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Noise-enhanced energy transduction of molecular machinery

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Abstract

We have numerically investigated the enhance effect of noise on the energy transduction of molecular machinery. The energy transduction is enhanced with the increase of relative amplitude of the limit-cycle oscillation in polymer chain. And noise can enlarge the relative amplitude through a mechanism of stochastic resonance (SR). In the simulation, two different types of SR, internal signal SR (ISSR) and explicit ISSR (EISSR) are studied, respectively. And the similarity as well as difference between them was presented. The potential application of the enhance effect of energy transduction is then discussed. © 2002 Elsevier Science B.V. All rights reserved.

1. Introduction

The constructive roles of random noise on various fields have been studied extensively in the last decade [1,2]. One important effect of them is stochastic resonance (SR) [3,4], a counter-intuitive phenomenon wherein noise with an appropriate level can optimize the response of a nonlinear system to a weak periodic signal. Since SR was put forward by Benzi et al. in the study of glacial period [5], it has been investigated widely on physical [6–8], chemical [9–15] and biological [16,17] systems theoretically and experimentally.

In many real chemical or biological systems, one should note that 'noise' does not means artificial agitation or error, but corresponds to thermal fluctuation. In earlier studies of SR, the occurrence of SR has three essential ingredients: nonlinear system, weak periodic signal and random noise. However, with the development of SR studies, some types of SR that do not have all three elements are found and investigated [18]. For example, internal signal SR (ISSR) has been found by investigating a two-dimensional autonomous system, which is in a state near a saddle-node bifurcation [19,20]. In recent research it was found that some chemical reaction systems show ISSR near a Hopf bifurcation [12]. Recently another attractive type of SR, explicit internal signal SR (EISSR), has been found when investigating the effect of parameter noise on the period-1 oscillation of a Belousov–Zhabotinsky (BZ) reaction system [21]. EISSR is thought to be having completely different mechanism with common ISSR, which is caused by the noise-induced coherent oscillation (NICO), while the occurrence of EISSR need to avoid crossing bifurcation.

Recently a working hypothesis on the mechanism of molecular machinery was proposed [22].

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And then an experiment trying to verify the hypothesis was made successfully [23]. It was mentioned that suitable nonequilibration in life generates a limit-cycle oscillation and that such a nonlinear oscillation is the essential process in energy transduction. It has recently been reported that it is the hydrolysis of ATP that drives the rotation of the ring-shaped sub-domain of ATP synthase [24]. Therefore, a uni-directional mechanical motion is generated with the dissipation of chemical energy in the molecular machinery. That is something like rowing, when we oar in one direction instead of two directions, the boat can move. And the more force we use in the direction, the faster the boat can move. Based on this consideration, it is reasonable that we can use the relative amplitude of the oscillation to stand for the efficiency of the process of energy transduction. Although the dynamics of proteins in energy transduction has been investigated extensively in the past years, very limited attention is paid to the effect of random extra stimulation. In the present Letter, we adopted this hypothesis to study the dynamics of a polymer chain without external signals. Our numerical simulation shows that a fluctuation at the environmental parameter in certain levels can enhance the oscillation in different circumstance, which means the more effective energy transduction. In this way noise plays a constructive role in the energy transduction process at the molecular chain level.

2. The model

The model used in the present Letter was previously proposed by Yoshikawa and Noguchi [22] to account for the dynamical behavior of a polymer chain with double minima in the free energy profile. Here we used it to study the effect of noise in the context of implicit and explicit internal signal SR.

The key property of this model is a first-order phase transition of single chains. The model can be described as

$$\xi \frac{d\alpha}{dt} = -4\alpha^3 + 12\alpha^2 - 10\alpha + \tau,$$

$$\frac{d\tau}{dt} = h - \tau\alpha^2, \qquad (1)$$

where ξ is a constant. τ is the reduced temperature in the chain, $\tau = \gamma(T - T_0)$; T and T_0 are the temperature of the chain and the environment, respectively, Y is a constant. h is the rate of energy input with dissipation proportional to the surface area S. It is noted here that h corresponds to the rate of the consumption of ATP molecules for the motor protein. Because h is a parameter that only have relation with environment, we choose it as the control parameter during simulation. α is a 'order parameter' derived from the free energy profile of the system

$$F/k_B T = r^2 + r^{-2} + B(1 - \theta/T)r^{-3} + Cr^{-6}, \qquad (2)$$

where B and C are the parameters related to the structure of the polymer. $r = R/R_c$ is the normalized size the chain, here R is the actual size and R_c is the size of the coil state, which is the longest size the chain can reach. θ is the temperature where the pair wise changes between repulsion and attraction. By simplifying Eq. (2) with α, the free energy can be written as

$$F = \alpha^4 - 4\alpha^3 + 5\alpha^2 - \tau\alpha \qquad (3)$$

and see [22] for details about this model.

This model has two stable Hopf bifurcation point at 1.0231 and 2.3691. When h is between 1.0231 and 2.3691, the system shows a limit-cycle oscillation. See Fig. 1a for the bifurcation diagram.

To study SR in the system we apply noise to the parameter h as

$$h = h_0[1 + \xi(t)], \qquad (4)$$

where h_0 is the constant value of h at stable steady state or first-period oscillation state, $\xi(t)$ is the Gaussian white noise with zero mean value $\langle\xi(t)\rangle = 0$ and autocorrelation function $\langle\xi(t_1)\xi(t_2)\rangle = \beta^2 \cdot \delta(t_1 - t_2)$, where β denotes the noise intensity. Eqs. (1) and (4) were integrated by a simple forward Eular algorithm with a fixed time step of 0.01 s. In each calculation the time evolution of the system lasted 10 000 s to guarantee the stable of the oscillation. To quantify noise-induced or noise-enhanced phenomena in the system, the time series of the 'order parameter' was analyzed by Fourier

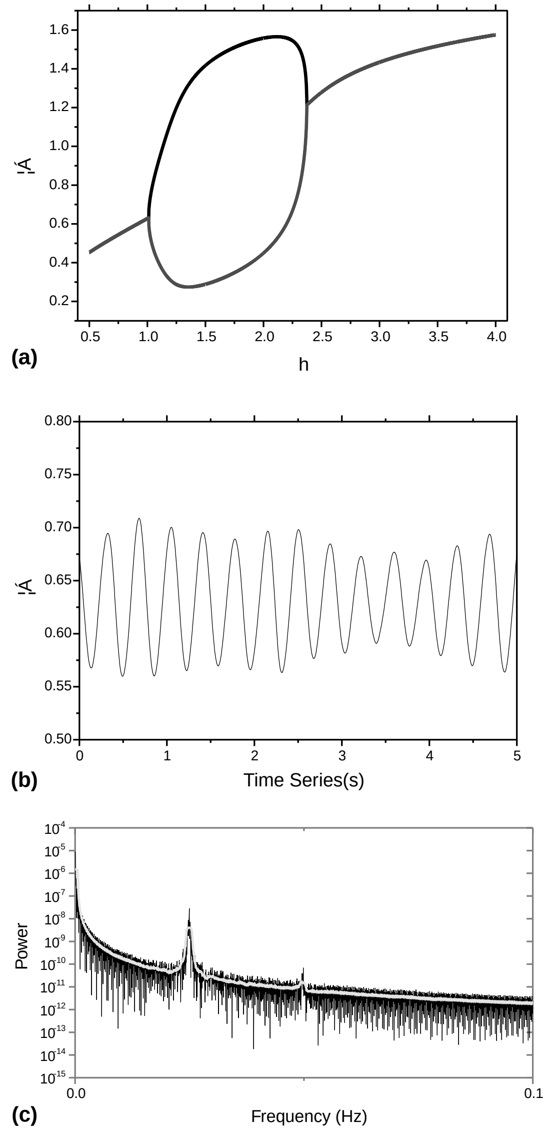

Fig. 1. (a) The bifurcation diagram of the model. (b) Noise-induced oscillation with $\beta = 0.05$ and a noise plus length of 0.15 s (c) The Fourier power spectrum of noise-enhanced oscillation of the parameter α. The noise length is 0.15 s.

power spectrum. We use signal-to-noise ratio (SNR) to quantify the relative amplitude of the oscillations. During the simulation, the value of the constant ξ is 1.0, and the initial value of α and τ are 0.6248 and 2.5254, respectively. The output power spectrum was averages over 20 steps for a smoother curve.

3. Results and discussion

In this Letter, we concentrate on two phenomena: ISSR and EISSR. They differ only by h_0, the mean value of energy input h. In the first part of this Letter, we set h_0 equal to 1.0106, which is in steady state near a Hopf bifurcation. In the second part, we let h_0 equal to 1.0232, which is in the period-1 oscillation. The oscillation properties of each part are studied.

3.1. Internal signal SR

When h_0 is in steady state near a Hopf bifurcation, the state is stable after long time. Noise, however, can induce stable limit-cycle oscillation. Fig. 1b shows such an oscillation. The system can enter deeper oscillatory region with larger noise intensity, which means the increment of the amplitude of stochastic oscillations (this is decided by the super criticality of the Hopf bifurcation point).

With this type of oscillation, we can calculate SNRs in the Fourier power spectrum. Fig. 1c shows a typical Fourier power spectrum in the simulation, where one can see that a clear peak appears. In the spectrum, we can see clearly that noise can induce intrinsic signal even without input signal. The SNR was calculated as the ratio of normalized peak height (to the noise background) to the relative width at half-maximum.

Fig. 2a shows the relationship between SNRs and noise intensity, one can see that with the increment of noise intensity the SNRs go through a peak, which indicates the occurrence of the SR. Because there is no input signal, it means the occurrence of ISSR.

3.2. Explicit internal signal SR

When h_0 is in the period-1 oscillation, the system shows oscillation even without any noise or signal. However, we can study the effect of noise in similar way. The Fourier power spectrum of this type of oscillation is also like that above. Fig. 2b shows the SNRs versus noise intensity, one can see that with the increment of noise intensity the SNRs also go through a peak. Since there is no

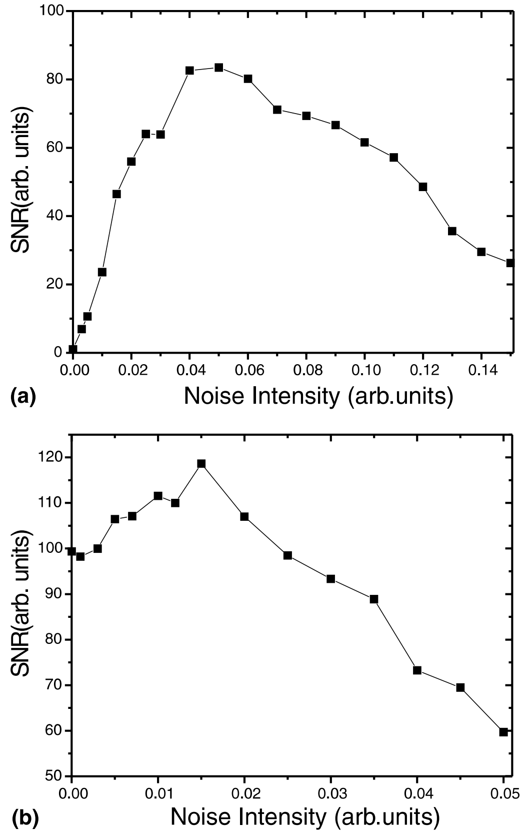

Fig. 2. (a) SNR as a function of noise intensity with $h_0 = 1.0106$ and noise length of 0.15 s. Solid line is drawn as a guide the eye. (b) SNR as a function of noise intensity with $h_0 = 1.0232$ and noise length of 0.15 s. Solid line is drawn to guide the eye.

input signal and the system is in the period-1 oscillation, it means the occurrence of EISSR.

In the present Letter, we have investigated the phenomena of ISSR and EISSR in a model of molecular machinery. When the system is located near the Hopf bifurcation, the fluctuation in the external energy input can induce the oscillation of the 'order parameter' that is related to the structure of the molecular machinery, which was proved to be a important process during energy transduction. More importantly, with the increment of the noise intensity, the strength of the noise-induced oscillation goes through a maximum, which implies that an optimal amount of noise can considerably enhance the efficiency of the energy transduction process. On the other hand, even when the system is already inside the oscillation region, a small amount of noise can still enhance the strength of the oscillation. Since the external fluctuations for molecular machinery are unavoidable, the system may be able to take advantages of these fluctuations through ISSR and EISSR. As energy transduction play an important role in many biological functions, how can we use the advantages to play functional roles in molecular machinery? Further theoretical and experimental work will be of great help to answer the question.

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