[nex107] Catalyst driven chemical reaction: dynamics

In the chemical reaction $A + X \leftrightarrow A + Y$, the molecule A is a catalyst at constant concentration. The total number of reacting molecules, $n_x + n_y = N$, is also constant. K_1 is the probability per unit time that a molecule X interacts with a molecule A to turn into a molecule Y, and K_2 is the probability per unit time that a Y interacts with an A to produce an X. The dynamics may be described by a master equation for $P(n,t)$, where $n \equiv n_x, n_y = N - n$. The transition rates are

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

(a) Solve the equations of motion for $\langle\langle n(t)\rangle\rangle$, $\langle\langle n^2(t)\rangle\rangle$ as constructed in [nex46]. Use initial values $\langle\langle n(0)\rangle\rangle = n_0$, $\langle\langle n^2(0)\rangle\rangle = 0$.
(b) Plot $\langle\langle n(t)\rangle\rangle$, $\langle\langle n^2(t)\rangle\rangle$ in separate frames for $n_0 = 0$, $K_1 = \gamma$, $K_2 = 1 - \gamma$, and various γ. This fixes the time scale. Identify any interesting features in the curves and try to explain them.

Solution: