[tex188] Hosts and tags at level 2

Consider a system of N_A orbitals. It takes two orbitals to accomomdate a host particle at level 2 and one more orbital for each tag the carry along as illustrated in [tln91]. The cominatorics of such a system is specified by two species of particles with the following interaction coefficients and capacity constants:

$$g_{\rm hh} = 2, \quad g_{\rm th} = -1, \quad g_{\rm ht} = 1, \quad g_{\rm tt} = 0; \quad A_{\rm h} = N_A - 1, \quad A_{\rm t} = 0.$$

(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 $\bar{N}_{\rm h}^{(\rm max)}$ at fixed $\bar{N}_{\rm t}$ which maximizes $\bar{S}$. Include the function $\bar{N}_{\rm h}^{(\rm max)}(\bar{N}_{\rm t})$ as a dashed line in the contour plot.
(d) Construct from this information a function $\bar{S}_{\rm max}(\bar{N})$, 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 $\bar{S}_{\rm max}(\bar{N})$. Mark and explain all landmarks on that curve.

Solution: