In this manuscript I will reproduce and rederive the results presented in section IIA-C of the paper: *“Noise-induced symmetry breaking far from equilibrium and the emergence of biological homochirality”* by Farshid Jafarpour and et al.

**1 – Analytical model**

Starting from the stochastic model for the system, given by the equation (9):

the stoichiometry matrix denoted by , is derived by considering the fact that only 4 types of transitions are happening in this model, namely: one A molecule gets converted to D molecule (both in autocatalysis and non-autocatalysis reaction) and vice versa, and one A molecule gets converted to one L molecule and vice versa. So, simply the stoichiometries of the species in the transitions will be the elements of the matrix, each row corresponding to one of the transitions:

Next is to derive the rate of each transition represented in matrix . Each row of is a vector :

can be thought of, as a change in the state of the system ( are the concentration of respectively). Multiplied by , the dimensions of , becomes the same as the state .

So, represents the transition rate from state to the state . The transition rates are derived from the rule of mass action. There are two contributors for the transition , one from the autocatalysis reaction and the other from non-autocatalysis reaction. So:

.

The rest are derived in the same fashion:

(**II)**

By considering all the four possible transitions in the system, the rate of the change in the probability of finding the system in state : , is given by:

By defining , the above equation can be re-written as:

Not that we have used: . Now, by performing a Taylor expansion we can re-write in terms of derivatives of :

In the limit , we can approximate by the first two terms.

Let’s remind ourselves that , is a matrix consisting of 4 rows (representing transitions) denoted by . So, we can absorb each row together with the corresponding term into one single vector:

**(III)**

is the drift vector.

The same procedure should be taken for the second term. To make it more lucid, I concentrate only on the first transition, namely index . So, the second term looks like:

So, we can form a matrix and put in all the possible products of the rows in vector , which we denote by (The Kronecker product) and multiply them with .

But we should repeat this for all the other three transitions and sum them all to get the right

is like a diffusionmatrix.

This way we can rewrite in a more compact form as:

**(IV)**

Which is in form of a Fokker-Plank equation and gives us the dynamics of the probability of finding the system in state , in time . Like every Fokker-Plank equation, there is a corresponding Stochastic Differential Equation (SDE) to the above equation. As a famous example, take the diffusion equation for a Brownian particle which looks like:

Which is also in the form of a Fokker-Plank equation, in absence of a drift. There is a well-known corresponding SDE equation to the above equation:

Where, is a Gaussian white noise. The latter equation simply describes the movement of the Brownian particle in diffusion regime.

In analogy to the Brownian particle case, the SDE corresponding to equation **(III)**, can be written as:

**(V)**

Where, satisfies the relation and is a Gaussian white noise.

There are a couple of differences between **(V)** and Brownian particle case, which can be understood intuitively. First that we have a vector equation here, and the diffusion is no longer a scalar, instead a matrix. So, it is easy to see why should satisfy .Moreover, unlike the diffusion case, we have a drift here, which is analogous to a long-term velocity for the Brownian particle if it was under the effect of an external field.

The matrix **G** is found to be (as explained in the paper appendix 1 ):

**(VI)**

Where: and

We proceed by performing a change of variables, introducing a new set of variables defining the state of the system:

It is argued in the paper that and can be regarded as constants., is the value r approaches quickly and we will evaluate it shortly. It’s trivial to express the older variables in terms of the new ones, by using the inverse of the above transformation matrix:

**(VII)**

, ,

Next is to evaluate . Back to equation **(V)** if r is to settle on a value, it has to satisfy:

Where I have inserted the corresponding row from **(III)**. The noise terms will only create a small region around . So, by ignoring the noise and inserting the values for and from **(VII)**, we can write down the equation satisfying :

After a few algebraic manipulations we get:

So finally, reads:

It is useful at this point, to derive an expression for in the limit , revoking

Therefore, we get the below simple expression for in the limit :

**(VIII)**

Now back to equation **(V)**, the dynamics of the system is on , so we proceed to find an expression for . We insert the relations **(VI)** and **(VII)** into **(V)**, to get the below set of equations:

The equation from the first row gives us the same expression for as we derived (ignoring the noise). We can subtract the second and third row from each other to ger an expression for . I will skip the algebraic steps in between and write down the final result:

Where I have used the relation for two Gaussian noises, to convert them to one single noise with a variance . Now we can use the result we derived in (VIII) to write down the simpler result in the limit :

**(!)**

The first term in **(!)** together with the first term in the square roots,agrees well with equation 27 in the paper but Unfortunately, I could not find out where the term comes from in the square roots.

Anyway, the correct equation from the paper reads:

**(IX)**

Once again, we switch to the Fokker-Plank equation corresponding to the SDE in **(IX) (**equation 28 in the paper). We seek the steady state solution to equation 28, which is found to be:

**(X)**

And is the normalization for the probability density. The value of indicates the dominance of non-autocatalysis reactions over autocatalysis(self-replicator) ones.

**2 – Simulations and comparison with analytical result**

To simulate the model presented in the previous section, I used the python package for Gillespie simulations, named *gillespy2*. The code defines a class with specifics of the reactions described in the previous section. Then in a loop, 10000 samples are drawn for the values of .

***Important:***

Please before running the code, enter the below command to make sure the required packages are installed:

pip install gillespy2 --user --upgrade

I set the value of and varied the ratio to simulate the different scenarios for . The figures in the next page show the results of simulations compared with the analytical model.

the analytical curve agrees almost well with the simulation points for all values of .









