Fundamentals of Statistical and Thermal Physics
Chapter 7
-
Simple applications of statistical mechanics

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Review of Chapter 6

- From **Statistical Mechanics** to **macroscopic observables**

1. Derive the partition function $Z \equiv \sum_r e^{-\beta E_r}$
2. Express macroscopic observables in terms of **Z**
3. Find **Z** for different systems

Example - Ideal monatomic gas

1. Define the total energy $$E = \sum_{i=1}^{N} \frac{p_i^2}{2m} + U(r_1, r_2, \ldots, r_N)$$

2. Calculate the partition function

$$Z' = \int exp\left\{-\beta\left[\frac{1}{2m}(p_1^2 + \cdots + p_N^2) + U(r_1, \ldots, r_N)\right]\right\} \frac{d^3r_1 \cdots d^3r_N d^3p_1 \cdots d^3p_N}{h_0^{3N}}$$

Example - Ideal monatomic gas

$$\ln Z' = N\left[\ln V - \frac{3}{2}\ln\beta + \frac{3}{2}\ln\left(\frac{2\pi m}{h_0^2}\right)\right]$$

3. Calculate macroscopic observables from Z

$$\bar{P} = \frac{1}{\beta}\frac{\partial \ln Z'}{\partial V} = \frac{1}{\beta}\frac{N}{V} = \frac{NkT}{V}$$

$$\bar{E} = -\frac{\partial}{\partial\beta}\ln Z' = \frac{3}{2}\frac{N}{\beta} = N(\frac{3}{2}kT)$$

$$C_v = \left(\frac{\partial\bar{E}}{\partial T}\right)_V = \frac{3}{2}Nk \stackrel{molar}{=} \frac{3}{2}R$$

Example - Harmonic oscillator

$$E = \frac{p^2}{2m} + \frac{1}{2}k_0 x^2$$

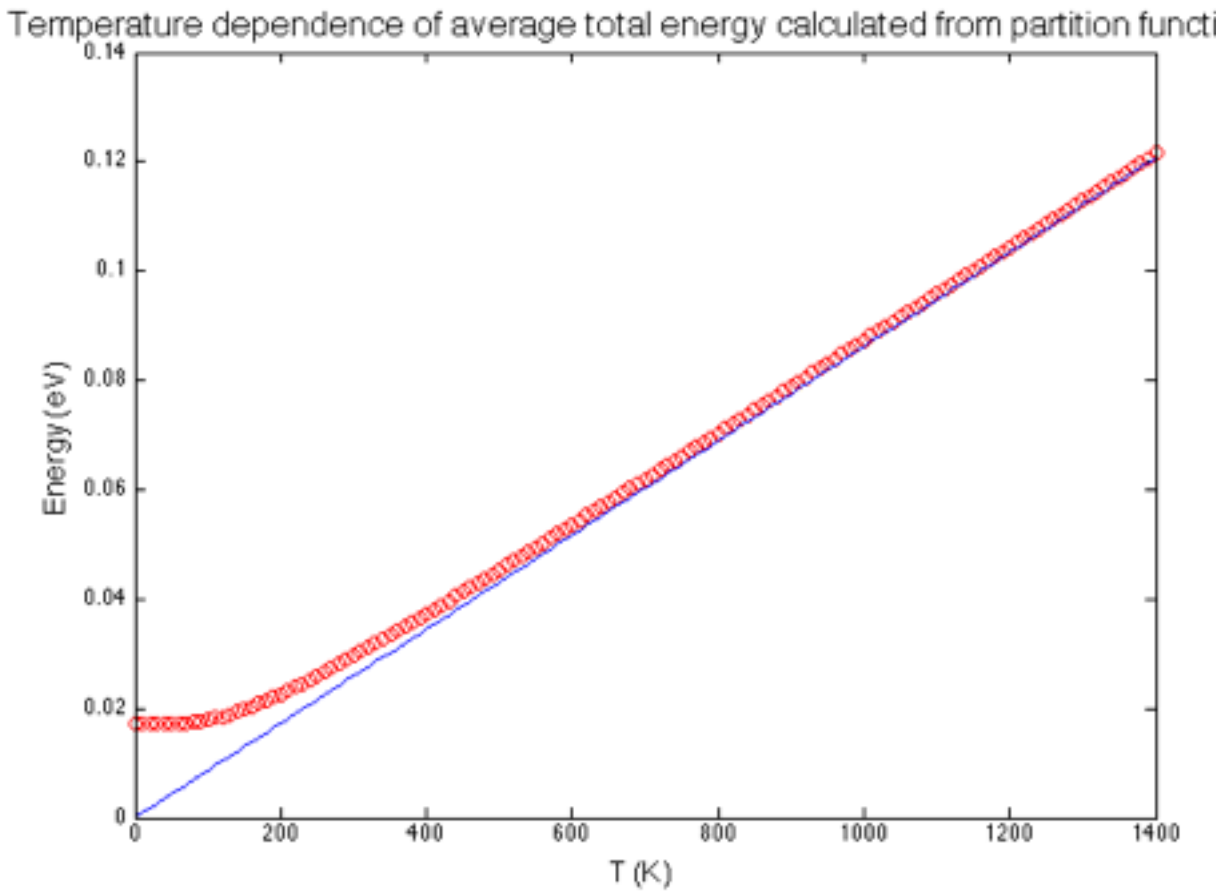
- **Classical:** by equipartition theorem

$$\boxed{\bar{E} = \frac{1}{2}kT + \frac{1}{2}kT = kT}$$

- **Quantum:** $$E_n = (n + \frac{1}{2})\hbar\omega$$

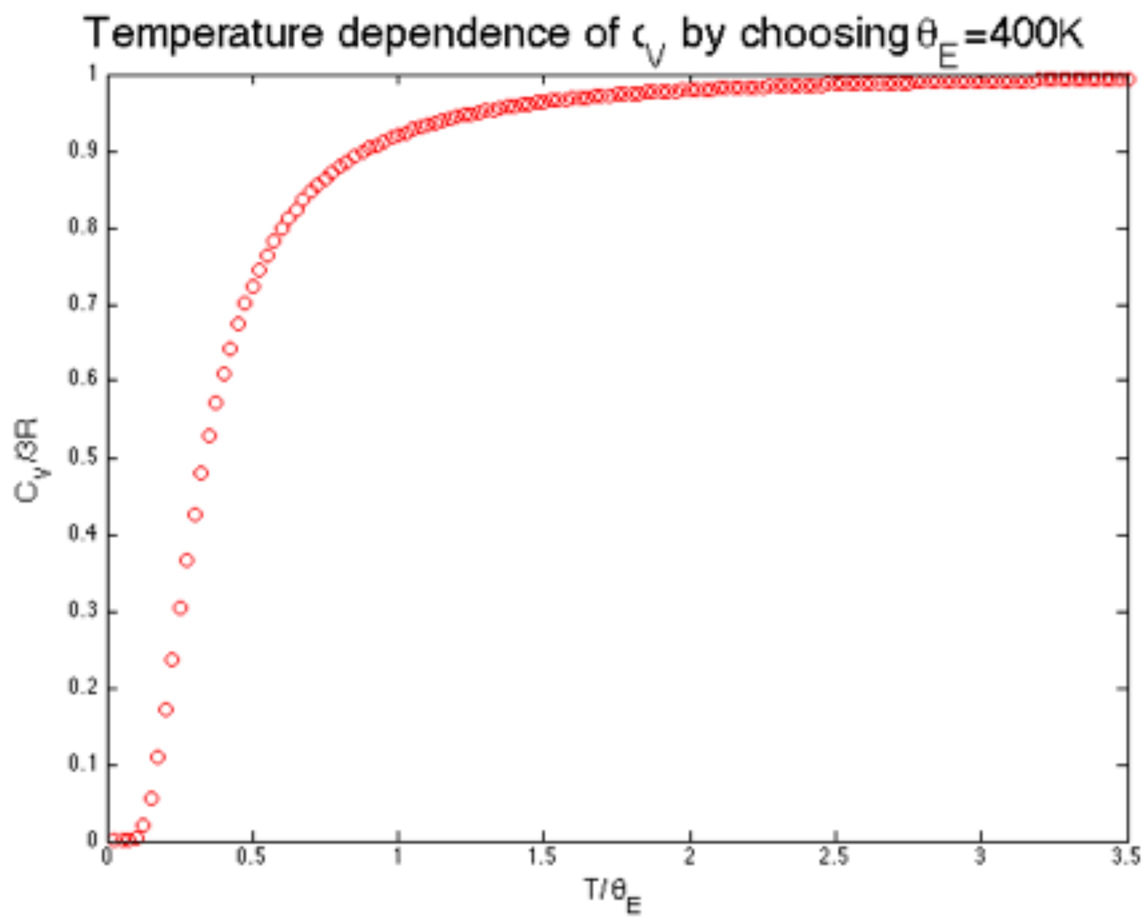
$$Z \equiv \sum_{n=0}^{\infty} e^{-\beta E_n} = \sum_{n=0}^{\infty} e^{-(n+\frac{1}{2})\beta\hbar\omega}$$

$$\boxed{\bar{E} = -\frac{\partial}{\partial\beta}\ln Z = \hbar\omega\left(\frac{1}{2} + \frac{1}{e^{\beta\hbar\omega} - 1}\right)}$$



$$\beta\hbar\omega = \frac{\hbar\omega}{kT} = \frac{\theta_E}{T}$$

$$c_V = \left(\frac{\partial \bar{E}}{\partial T}\right)_V = 3R\left(\frac{\theta_E}{T}\right)^2 \frac{e^{\theta_E/T}}{(e^{\theta_E/T}-1)^2}$$



Thank you