Recitation 15 – Entropy, Temperature and Heat Capacity

Last week you solved a problem involving a nanoparticle consisting of 27 copper atoms. More specifically, you estimated the entropy and temperature of the particle in macrostates having 0, 1 and 2 vibrational energy quanta. Knowing the stiffness of the atomic bond between copper atoms and the mass of a copper atom, you found that the vibrational energy quantum is 3.24×10^{-21} J. The table below summarizes your other findings, including the expected result that the low-energy states of the nanoparticle have very low (near absolute zero) temperatures.

q	#ways	E (J)	S (J/K)	ΔE (J)	ΔS (J/K)	T (K)
0	1	0	0			
				3.24×10^{-21}	0.6066×10^{-22}	53.42
1	81	3.24×10^{-21}	0.6066×10^{-22}			
				3.24×10^{-21}	0.5124×10^{-22}	63.25
2	3321	6.48×10^{-21}	0.1119×10^{-21}			

You then used these results to estimate the heat capacity per copper atom at such low temperatures and found that $C_{atom}\approx1.2\times10^{-23}J/K$, much smaller than the classical prediction of $3k\approx4.14\times10^{-23}J/K$.

Problem 1

Consider the copper nanoparticle you studied last week but in states with higher energy (about one quantum per oscillator).

a) Show your work as you compute the information that completes the table on the next page. Use the full accuracy of your calculator to avoid losing precision when computing entropy and temperature differences.

q	E (J)	S (J/K)	ΔE	ΔS	T
80		$0.14923128 \times 10^{-20}$			
			J	J/K	K
81		$0.15017927 \times 10^{-20}$			
			J	J/K	K
82		$0.15111889 \times 10^{-20}$			

b) Use information from the table above to estimate the copper nanoparticle's heat capacity when it has 81 quanta of energy. What is the corresponding heat capacity per copper atom? How does it compare to the classical estimate of the heat capacity per atom, 3 times Boltzmann's constant?

[Checkpoint 1]

Problem 2

In the preceding problems you computed estimates of the heat capacity per atom of a copper nanoparticle with different amounts of thermal energy. Are the values you obtained related to the classical estimate of the heat capacity per atom, 3 times the Boltzmann constant, as you expected? Explain briefly.

[Checkpoint 2]