[tex187] Hosts and tags at level 1

Consider a system of N_A orbitals, where each orbital can be populated by one host, which, in turn, can accommodate an unlimited number of tags. The combinatorics of such a system is specified by two species of particles with the following interaction coefficients and capacity constants [tsc20]:

$$g_{\rm hh} = 1$$
, $g_{\rm th} = -1$, $g_{\rm ht} = g_{\rm tt} = 0$; $A_{\rm h} = N_A$, $A_{\rm t} = 0$.

(a) Derive a compact expression for the scaled configurational entropy $\bar{S} \doteq S/N_A$ as a function of the densities $\bar{N}_{\rm h} \doteq N_{\rm h}/N_A$ of hosts and $\bar{N}_{\rm t} \doteq N_{\rm t}/N_A$ of tags.

(b) Produce of contour plot of the function $\bar{S}(\bar{N}_{\rm h}, \bar{N}_{\rm t})$. (c) Determine the value of $\bar{N}_{\rm h}^{(\max)}$ at fixed $\bar{N}_{\rm t}$ which maximizes \bar{S} . Include the function $\bar{N}_{\rm h}^{(\max)}(\bar{N}_{\rm t})$ as a dashed line in the contour plot.

(d) Construct from this information a function $\bar{S}_{\max}(\bar{N})$, which represents the maximum configurational entropy as a function of the total number $\bar{N} = \bar{N}_{\rm h} + \bar{N}_{\rm t}$ of particles. Produce a plot of $\bar{S}_{\max}(\bar{N})$. Mark and explain all landmarks on that curve.

Solution: