Hosts and caps [pln10]

Consider a system of N_A orbitals. Each orbital may be vacant, singly occupied, or doubly occupied, contributing energies 0, ϵ_1, or $\epsilon_1 + \epsilon_2$, respectively, to the system.

The first (second) particle placed into an orbital is categorized as host (cap). Their activation energies are ϵ_1 and ϵ_2, respectively. Hosts and caps are effectively distinguishable even if $\epsilon_1 = \epsilon_2$. They are not mergeable.

Multiplicity of microstates with N_1 hosts and N_2 caps:

$$W(N_1, N_2) = \begin{pmatrix} d_1 + N_1 - 1 \\ N_1 \end{pmatrix} \begin{pmatrix} d_2 + N_2 - 1 \\ N_2 \end{pmatrix},$$

$$d_m = A_m - \sum_{m'} g_{mm'}(N_{m'} - \delta_{mm'}), \quad \mathbf{g} = \begin{pmatrix} 1 & 0 \\ -1 & 1 \end{pmatrix}, \quad A_1 = N_A, \quad A_2 = 0.$$

The system without particles has only capacity for hosts ($A_1 = N_A$), not for caps ($A_2 = 0$). Adding hosts decreases capacity for further hosts ($g_{11} = 1$), but increases capacity for caps ($g_{21} = -1$). Adding caps does not affect capacity for hosts ($g_{12} = 0$) but decreases capacity for further caps ($g_{22} = 1$).

In the following, the state of each orbital is encoded as vacant (0), occupied by a host (1), or occupied by a host and a cap (2).

Microstates for $N_A = 2$:

00
10 01
20 02, 11
21 12
22

Microstates for $N_A = 3$:

000
100 010 001
110 101 011, 200 020 002
111, 210 201 021 120 102 012
211 121 112, 220 202 022
221 212 122
222