[nex107] Isomeric transition II: dynamics

A molecule exist exists in two isomeric arrangements of atoms, X and Y. In the presence of a catalyst, transitions happen at rates K_1 and K_2:

$$X \underset{K_2}{\overset{K_1}{\rightleftarrows}} Y.$$

The approach to equilibrium is governed by a master equation (12) with transition rates,

$$W(m|n) = K_1 n \delta_{m,n-1} + K_2 (N-n) \delta_{m,n+1},$$

where the number of isomers are $n_X = n$ and $n_Y = N - n$ with constant N. Processes of given overall time scale depend on a single parameter, controlled by the density of the catalyst. We set

$$K_1 = \gamma, \quad K_2 = 1 - \gamma \quad : \ 0 < \gamma < 1.$$

(a) Solve the equations of motion for mean $\langle\langle n(t)\rangle\rangle$ and variance $\langle\langle n^2(t)\rangle\rangle$ established in [nex46] from the first two jump moments of the process:

$$\frac{d}{dt}\langle n\rangle = -\langle n\rangle + (1-\gamma)N, \qquad \frac{d}{dt}\langle\langle n^2\rangle\rangle = -2\langle\langle n^2\rangle\rangle + (2\gamma - 1)\langle n\rangle + (1-\gamma)N.$$

(b) Plot $\langle\langle n(t)\rangle\rangle$, $\langle\langle n^2(t)\rangle\rangle$ in separate frames for $n_0 = 0$ and $\gamma = 0.1, 0.5, 0.9$. Identify and explain any interesting features in the curves.

Solution: