Phase diagram analysis of noise-induced transition in an autocatalytic reaction

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Abstract. We present the analysis of the genetic model of autocatalytic chemical reactions proposed by Arnold et al. This model, when subjected to multiplicative white noise modelling environmental fluctuations, can undergo a sudden change from a unimodal state to a bimodal one, while no such transition occurs if the noise is absent. Here, this noise-induced transition is studied analytically by investigating the so-called critical surface in the three-dimensional parameter space.

1. Introduction

Noise-induced phenomena have become a subject of widespread interest in recent decades, because of their observations in various nonlinear systems in physics, chemistry and biology [1,2]. In particular, autocatalytic reaction occurring in a random environment

$$A + X + Y \underset{k_1}{\overset{k_2}{\leftrightarrows}} 2Y + A^* \,, \qquad B + X + Y \underset{k_3}{\overset{k_4}{\leftrightarrows}} 2X + B^* \,,$$

is one of the most studied models in chemistry. The reaction dynamics is governed by the following stochastic differential equation (SDE) for the concentration $x(t)$,

$$dx(t) = [\alpha - x(t) + \lambda x(t)(1 - x(t))]\, dt + \sigma x(t)(1 - x(t)) dw(t)\,, \quad x(t) \in [0, 1] \tag{1}$$

where $\alpha \in [0, 1]$, $\lambda \in \mathbb{R}$, $\sigma > 0$. This SDE is interpreted in the Stratonovirch sense according to the well-known results of Van Kampen [3], Wong-Zakai [4] and Blankenship [5]. Such chemical interpretation was proposed by Arnold, Horsthemke and Lefever in [6].

It was shown in [1] that this equation also describes the time dependence of gene frequency in a haploid population where there are only two possible alleles with corresponding frequencies x and $1 - x$. For this reason, the model was named "genetic model".

The solutions of Eq.(1) form the Markovian diffusion process $x(t) \in [0, 1]$ at any initial condition $x(0) \in [0, 1]$. In thermodynamic equilibrium states, this process has the stationary probability density

$$p(x) = \frac{C}{x(1 - x)} \left(\frac{x}{1 - x} \right)^{\beta} \exp \left\{ \frac{2}{\sigma^2} \left(\frac{\alpha - 1}{1 - x} - \frac{\alpha}{x} \right) \right\} , \tag{2}$$

$$C = \frac{e^{2/\sigma^2}}{2K_{-\beta}\big(4\sigma^{-2}\sqrt{\alpha(1-\alpha)}\big)}\left[\frac{1-\alpha}{\alpha}\right]^{\beta/2}, \quad \beta = \frac{2(2\alpha+\lambda-1)}{\sigma^2},$$

here $K_{-\beta}(.)$ is the modified Bessel function of the second kind with index $(-\beta)$ defined as

$$K_{-\beta}(z) = \frac{1}{2}\int\limits_{-\infty}^{\infty} e^{-z\,\mathrm{ch}\,u+\beta u}du\,, \quad \mathrm{Re}\,z > 0\,.$$

2. The analysis of critical surface

In our system coupled to a fluctuating environment, a phase transition can occur whenever the density function $p(x)$ qualitatively changes. In fact, this function may have different mode numbers, depending on the value of parameters λ, σ^2, α. Therefore, the three-dimensional parameter space is divided into domains in such a way that there is a certain mode number in each of them. This partition, on the analogy of thermodynamics, is called the phase diagram, while the surface Σ dividing these domains is called the critical surface. Our paper is devoted to the surface investigation.

Since any changes in the mode number of $p(x)$ corresponds to changes in the solution number of the equation $dp(x)/dx = 0$ which can be written as

$$S(x) \equiv \alpha - x + \lambda x(1-x) - \frac{\sigma^2}{2}x(1-x)(1-2x) = 0\,, \qquad x \in (0,1)\,, \tag{3}$$

we find the degeneracy condition of solutions. This is equivalent to the existence of such a multiple root x_0 that $S(x_0) = S'(x_0) = 0$. Then apply the Euclid algorithm for polynomials $S(x)$ and $S'(x)$. As a result, we obtain the equation of the critical surface:

$$P(\lambda,\sigma^2,\varepsilon) \equiv \lambda^4+\lambda^2\Big(1-5\sigma^2-\sigma^4/2\Big)-\lambda\varepsilon(9\sigma^4+18\sigma^2-4\lambda^2)-4\sigma^2\Big(1-\sigma^2/4\Big)^3-27\sigma^4\varepsilon^2 = 0\,, \tag{4}$$

where $\varepsilon = \alpha - 1/2$. At this time, the root x_0 is given by

$$x_0 = \frac{1}{2} - \frac{2\lambda(1+2\sigma^2)+18\varepsilon\sigma^2}{\Delta}\,, \quad \Delta = 4\lambda^2 + 3\sigma^4 - 12\sigma^2\,.$$

In order that x_0 be the bifurcation point of $p(x)$, it is necessary and sufficient that $0 < x_0 < 1$ which is equivalent to the following inequality

$$G_+(\lambda,\sigma^2,\varepsilon)G_-(\lambda,\sigma^2,\varepsilon) \geq 0\,, \tag{5}$$

by introducing the hyperbolas

$$G_\pm(\lambda,\sigma^2,\varepsilon) \equiv \Delta \pm 4\big[\lambda(2\sigma^2+1)+9\varepsilon\sigma^2\big] = 0\,. \tag{6}$$

The inequality (5) defines the allowable domain for the location of the points of the critical surface, whose boundaries are the hyperbolas $G_\pm(\lambda,\sigma^2,\varepsilon) = 0$. It is crucial as the surface (4) is not connected.

Let Σ_ε be the intersection of the surface defined by Eq.(4) with the plane $\varepsilon = \mathrm{const}$ and (λ_*,σ_*^2) be the coordinates of the contacting points between the curve Σ_ε and the ellipse $\Delta = 0$. Then

$$\lambda_* = -\frac{9\varepsilon\sigma_*^2}{1+2\sigma_*^2}\,. \tag{7}$$

If exclude λ_* from this relation by using $\Delta = 0$, the single-valued function $\sigma_*^2(\varepsilon)$ is derived from the equation

$$4(\sigma_*^2 - 1)^3 = 27\sigma_*^2(1 - 4\varepsilon^2)\,, \quad \sigma_*^2 > 1 \tag{8}$$

due to the convexity of the left-hand side function.

Now, we represent the polynomial $P(\lambda, \sigma^2, \varepsilon)$ as Taylor's power series of $(\lambda - \lambda_*)$ and $(\sigma^2 - \sigma_*^2)$, which, after introducing the variable substitution

$$\lambda = \lambda_* + \rho\cos\varphi\,, \quad \sigma^2 = \sigma_*^2 + \rho\sin\varphi\,, \tag{9}$$

has the form

$$P(\lambda, \sigma^2, \varepsilon) = -3(\sigma_*^2 - 1)^2(\rho\sin\varphi)^2\,Q_2(z) + \frac{1}{6}(\rho\sin\varphi)^3\,Q_3(z) + \frac{1}{16}(\rho\sin\varphi)^4\,Q_4(z)\,,$$

where $z = \mathrm{ctg}\varphi$, $z_* = \mathrm{ctg}\varphi_* = \lambda_*/3\sigma_*^2$, $Q_2(z) = (z - z_*)^2$, $Q_4(z) = (4z^2 - 1)^2$ and

$$Q_3(z) = 8z_*(7\sigma_*^2 - 1)z^3 - 6(\sigma_*^2 + 5)z^2 + 18z_*(1 + \sigma_*^2)z + \frac{3}{2}(\sigma_*^2 - 3)\,.$$

The Eq.(4) now becomes

$$\frac{1}{16}\rho^2 Q_4(z)\sin^2\varphi + \frac{1}{6}\rho Q_3(z)\sin\varphi - 3(\sigma_*^2 - 1)^2 Q_2(z) = 0\,, \tag{10}$$

and its solutions read

$$\rho_\pm(\varphi) = \frac{4}{3Q_4(z)\sin\varphi}\Big(- Q_3(z) \pm \sqrt{Q_3^2(z) + 27(\sigma_*^2 - 1)^2 Q_4(z) Q_2(z)}\Big)\,. \tag{11}$$

These two functions describe the curve Σ_ε at such φ that $\rho_\pm(\varphi) \geq 0$. This means that Σ_ε is defined by $\rho_+(\varphi)$ for $\varphi \in [0, \pi]$ and by $\rho_-(\varphi)$ for $\varphi \in [-\pi, 0]$. From Eq.(11), it is not difficult to show that

$$\rho_+(\varphi) = \frac{\sqrt{5}|Q_3(\pm 1/2)|}{12(z^2 - 1/4)^2}\big(1 + o(1)\big) \quad \text{when} \quad z \to \pm\frac{1}{2}\,.$$

Lemma 1. Σ_ε is a biconnected curve consisting of two components Σ_+ and Σ_- where $\Sigma_+ \equiv \rho_+(\varphi)$ at $\varphi \in [\psi, \pi - \psi]$, $\psi = \mathrm{arcctg}\,(1/2)$, while Σ_- is the glue of simple curves

$$\rho_+(\varphi), \quad \varphi \in [0, \psi)\,; \quad \rho_-(\varphi), \quad \varphi \in [-\pi, 0]; \quad \rho_+(\varphi), \quad \varphi \in (\pi - \psi, \pi].$$

□ This statement follows from the fact that connected curve component must be defined as a continuous function and both $\rho_\pm(\varphi)$ tend to the same finite limit at $\varphi \to 0, \pi$. ■

Theorem 1. Σ_+ is composed of two branches stitched at the contacting point (λ_*, σ_*^2).
□ In the neighborhood of the point (λ_*, σ_*^2), the asymptotic formula of Σ_+, in terms of local Cartesian coordinates u and v, has the form

$$u = \mathrm{const}|v|^{2/3} \quad \text{when} \quad v \to 0\,. \tag{12}$$

In fact, from Eq.(11), we find

$$\rho_+(\varphi) = \varkappa(z - z_*)^2 + O\left((z - z_*)^3\right) \quad \text{when} \quad z \to z_*\,, \quad \varkappa = \frac{81\sigma_*^4(1 + z_*^2)^{1/2}}{4(\sigma_*^2 - 1)}\,.$$

Hence $\rho_+(\varphi)$ is presented by $u^2 + v^2 = \varkappa^2 \arctan^4(v/u)$ where $\varphi - \varphi_* = \arctan(v/u)$ and consequently it follows Eq.(12). ■

In order to establish which component of Σ_ε corresponds to the critical curve, we find the following expressions of $G_\pm(\lambda, \sigma^2, \varepsilon) = 0$ in the polar coordinates (ρ, φ)

$$\rho^{(\pm)}\big[4(1 \pm \sin 2\varphi) - \sin^2\varphi\big] + 2\big[2\cos\varphi\big(2(\lambda_* \pm \sigma_*^2) \pm 1\big) + \sin\varphi(3\sigma_*^2 \pm 4\lambda_* - 6 \pm 18\varepsilon)\big] = 0\,.$$

Then such angles $\varphi^{(\pm)}$ that $\rho^{(\pm)}(\varphi^{(\pm)}) = 0$ are given by

$$z^{(\pm)} = \frac{6z_* \mp 3(\sigma_*^2 - 2)}{2(2\sigma_*^2 + 1) \pm 12\sigma_*^2 z_*} \tag{13}$$

where $z^{(\pm)} = \operatorname{ctg}\varphi^{(\pm)}$. Note that the denominator is greater than zero due to $\sigma_*^2 > 1$.

Theorem 2. Σ_+ is the intersection of the critical surface Σ and the plane $\varepsilon = \text{const}$.
□ It can be seen from Eq.(4) and Eq.(6) that (0,0) and (λ_*, σ_*^2) are two common points of Σ_ε and the hyperbolas $G_\pm = 0$. Furthermore, the former is the intersection of Σ_- and $G_\pm = 0$ (as $\rho_-^2(\varphi_0) = \lambda_*^2 + \sigma_*^4$ where $\operatorname{ctg}\varphi_0 = \lambda_*/\sigma_*^2$), while the latter is the intersection of Σ_+ and $G_\pm = 0$ $(\rho_+(\varphi_*) = 0)$.

We now prove that the component Σ_- is contained inside the domain $G_+G_- < 0$. In fact, the derivative $(d\sigma^2/d\lambda)$ of the implicit function $\sigma^2(\lambda)$ defined by Eq.(4) vanishes at $(0,0)$ while those derivatives of functions $\sigma^2(\lambda)$ described by $G_\pm = 0$ are

$$\left(\frac{d\sigma_\pm^2}{d\lambda}\right)_{(0,0)} = [3(1 \mp 3\varepsilon)]^{-1} \neq 0\,.$$

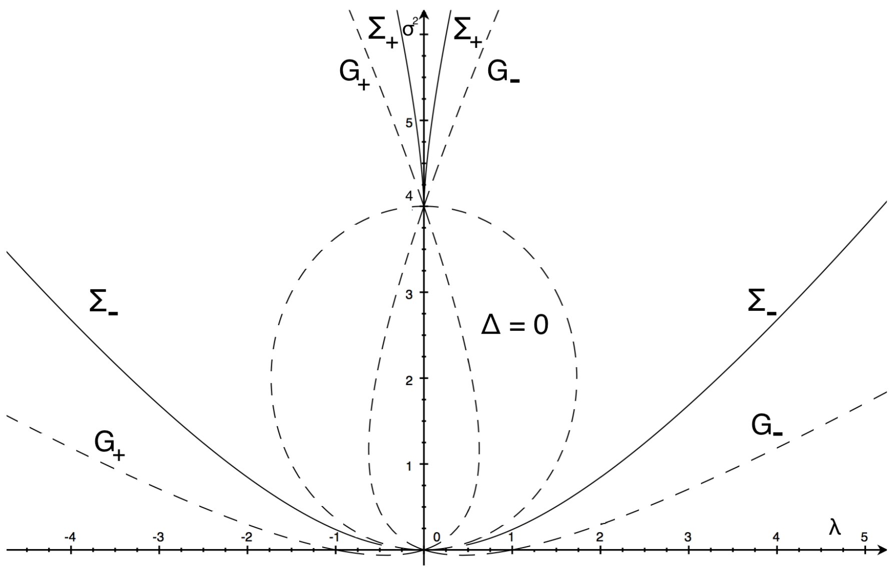
This means that for the points of Σ_-, being close enough to $(0,0)$, $G_+G_- < 0$ since $G_\pm(\lambda, 0, \varepsilon) = \pm 4\lambda + O(\lambda^2)$ when $\lambda \to 0$. Moreover, because (0,0) is the unique common point of Σ_- and $G_\pm = 0$, if the inequality $G_+G_- < 0$ is satisfied in the neighborhood of (0,0), it definitely holds for all others points (λ, σ^2) of Σ_-. Consequently, Σ_- is confined in this domain.

In contrast, the half-plane $(\lambda, \sigma^2 > 0)$ is divided by the component Σ_+ into two separate parts. Whenever one of the hyperbolas $G_\pm = 0$ crosses this component, it must go from one part to another part when φ continuously changes, passing through the contacting point ($\rho^{(+)}(\varphi^{(+)}) = 0$ and $\rho^{(-)}(\varphi^{(-)}) = 0$ respectively). However, this is impossible because of the existence of the cusp point $(0, \varphi_*)$. Since tangent of Σ_+ at this point is a ray radiating from it, for the proof of this fact it is sufficient that $\varphi^{(-)} > \varphi_* > \varphi^{(+)}$ i.e. $z^{(+)} < z_* < z^{(-)}$ which follows from Eq. (13). Therefore, only Σ_+ fulfills the condition (5) and represents the critical curve. ■

As an illustration for the obtained result, we demonstrate here the critical curve in the case of $\alpha = 1/2$, which is defined as

$$\lambda^2 = \frac{1}{2}\Big[\frac{\sigma^4}{2} + 5\sigma^2 - 1 - (2\sigma^2 + 1)^{3/2}\Big]\,.$$

The inverse function $\sigma^2(\lambda)$ is depicted in Pic. 1.



Pic. 1. Phase diagram in the symmetrical case $\alpha = 1/2$. The components Σ_+ and Σ_- are presented by the solid lines, while the hyperbolas $G_\pm = 0$ and the ellipse $\Delta = 0$ are drawn by dotted lines.

3. Conclusion

In contrast to the previous work of Horsthhemke et al., the complete analysis of the critical surface Σ of the model is obtained. This surface divides the parameter space into two domains where qualitatively different stationary dynamical regimes of the system are observed. From the physical point of view, for sufficiently slow variations of the parameters, the switch between these regimes represents a transition between two "phases": the unimodal one and the bimodal one. The dynamical regime in the bimodal phase consists of temporal intervals consequentially replacing each other and having random lengths. In these intervals reactant relative concentrations fluctuate nearby the two maxima of the density function $p(x)$.

4. References

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