[nex46] Catalyst driven chemical reaction: stationary state

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 $n \doteq n_x, n_y = N - n$. The transition rates are

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

To calculate the mean value $\langle\langle n(t)\rangle\rangle$ and the variance $\langle\langle n^2(t)\rangle\rangle$ proceed as in [nex44] via the equations of motion, $d\langle n\rangle/dt = \langle\alpha_1(n)\rangle$, $d\langle n^2\rangle/dt = \langle\alpha_2(n)\rangle + 2\langle n\alpha_1(n)\rangle$, with jump moments $\alpha_l(m) = \sum_n (n-m)^l W(n|m)$.
(a) Construct the equations of motion for $\langle\langle n(t)\rangle\rangle$, $\langle\langle n^2(t)\rangle\rangle$.
(b) Infer the long-time asymptotic values $\langle\langle n(\infty)\rangle\rangle$, $\langle\langle n^2(\infty)\rangle\rangle$ directly.
(c) Plot $\langle\langle n(\infty)\rangle\rangle$, $\langle\langle n^2(\infty)\rangle\rangle$ versus γ for $K_1 = \gamma$, $K_2 = 1 - \gamma$ (thus fixing the time scale) and explain the location of the maximum for each quantity.

Solution: