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HW for 11/20/17

T4D.5
T4D.6
T5M.1

$e^{\frac{1}{2}-1} = \left(\frac{1}{\sqrt{e}}\right)^2 = \ldots$

$\frac{\varepsilon}{k_B}$

T4D.5

When T becomes large compared to $T_E = \frac{\varepsilon}{k_B}$, then $u \equiv \varepsilon/k_B T = \frac{1}{t}$ becomes very small and $e^{\varepsilon/k_B T} = e^u$ becomes close to 1. Under such circumstances, we can approximate $e^u \approx 1 + u$. In this limit, show that equation T4.42 becomes $\frac{dU}{dT} \approx 3Nk_B$

Equation T4.42 is $\frac{dU}{dT} = \frac{3Nk_B e^{1/t}}{t^2(e^{1/t}-1)^2}$, $t \equiv \frac{k_B T}{\varepsilon}$

When T is very large compared to $T_E = \frac{\varepsilon}{k_B}$, $e^{\frac{1}{t}} = e^u$ is approximated as $1 + u = 1 + \frac{1}{t}$.

Plugging this into Eq. T4.42, we get

$$\frac{dU}{dT} \approx \left\{3Nk_B\left(1+\tfrac{1}{t}\right)\right\} \Big/ \left[t^2\left(1+\tfrac{1}{t}-1\right)^2\right]$$

$$\Rightarrow \left[3Nk_B\left(1+\tfrac{1}{t}\right)\right] \Big/ \left(t^2 \cdot \tfrac{1}{t^2}\right) \Rightarrow \frac{dU}{dT} \approx 3Nk_B\left(1+\tfrac{1}{t}\right)$$

Because $\frac{1}{t}$ is very small, we can say that $1 + \frac{1}{t} \approx 1$. So

$\frac{dU}{dT} \approx 3Nk_B$

T4D.6

When $T \ll T_E$ ($t = k_B T/\varepsilon \ll 1$), $1/t \gg 1$. What does an Einstein solid's heat capacity $\frac{dU}{dT}$ become in this limit? You should find that the quantity goes to zero, but show HOW it goes to zero.

Eq. T4.42 states $\frac{dU}{dT} = \frac{3Nk_B \cdot e^{1/t}}{t^2(e^{t}-1)^2}$

When $T \ll T_E$, $1/t \gg 1$. This means that $e^{1/t} \gg 1$. So $e^{1/t} - 1 \approx e^{1/t}$.

$\Rightarrow \frac{dU}{dT} \approx \frac{3Nk_B e^{\frac{1}{t}}}{t^2 \cdot (e^{1/t})^2} = \frac{3Nk_B}{t^2 e^{1/t}}$

When $T \ll T_E$, $t \ll 1$ so t^2 is VERY SMALL. But $\frac{1}{t}$ is as big as t is small. $e^{\frac{1}{t}}$ then is a truly ginormous number, so big that multiplying it by t^2 will not have much of an effect. In the limit that $T \ll T_E$, the denominator goes to infinity, and so $\frac{3Nk_B}{t^2 e^{1/t}} = \frac{dU}{dT}$ goes to zero.

TSM.1

Consider a diatomic gas at temperatures T_1 and T_2 such that $\tau_1 \equiv k_B T_1/\varepsilon = 0.29$ $\tau_2 = 0.31$ for the gas's rotational excitation mode.

a) Evaluate the partition function directly as a sum for each temp, keeping what you think is a sufficient # of terms needed to ensure six significant figures of accuracy

$$Z = \sum_{j=0}^{\infty} (2j+1)e^{-j(j+1)\frac{\varepsilon}{k_B T}} \rightarrow Z_1 = \sum_{j=0}^{10000} (2j+1)e^{-j(j+1)\cdot\frac{1}{0.29}} \approx 1.00303$$

$$Z_2 = \sum_{j=0}^{10000} (2j+1)e^{-j(j+1)\cdot\frac{1}{0.31}} = 1.00473$$

b) For T_1, T_2, compute $\sum \Pr(E_j)E_j$ in terms of ε directly as a sum with the same # of terms,

$$E_j = j(j+1)\varepsilon$$

$$E_{avg} = \sum_{j=1}^{10000} j(j+1)\varepsilon\cdot(2j+1)e^{-j(j+1)\frac{1}{\tau}} = \varepsilon\sum_{j=1}^{10000} j(j+1)(2j+1)e^{-j(j+1)\frac{1}{\tau}}$$

$E_{avg,1} = \varepsilon\cdot 0.00606763$

$E_{avg,2} = \varepsilon\cdot 0.00946797$

c) Use $\frac{dE_{avg}}{d\tau} \approx \left[\frac{E_{avg}(\tau_2)-E_{avg}(\tau_1)}{\tau_2-\tau_1}\right]$ Use this to compute an estimate $\frac{dE_{avg}}{dT}/k_B$ at $\tau = 0.30$

$$\frac{dE_{avg}}{dT}/k_B = \frac{dE_{avg}}{d\tau\,\varepsilon} \approx \frac{\varepsilon\cdot(0.00946797-0.00606763)}{\varepsilon\cdot\ 0.31-0.29} = 0.340034$$

d) The answer is close-ish (should be about 30% less).

Evals:

T4D.5: Check plus

T4D.6: check plus

TSM.1: Check minus (