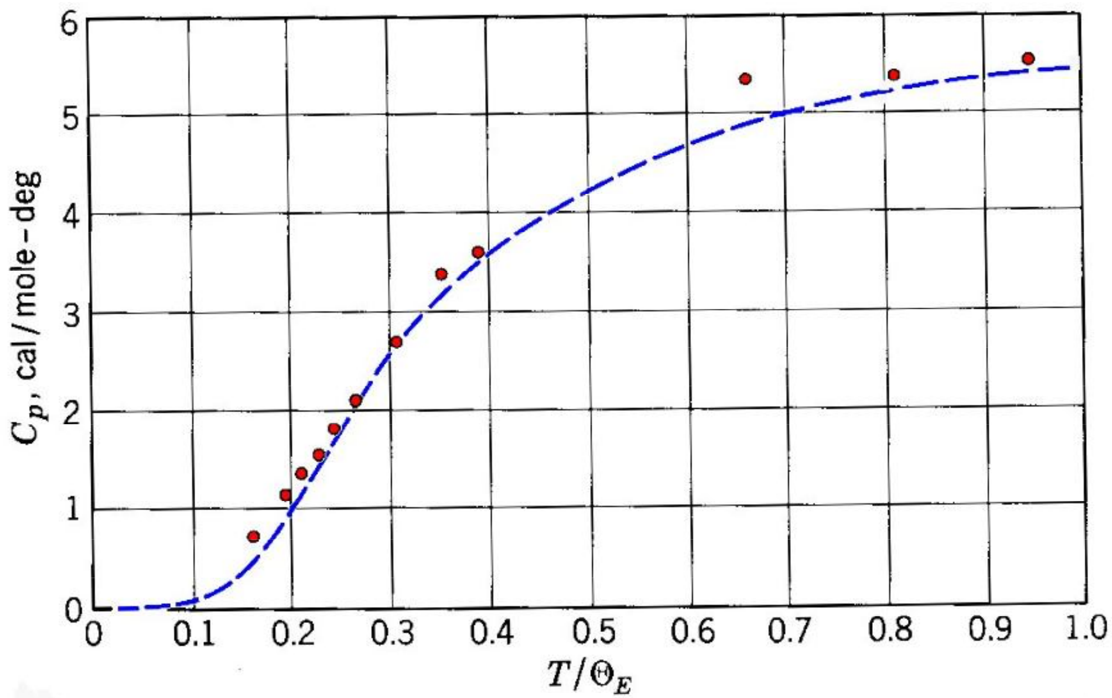
$$c_V = \frac{\partial E}{\partial T} = -\frac{1}{k_B T^2}\frac{\partial E}{\partial \beta}$$



Di-atomic molecules



Einstein Model (1907): Each atom in a solid is an independent 3D oscillator



Comparison of experimental values of the heat capacity of diamond with values calculated on the Einstein model, using the characteristic temperature $\Theta_E = \hbar\omega/k_B = 1320°K$. [After A. Einstein, Ann. Physik **22**, 180 (1907).]

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e = FullSimplify[-D[Log[Sum[ Exp[- b (n + 1 / 2) ], {n, 0, Infinity}]], b]]
cv = - b b D[e, b]
Plot[e /. b → 1 / T, {T, 0, 2}]
Plot[cv /. b → 1 / T, {T, 0, 2}]
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$$\frac{1}{2}\,\mathrm{Coth}\left[\frac{b}{2}\right]$$

$$\frac{1}{4}\,b^2\,\mathrm{Csch}\left[\frac{b}{2}\right]^2$$