Assignment 3

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2. 某金属晶体于300K时，其摩尔热容为2R，试应用爱因斯坦晶体模型计算晶体中原子的振动频率。

2. The molar heat capacity of a metal crystal at 300K is 2R. Try to apply the Einstein crystal model to calculate the vibration frequency of atoms in the crystal.

3. 两个体积相同的容器1、2之间由活栓联结，火栓关闭时，容器1中有1*mol* He，容器2为真空，整个装置与环境绝热。试论证： a) 活栓关闭时, 体系的微观状态数为$(x\_{1}+x\_{2}+\cdots \cdots +x\_{m})^{n}$$Ω\_{ini}$$=\frac{q^{\tilde{N}\_{0}}}{\tilde{N}\_{0}!}e^{-βE}, $活栓打开后$(x\_{1}+x\_{2}+\cdots \cdots +x\_{m})^{n}$$Ω\_{fin}$$=\frac{(2q)^{\tilde{N}\_{0}}}{\tilde{N}\_{0}!}e^{-βE}$；b) 将活栓重新关上，体系的微观状态数等于 的可几率为，而体系的熵值在这时下降10-6或更多熵单位的可几率则为。



3. Two containers 1 and 2 of the same volume are connected by a stopcock. When the stopcock is closed, there is 1 mol He in container 1, container 2 is vacuum, and the entire device is adiabatic from the environment. Please prove: a) When the stopcock is closed, the number of microscopic states of the system is $(x\_{1}+x\_{2}+\cdots \cdots +x\_{m})^{n}$$Ω\_{ini}$$=\frac{q^{\tilde{N}\_{0}}}{\tilde{N}\_{0}!}e^{-βE}.$ After the stopcock is opened, the number of microscopic states of the system is $(x\_{1}+x\_{2}+\cdots \cdots +x\_{m})^{n}$$Ω\_{fin}$$=\frac{(2q)^{\tilde{N}\_{0}}}{\tilde{N}\_{0}!}e^{-βE}$. b) When the stopcock is closed again, the probability that the number of microscopic states of the system is equal to is , and the probability that the entropy value of the system drops by 10-6 or more entropy units at this time is .

4. 设A、B两组分在二维平面上形成理想固溶体，以NA和NB分别表示其中A、B分子数。a) 如果A、B均为单原子分子，则在二维固溶体点阵上，各有几个运动自由度？采用爱因斯坦模型，写出固溶体中A、B分子的配分函数。b) 确定体系的正则配分函数。c) 导出此二维固溶体混合熵以及热容表达式。

4. Assume that components A and B form an ideal solid solution on a two-dimensional plane, and let NA and NB represent the number of A and B molecules respectively. a) If A and B are both monatomic molecules, how many degrees of freedom do they have on the two-dimensional solid solution lattice? Using the Einstein model, write the partition function of A and B molecules in the solid solution. b) Determine the canonical partition function of the system. c) Derive the mixing entropy and heat capacity of this two-dimensional solid solution.

5. 有A、B两组分同时在固体S表面吸附，并遵从Langmuir假设。以M表示固体表面的吸附位数，NA和NB表示吸附在固体表面上的A、B分子数。a) 应用正则系综法导出体系的混合吸附等温方程。b) 应用巨正则系综法导出体系的混合吸附等温方程。c) 证明两种求导方法结果是一致的。

5. There are two components A and B coadsorbed on the surface of solid ***S***, and they obey the Langmuir hypothesis. *M* represents the number of adsorption sites on the solid surface, and *NA* and *NB* represent the number of A and B molecules adsorbed on the solid surface. a) Use the canonical ensemble method to derive the mixed adsorption isotherm equation of the system. b) Use the grand canonical ensemble method to derive the mixed adsorption isotherm equation of the system. c) Prove that the results of the two derivations are consistent.