Supplementary Information On

Stochastic dynamics of gene switching and energy dissipation for gene expression

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1 DETAILED DERIVATION FROM CHEMICAL MASTER EQUATIONS TO STEADY-STATE DISTRIBUTIONS

Since it is difficult to obtain the theoretical results of chemical master equations, the method of probability-generating functions is used to change chemical master equations into differential equations which may be solved with mathematical skill. Based on this method, two factorial probability-generating functions $G_i(z) = \sum_{m=0}^{\infty} P_i(m) z^m$ with $i = 0, 1$ are introduced. Substituting these into Eq.2:

$$\begin{aligned} &k_{\text{off}}G_1(z) - k_{\text{on}}G_0(z) + k_2 z G_1'(z) - ak_1 G_0(z) + ak_3(z-1)G_0(z) - (z-1)G_0'(z) = 0, \\ &-k_{\text{off}}G_1(z) + k_{\text{on}}G_0(z) - k_2 z G_1'(z) + ak_1 G_0(z) + ak_3(z-1)G_1(z) - (z-1)G_1'(z) = 0. \end{aligned} \tag{S1}$$

Here, all parameters have been normalized by k_4 as mentioned in Sec.II. It is found from Eq. S1 that

$$(e^{-ak_3 z}G_0)' = -(e^{ak_3 z}G_1)'. \tag{S2}$$

$e^{-ak_3 z}G_i$ is set as H_i for simplicity. From Eq. S2, we can determine that $H_0' = -H_1'$. This allows us to obtain H_0 from H_1. In the following, we will only focus on the expression of H_1, which can be deduced from Eq. S1 as

$$A(z)H_1'' + B(z)H_1' + CH_1 = 0 \tag{S3}$$

in which $A(z) = (k_2+1)z - 1$, $B(z) = ak_2k_3z + k_{\text{off}} + k_{\text{on}} + ak_1 + k_2 + 1$, and $C = ak_2k_3$. Until now, it seems difficult to obtain the analytical distribution because the coefficients of Eq. S3 are dependent on the variable z. Another transformation of the form $H_1(z) = e^{mz}W(nz+p)$ (here, m, n and p are undetermined constants) is introduced in Eq. S3, and hence a solvable differential equation about W is obtained as

$$\omega W''(\omega) - (\beta - \omega)W'(\omega) - \alpha W(\omega) = 0 \tag{S4}$$

where

$$\omega = \frac{ak_2k_3}{k_2+1}z - \frac{ak_2k_3}{(k_2+1)^2},$$
$$\alpha = \frac{ak_2k_3}{(k_2+1)^2} + \frac{k_{\text{on}}+k_{\text{off}}+ak_1}{k_2+1},$$
$$\beta = \frac{ak_2k_3}{(k_2+1)^2} + \frac{k_{\text{on}}+k_{\text{off}}+ak_1}{k_2+1} + 1. \tag{S5}$$

There are two independent solutions of Eq. S4. One is expressed by the Tricomi function of the form $U(\alpha,\beta;\omega)$. This result is inadmissible because it is required that $P_1(m) \to 0$ for $m\to\infty$. The other solution is expressed by the confluent hypergeometric function of the form ${}_1F_1(\alpha,\beta;\omega)$. The analytical expressions for the probability-generating functions are presented as below

$$\begin{aligned} G_0(z) &= A_0[e^{ak_3(z-1)} - e^{ak_3z/(k_2+1)}{}_1F_1(\alpha-1,\beta-1;\omega)], \\ G_1(z) &= A_0e^{ak_3z/(k_2+1)}{}_1F_1(\alpha,\beta;\omega) \end{aligned} \tag{S6}$$

Furthermore, based on the relationship between probability distribution and generating function:

$$P_i(m) = \frac{1}{m!}\frac{d^m}{dz^m}G_0(z)|_{z=0}. \tag{S7}$$

The analytic results of probability distributions are obtained and shown in the text (i.e., Eq.3 in Sec.II).

2 THE RESULTS OF NUMERICAL SIMULATIONS

The direct method to verify our analytical results is numerical simulations. The approximate probability distributions of $P_i(m)$ obtained by Monte Carlo simulation are given in Fig.S1.

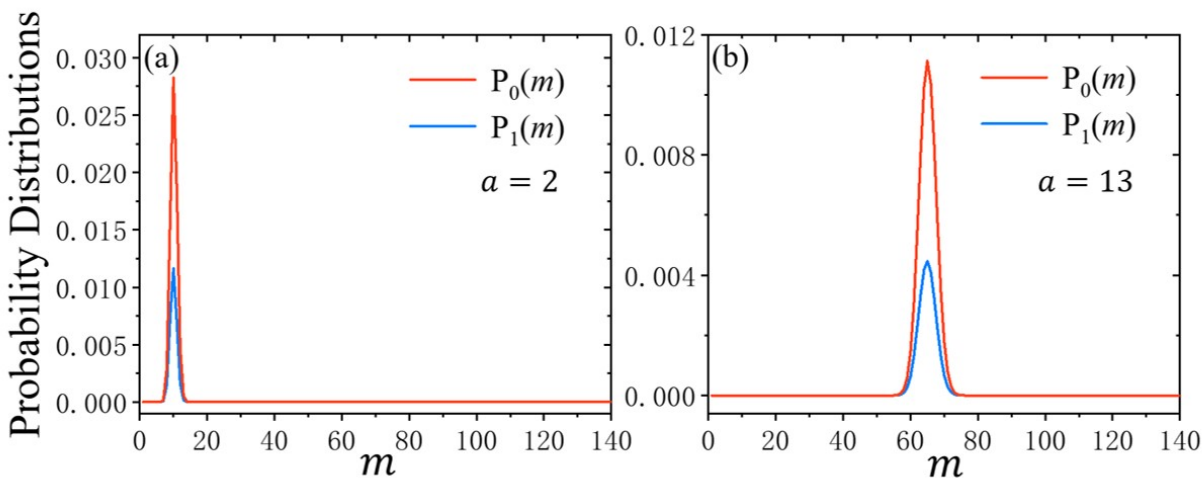

Figure S1. The numerical simulated results about probability distribution functions of the gene's states . The parameters are the same with Fig.3(a) and (b): $k_1 = 20$, $k_2 = 10$, $k_3 = 1.5$, $k_{\text{on}} = k_{\text{off}} = 2$. $P_0(m)$ is the probability of the gene's "off" state indicated with orange curve, $P_1(m)$ is the probability of gene's "on" state indicated with blue curve.

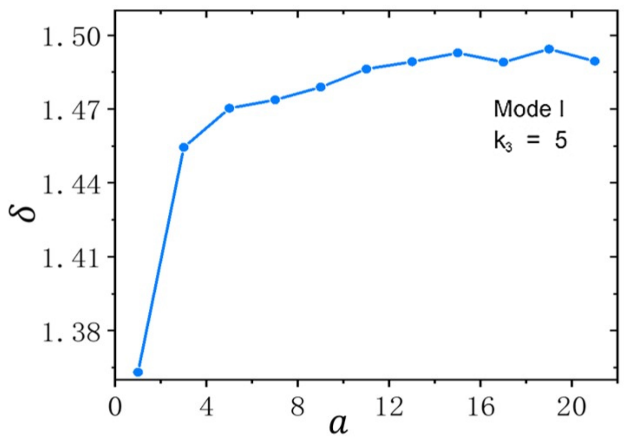

Figure S2. The numerical simulated results about gene's state dominance factor δ which is consistent with that in Fig.4(c). δ will increase with the increasing of the strength of external signal in Mode I. The values of other parameters are listed in Table I.

Moreover, the curve between δ and a which is obtained by Monte Carlo simulation with the same set of parameters in Fig.4(c) is shown in Fig.S2. It is obviously that the trend of δ is similar with the curve in Fig.4(c).

3 THE COMPARISONS BETWEEN THE TOTAL ENERGY DISSIPATION AND THE ENERGY DISSIPATION IN THE SYNTHESIS-DEGRADATION PROCESS OF ROCK IN MODE I AND II

The Fig.S3 shows the trends of the total energy dissipation (i.e., EP) and the energy dissipation in the synthesis-degradation process of ROCK (i.e., EP_m) with the increase of the strengthen of external stimulations (i.e., a) in Mode I and II. It is obviously that their trends are consistent as a increases in its respective modes. Specifically, EP and EP_m increase simultaneously in Mode I and decrease simultaneously in Mode II with the enhancing of the strengthen of external stimulations (i.e., a). Moreover, the difference between EP and EP_m diminishes both in Mode I and Mode II when a increases.

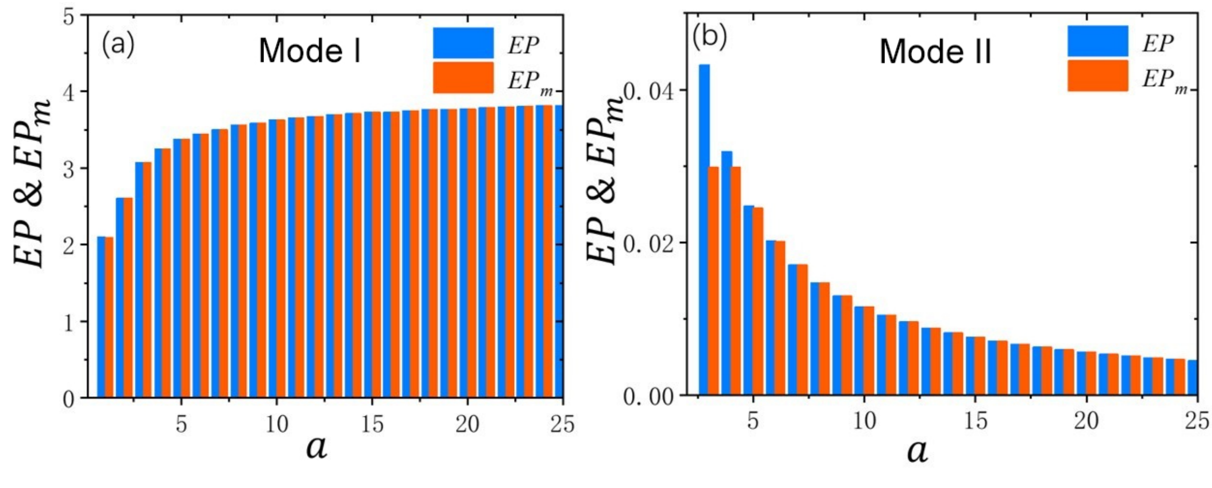

Figure S3. The comparisons between the total energy dissipation and the energy dissipation in the synthesis-degradation process of ROCK in Mode I and II. The values of all parameters are listed in Table I.

4 PARAMETERS TABLE

The values of the main parameters used in calculations are given in Table I. All these parameters have been normalized by the degradation rate of ROCK (i.e., k_4).

Table I: The values of parameters used in calculations

Parameters	Value
The reaction rate of positive control (k_1)	20
The reaction rate of negative control (k_2)	10
The synthetic rate of ROCK (k_3)	1.5 (Mode I) or 5 (Mode II)
The basic switch rate of gene to "on" state (k_{on})	2
The basic switching rate of gene to "off" state (k_{off})	2