5. Consider a system of N distinguishable particles with only 3 possible energy levels: 0, ϵ and 2ϵ. The system occupies a fixed volume V and is in thermal equilibrium with a reservoir at temperature T. Ignore interactions between particles and assume that Boltzmann statistics applies.

   (a) What is the partition function for a single particle in the system? (1 point).

   (b) What is the average energy per particle? (1 points).

   (c) What is probability that the 2ϵ level is occupied in the high temperature limit, $k_B T \gg \epsilon$? Explain your answer on physical grounds. (1 point).

   (d) What is the average energy per particle in the high temperature limit, $k_B T \gg \epsilon$? (1 point).

   (e) At what approximate temperature is the ground state 1.1 times as likely to be occupied as the 2ϵ level? (1 point).

   (f) Find the heat capacity of the system, c_v, analyze the low-T (when $k_B T \ll \epsilon$) and high-T ($k_B T \gg \epsilon$) limits, and sketch c_v as a function of T. Explain your answer on physical grounds. (5 points).

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Stat Mech #2

System: N distinguishable particles

3 possible energy levels $(0, \epsilon, 2\epsilon)$

V is a fixed volume

T is temperature of heat reservoir, in thermal equilibrium

* Ignore particle interactions, assume Boltzmann statistics

a) What is the partition function for a single particle?

$$Z = \sum_i e^{-\beta E_i}$$

$$= e^{-\beta 0} + e^{-\beta\epsilon} + e^{-\beta 2\epsilon}$$

$$= 1 + e^{-\beta\epsilon} + e^{-2\beta\epsilon}$$

b) What is the avg. energy per particle

$$\langle E \rangle = \frac{-\partial}{\partial\beta} \ln(z)$$

$$= \frac{-\partial}{\partial\beta} \ln\left(1 + e^{-\beta\epsilon} + e^{-2\beta\epsilon}\right)$$

$$= \frac{-\epsilon e^{-\beta\epsilon} - 2\epsilon e^{-2\beta\epsilon}}{1 + e^{-\beta\epsilon} + e^{-2\beta\epsilon}}$$

c) What is the probability that the 2ϵ energy level is occupied in the high T limit ($k_B T >> \epsilon$)? Explain answer on physical grounds

$$P = \frac{1}{z} e^{-\beta E}$$

$$= \frac{e^{-2\beta\epsilon}}{1 + e^{-\beta\epsilon} + e^{-2\beta\epsilon}}$$

$$= \frac{1}{e^{2\beta\epsilon} + e^{\beta\epsilon} + 1}$$

$$= \frac{1}{3}$$

d) What is the avg energy per particle in the high T limit?

$$\langle E \rangle = -\frac{\partial}{\partial \beta} \ln(z)$$

$$= \frac{-\epsilon e^{-\beta\epsilon} - 2\epsilon e^{-2\beta\epsilon}}{1 + e^{-\beta\epsilon} + e^{-2\beta\epsilon}}$$

$$= \frac{-\epsilon - 2\epsilon}{3}$$

$$= -\epsilon$$

e) At what approximate T is the ground state 1.1 times as likely to be occupied as the 2ϵ level?

$$\frac{P_0}{P_{2\epsilon}} = 1.1 = \frac{\frac{1}{z} e^{-\beta 0}}{\frac{1}{z} e^{-\beta 2\epsilon}}$$

$$1.1 = \frac{e^{-\beta 0}}{e^{-2\beta\epsilon}}$$

$$1.1 = \frac{1}{e^{-2\beta\epsilon}}$$

$$e^{2\beta\epsilon} = \frac{1}{1.1}$$

$$2\beta\epsilon = \ln\left(\frac{1}{1.1}\right)$$

$$\frac{1}{k_B T} = \frac{1}{2\epsilon} \ln\left(\frac{1}{1.1}\right)$$

$$T = \frac{2\epsilon}{k_B \ln\left(\frac{1}{1.1}\right)}$$

f) Find the heat capacity of the system in both the high and low T limits. Sketch C_v as a function of T. Explain your answer on physical grounds.

$$C_v = \left(\frac{\partial U}{\partial T}\right)_V$$

$$U = -\frac{\partial}{\partial \beta} \ln(z)$$

$$= -\frac{\partial}{\partial \beta} N \ln\left(1 + e^{-\beta\epsilon} + e^{-2\beta\epsilon}\right)$$

$$= \frac{N(-\epsilon e^{-\beta\epsilon} - 2\epsilon e^{-2\beta\epsilon})}{1 + e^{-\beta\epsilon} + e^{-2\beta\epsilon}}$$

$$C_V = \frac{\partial U}{\partial T}$$

$$= \frac{\partial}{\partial T}\left[\frac{-N\epsilon(e^{-\beta\epsilon} + 2e^{-2\beta\epsilon})}{1 + e^{-\beta\epsilon} + e^{-2\beta\epsilon}}\right]$$

$$= \frac{\partial}{\partial T}\left[\frac{-N\epsilon(e^{\beta\epsilon} + 2)}{e^{2\beta\epsilon} + e^{\beta\epsilon} + 1}\right]$$

$$= \frac{\partial}{\partial T}\left[\frac{-N\epsilon(e^{\epsilon/kT} + 2)}{e^{2\epsilon/kT} + e^{\epsilon/kT} + 1}\right]$$

$$= \frac{-N\epsilon \frac{-\epsilon}{kT^2} e^{\epsilon/kT}}{e^{2\epsilon/kT} + e^{\epsilon/kT} + 1} + -N\epsilon(e^{\epsilon/kT} + 2)(e^{2\epsilon/kT} + e^{\epsilon/kT} + 1)^{-2} \cdot \left(-\frac{2\epsilon}{kT^2} e^{2\epsilon/kT} + -\frac{\epsilon}{kT^2} e^{\epsilon/kT}\right)$$

$$=$$

f) $C_V = +N\epsilon \frac{\epsilon}{kT^2} e^{\epsilon/kT}\left(e^{2\epsilon/kT}+e^{\epsilon/kT}+1\right)^{-1} - N\epsilon\left(e^{\epsilon/kT}+2\right)\left(\frac{2\epsilon}{kT^2}e^{2\epsilon/kT}+\frac{\epsilon}{kT^2}e^{\epsilon/kT}\right)\left(e^{2\epsilon/kT}+e^{\epsilon/kT}+1\right)^{-2}$

$= \frac{N\epsilon^2}{kT^2}\left[e^{\epsilon/kT}\left(e^{2\epsilon/kT}+e^{\epsilon/kT}+1\right)^{-1} - \left(e^{\epsilon/kT}+2\right)\left(e^{2\epsilon/kT}+e^{\epsilon/kT}\right)\left(e^{2\epsilon/kT}+e^{\epsilon/kT}+1\right)^{-2}\right]$

* in the high T limit

$C_V \to 0$

* in the low T limit

$C_V \to \infty$