Assignment 3 (PHYC90010)
To be handed in by the 17th of May (5pm)

In the stratosphere and mesosphere of the Earth, between altitudes of 30 km and 90 km, solar ultraviolet radiation dissociates oxygen molecules (O_2) to form oxygen atoms (O). An oxygen atom and molecule can then combine to form an ozone molecule in an excited state (O_3^*). In turn, the excited ozone molecule decomposes into its original constituents, unless it collides promptly with some other atmospheric molecule, which carries away the excess energy. The forward and reverse reactions

$$\mathrm{O} + \mathrm{O}_2 \to \mathrm{O}_3^*,$$
$$\mathrm{O}_3^* \to \mathrm{O} + \mathrm{O}_2,$$

proceed with rate coefficients k_1 and k_2 respectively.

(a) Show that the master equation obeyed by the joint probability distribution function $p(x_0, x_3, t)$ of the atomic oxygen (x_0) and ozone (x_3) populations, assuming that the O_2 population is fixed at x_2, is given by [5]

$$\begin{aligned}\frac{\partial p(x_0, x_3, t)}{\partial t} &= k_1 x_2 (x_0 + 1) p(x_0 + 1, x_3 - 1, t) + k_2 (x_3 + 1) p(x_0 - 1, x_3 + 1, t) \\ &- (k_1 x_2 x_0 + k_2 x_3) p(x_0, x_3, t).\end{aligned}$$

(b) Derive the first-order partial differential equation satisfied by the generating function [10]

$$G(t, s_0, s_3) = \sum_{x_0=0}^{\infty} \sum_{x_3=0}^{\infty} s_0^{x_0} s_3^{x_3} p(t, x_0, x_3).$$

You should find

$$\frac{\partial G}{\partial t} = k_1 x_2 (s_3 - s_0) \frac{\partial G}{\partial s_0} + k_2 (s_0 - s_3) \frac{\partial G}{\partial s_3}.$$

(c) Assuming that there are exactly p oxygen atoms and zero ozone molecules initially, find the solution for $G(t, s_0, s_3)$. [10]

(d)

i. Calculate the mean number of ozone molecules in equilibrium ($t \to \infty$). [5]

ii. Calculate the covariance $\langle x_0\, x_3 \rangle$ at equilibrium ($t \to \infty$). [5]

iii. Are the numbers of oxygen atoms and ozone molecules correlated, anti-correlated, or uncorrelated at equilibrium? Explain the result physically. [5]

Total Marks 40