Section B. Statistical Mechanics and Thermodynamics

1. **Interstitials and Vacancies**

Consider a crystal lattice where the atoms can sit on a lattice site or they can sit on an "interstitial" site. Assume the number of atoms N is equal to the number of lattice sites. The ground state has all atoms on lattice sites, so there are no interstitials and no vacancies (a vacancy is a lattice site that is empty; an interstitial is an atom that sits on an interstitial site).

However, when the lattice is in thermal equilibrium at a nonzero temperature T, vacancies and interstitials are present at some nonzero equilibrium density. The number of interstitial *sites* is $N_i = \rho N$. The excess energy of an atom on an interstitial site is $\epsilon > 0$, and assume that there are otherwise no other interactions, so the crystal's energy is $E = K\epsilon$, where K is the number of interstitials. Each site can be occupied by at most one atom, so the number of vacancies is necessarily equal to the number of interstitials. Consider the thermodynamic limit of an infinite such crystal, with a given ρ and ϵ:

a) For a given density of interstitials per lattice site $n = K/N$ (and the same density of vacancies), what is the total entropy per lattice site, $s(n)$?

b) Calculate the equilibrium density of interstitials $n(T)$. Explain the leading behavior at low temperature T.