[nex108] Catalyst driven chemical reaction: total rate of reactions

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 $W(m|n) = K_1 n \delta_{m,n-1} + K_2(N-n)\delta_{m,n+1}$. The total rate of chemical reactions is defined as follows:

$$R(t) \doteq \sum_{nm} W(n|m)P(m,t).$$

(a) Express $R(t)$ in terms of $\langle\langle n(t)\rangle\rangle$.
(b) Use the result of $\langle\langle n(\infty)\rangle\rangle$ from [nex46] to calculate the total rate of chemical reactions in the stationary state. Set $K_1 = \gamma$, $K_2 = 1 - \gamma$ and compare the γ-dependence of $R(\infty)$ with that of $\langle\langle n^2(\infty)\rangle\rangle$ from [nex46], which is a measure of the fluctuations in the population of molecules.
(c) Use the result of $\langle\langle n(t)\rangle\rangle$ from [nex107] to calculate the time evolution of $R(t)$. Plot $R(t)$ for $n_0 = 0, K_1 = \gamma, K_2 = 1 - \gamma$ and various fixed values of γ. The time scale is thus set. Compare the graph of $R(t)$ with the graph of $\langle\langle n^2(t)\rangle\rangle$ from [nex107]. Explain the similarities and differences.

Solution: