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Consider an atom that has a lowest electronic state $^1S_0$ and a first excited state $^3S_1$ with energy ϵ_1 above the ground state. All higher states with energies above the first excited states have energies much greater than KT.

(a) For a gas of the atoms at temperature T, find the fraction of excited atoms.

start w/ partition function.

$$Z = e^{-\beta \epsilon_0} + e^{-\beta(\epsilon_0+\epsilon_1)}$$

the fraction of excited atoms is

$$\frac{e^{-\beta(\epsilon_0+\epsilon_1)}}{Z} = \frac{e^{-\beta\epsilon_0}e^{-\beta\epsilon_1}}{e^{-\beta\epsilon_0}+e^{-\beta\epsilon_0}e^{-\beta\epsilon_1}} = \boxed{\frac{e^{-\beta\epsilon_1}}{1+e^{-\beta\epsilon_1}}}$$

(b) give the internal energy of a gas of N atoms as function of temperature (i.e. $U(T)$) and compute from this the specific heat $c_V(T)$. Make a plot of $c_V(T)$

since we know that $E = -\frac{\partial}{\partial\beta}\ln Z$, we need the partition function for N atoms.

let N_0 be the number in ground state and N_1 the number in excited state such that $N = N_0 + N_1$. So,

$$Z = \frac{1}{N_0!}\left(e^{-\beta\epsilon_0}\right)^{N_0} + \frac{1}{N_1!}\left(e^{-\beta(\epsilon_0+\epsilon_1)}\right)^{N_1} \qquad (1)$$

or ?

$$Z = \frac{1}{N!}\left[e^{-\beta\epsilon_0} + e^{-\beta(\epsilon_0+\epsilon_1)}\right]^N$$

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I assume it is the second one b/c the math works for it. I am not sure of the physical reason.

$$\ln Z = N \ln\left(e^{-\beta\epsilon_0} + e^{-\beta(\epsilon_0+\epsilon_1)}\right) - \ln N!$$

Then

$$E = -\frac{\partial}{\partial\beta}\ln Z = -N\frac{\partial}{\partial\beta}\ln\left(e^{-\beta\epsilon_0} + e^{-\beta(\epsilon_0+\epsilon_1)}\right)$$

$$= -N\,\frac{-\epsilon_0 e^{-\beta\epsilon_0} - (\epsilon_0+\epsilon_1)e^{-\beta(\epsilon_0+\epsilon_1)}}{e^{-\beta\epsilon_0} + e^{-\beta(\epsilon_0+\epsilon_1)}}$$

$$\boxed{E = N\,\frac{\epsilon_0 + (\epsilon_0+\epsilon_1)e^{-\beta\epsilon_1}}{1+e^{-\beta\epsilon_1}}}$$

$$C_V = \left(\frac{\partial E}{\partial T}\right)_V = \left(\frac{\partial E}{\partial\beta}\right)_V\frac{\partial\beta}{\partial T} = \left(\frac{\partial E}{\partial\beta}\right)_V\left(-\frac{1}{kT^2}\right)$$

So,

$$C_V = -\frac{N}{kT^2}\left[\frac{-\epsilon_1(\epsilon_0+\epsilon_1)e^{-\beta\epsilon_1}}{1+e^{-\beta\epsilon_1}} + \frac{\epsilon_1\left[\epsilon_0+(\epsilon_0+\epsilon_1)e^{-\beta\epsilon_1}\right]e^{-\beta\epsilon_1}}{(1+e^{-\beta\epsilon_1})^2}\right]$$

$$= -\frac{N}{kT^2}\left[\frac{-\epsilon_1(\epsilon_0+\epsilon_1)e^{-\beta\epsilon_1}(1+e^{-\beta\epsilon_1}) + \epsilon_1\epsilon_0 e^{-\beta\epsilon_1} + \epsilon_1(\epsilon_0+\epsilon_1)e^{-2\beta\epsilon_1}}{(1+e^{-\beta\epsilon_1})^2}\right]$$

$$= -\frac{N}{kT^2}\left[\frac{-\epsilon_1(\epsilon_0+\epsilon_1)e^{-\beta\epsilon_1} + \epsilon_1\epsilon_0 e^{-\beta\epsilon_1}}{(1+e^{-\beta\epsilon_1})^2}\right]$$

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$$\Rightarrow \boxed{C_V = +\frac{N}{kT^2}\frac{\epsilon_1^2 e^{-\beta\epsilon_1}}{(1+e^{-\beta\epsilon_1})^2}}$$

← independent of ϵ_0! why?

$$\lim_{T\to 0} e^{-\beta\epsilon_1} = 0 \quad , \quad \lim_{T\to\infty} e^{-\beta\epsilon_1} = 1$$

so,

$$\lim_{T\to 0} C_V = 0 \qquad \lim_{T\to\infty} C_V = 0$$

since exponential goes faster than T^2

from $\frac{1}{T^2}$

So,