

Article ID: 1000-5641(2010)03-0134-08

On the fluctuation spectra with respect to complex functions of the three-state Markov processes

KUANG Neng-hui, CHEN Yong

(School of Mathematics and Computing Science, Hunan University of Science and Technology,
Xiangtan Hunan 411201, China)

Abstract: Explicit formulae for the autocorrelation functions and the fluctuation spectra with respect to complex functions of the irreducible three-state Markov processes were investigated. By the theory of cubic and quintic equations, the necessary and sufficient condition for the fluctuation spectra with respect to complex functions to be nonmonotonic on $[0, +\infty)$ was presented when there existed coinciding eigenvalues for the transition rate matrix, and the sufficient conditions for the fluctuation spectra with respect to complex functions to be nonmonotonic on $[0, +\infty)$ were given when there existed distinct nonzero eigenvalues.

Key words: power spectral density; autocorrelation function; nonequilibrium steady state; three-state Markov processes

CLC number: O211.62 **Document code:** A

关于三状态马氏过程的复函数的功率谱密度

匡能晖, 陈 勇

(湖南科技大学 数学与计算科学学院, 湖南湘潭 411201)

摘要: 得到了关于不可约的三状态马氏过程的复函数的自相关函数与功率谱密度的显式表达式. 由三次和五次方程理论得到: 当转移速率矩阵存在相同的特征值时, 给出复函数的功率谱密度在 $[0, +\infty)$ 上非单调的一个充要条件; 当转移速率矩阵存在不同的非零特征值时, 给出复函数的功率谱密度在 $[0, +\infty)$ 上非单调的一些充分条件.

关键词: 功率谱密度; 自相关函数; 非平衡稳定状态; 三状态马氏过程

0 Introduction

We address the simplest nonequilibrium problem — the three-state cyclic Markovian model (which can be traced back to the so-called Onsager triangle) with a generally violated detailed

收稿日期: 2009-09

基金项目: 湖南省教育厅资助科研项目(06C300)

第一作者: 匡能晖, 男, 讲师, 研究方向为随机过程及其应用. E-mail: knh@hnust.edu.cn.

balance. This basic model, apart from a fundamental significance, has numerous applications, in particular, in biophysics.

As indicated in Refs. [1–3], if a Markov process is reversible, then the fluctuation spectra are monotonic over $[0, +\infty)$. As pointed in Refs. [4–6], the irreversibility of the underlying Markov process is equivalent to the existence of some nonmonotonic fluctuation spectrum, and there exist irreversible processes such that the fluctuation spectra with respect to real functions are all monotonic. In some literatures (see, e. g., Ref. [7]), the steady distribution of a system driven by an irreversible Markov process is sometimes referred to as a nonequilibrium steady state (briefly, NESS).

In Ref. [8], explicit formulae for the autocorrelation functions and the fluctuation spectra with respect to real functions of the irreducible three-state Markov processes are investigated, and the necessary and sufficient conditions for the fluctuation spectra with respect to real functions to be nonmonotonic on $[0, +\infty)$ are given. In this paper, we discuss the similar problems but with respect to complex functions.

1 Main results

We adopt the same notations as Ref. [8]. Throughout this paper $\xi = \{\xi_t : t \in \mathbf{R}^+\}$ always denotes an irreducible three-state Markov process, with its stationary distribution written as $\mu = (\mu_1, \mu_2, \mu_3)$ and the transition rate matrix written as

$$\mathbf{Q} = \begin{bmatrix} -a_1 & a_2 & a_3 \\ b_1 & -b_2 & b_3 \\ c_1 & c_2 & -c_3 \end{bmatrix},$$

where $a_1 = a_2 + a_3$, $b_2 = b_1 + b_3$, $c_3 = c_1 + c_2$, $\mu_1 + \mu_2 + \mu_3 = 1$, $\mu_i > 0$, $a_i, b_i, c_i \geq 0$, $i = 1, 2, 3$, and $a_1 b_2 c_3, b_1 + c_1, a_2 + c_2, a_3 + b_3 > 0$ (i. e. irreducible). Let $\alpha = a_1 + b_2 + c_3$, $\beta = k_1 + k_2 + k_3$, where k_i is the algebraic cofactor of the (i, i) entry of the matrix \mathbf{Q} . Then the eigen-equation of \mathbf{Q} is $\lambda(\lambda^2 + \alpha\lambda + \beta) = 0$. Denote by $-\lambda_1, -\lambda_2$ the nonzero eigenvalues of \mathbf{Q} . Let $\Delta = \alpha^2 - 4\beta$.

For a complex function $Z(x) = \varphi(x) + \mathbf{i}\psi(x)$ on the state space $S = \{1, 2, 3\}$, where $\varphi(x)$ and $\psi(x)$ are real functions, $\mathbf{i} = \sqrt{-1}$. Denote the autocorrelation function and the fluctuation spectrum of $\{Z(\xi_t)\}$ by $B_Z(t)$, $S_Z(\omega)$ respectively, which are defined as

$$B_Z(t) = \mathbf{E} \left[(Z(\xi_t) - \mu(Z)) \overline{(Z(\xi_0) - \mu(Z))} \right], \text{ if } t \in \mathbf{R}^+,$$

$$B_Z(t) = \overline{B_Z(-t)}, \text{ if } t \in \mathbf{R}^-, \quad S_Z(\omega) = \frac{1}{2\pi} \int e^{-i\omega t} B_Z(t) dt,$$

where \mathbf{E} is the expectation operator with respect to $\{\xi_t\}$, $\mu(Z) = \mathbf{E}[Z(\xi_t)]$ independent of time t because of stationarity, $\overline{Z(x)}$ denotes the conjugation of $Z(x)$.

Let $Z(1) = \varphi(1) + \mathbf{i}\psi(1)$, $Z(2) = \varphi(2) + \mathbf{i}\psi(2)$, $Z(3) = \varphi(3) + \mathbf{i}\psi(3)$, and denote $Z(i)$, $\varphi(i)$, $\psi(i)$ by Z_i , φ_i , ψ_i respectively, $i = 1, 2, 3$, and $y_i = Z_i - Z_{i+1}$, ($Z_4 = Z_1$), $i = 1, 2, 3$. Let

$$\gamma = \frac{\mu_1 a_2 + \mu_2 b_1}{2}, \delta = \frac{\mu_2 b_3 + \mu_3 c_2}{2}, \kappa = \frac{\mu_3 c_1 + \mu_1 a_3}{2}.$$

$$s = (\varphi_1\psi_2 - \varphi_2\psi_1) + (\varphi_2\psi_3 - \varphi_3\psi_2) + (\varphi_3\psi_1 - \varphi_1\psi_3).$$

Denote $E = \gamma|y_1|^2 + \delta|y_2|^2 + \kappa|y_3|^2$, $F = \mu_1\mu_2|y_1|^2 + \mu_2\mu_3|y_2|^2 + \mu_3\mu_1|y_3|^2$. By the stationarity, it is clear that the probability flux is

$$\mu_1a_2 - \mu_2b_1 = \mu_2b_3 - \mu_3c_2 = \mu_3c_1 - \mu_1a_3.$$

Let $\nu = \frac{\mu_1a_2 - \mu_2b_1}{2}$. The main results of this paper are the following.

Theorem 1 When $t \geq 0$, the autocorrelation function of $\{Z(\xi_t)\}$ belongs to one of the following three cases.

(1) If $\Delta \neq 0$, then

$$B_Z(t) = \frac{E - (2\nu s)\mathbf{i} - F\lambda_2}{\lambda_1 - \lambda_2} \exp(-\lambda_1 t) + \frac{E - (2\nu s)\mathbf{i} - F\lambda_1}{\lambda_2 - \lambda_1} \exp(-\lambda_2 t);$$

(2) If $\Delta = 0$ and the process $\{\xi_t\}$ is irreversible, then

$$B_Z(t) = F \exp(-\lambda_1 t) - [E - (2\nu s)\mathbf{i} - F\lambda_1]t \exp(-\lambda_1 t);$$

(3) If $\Delta = 0$ and the process $\{\xi_t\}$ is reversible, then

$$B_Z(t) = F \exp(-\lambda_1 t).$$

Theorem 2 The fluctuation spectrum of $\{Z(\xi_t)\}$ belongs to one of the following three cases.

(1) If $\Delta \neq 0$, then

$$S_Z(\omega) = \frac{1}{\pi} \frac{\omega^2 E + (2\alpha\nu s)\omega + \beta(\alpha F - E)}{\omega^4 + (\alpha^2 - 2\beta)\omega^2 + \beta^2};$$

(2) If $\Delta = 0$ and the process $\{\xi_t\}$ is irreversible, then

$$S_Z(\omega) = \frac{1}{\pi} \frac{\omega^2 E + (2\alpha\nu s)\omega + \beta(\alpha F - E)}{(\omega^2 + \beta)^2};$$

(3) If $\Delta = 0$ and the process $\{\xi_t\}$ is reversible, then

$$S_Z(\omega) = \frac{F}{\pi} \frac{2\alpha}{4\omega^2 + \alpha^2}.$$

When $\Delta = 0$ and the process $\{\xi_t\}$ is reversible, due to $\alpha > 0, F \geq 0$, hence $S_Z(\omega)$ is decreasing on $[0, +\infty)$, which means that the fluctuation spectra of $\{Z(\xi_t)\}$ are monotonic on $[0, +\infty)$ for any complex function $Z(x)$.

When $\Delta = 0$ and the process $\{\xi_t\}$ is irreversible, we obtain the following conclusion.

Theorem 3 If $\Delta = 0$ and the process $\{\xi_t\}$ is irreversible, then the fluctuation spectrum of $\{Z(\xi_t)\}$ is nonmonotonic on $[0, +\infty)$ if and only if

- (1) $\nu s > 0$; or
- (2) $\nu s = 0, 2\alpha F - 3E < 0$; or
- (3) $\nu s < 0, \Delta_2 \geq 0$, and $A \leq 0$,

where $\Delta_2 = 3\alpha^2\nu^2s^2 - \beta E(2\alpha F - 3E)$,

$$A = 9\alpha^3\nu^3s^3 - (9\alpha\beta\nu s)E(\alpha F - E) - \sqrt{3[3\alpha^2\nu^2s^2 - \beta E(2\alpha F - 3E)]^3}.$$

When $\Delta \neq 0$, we obtain the following result.

Theorem 4 If $\Delta \neq 0$, and if one of the following conditions holds

- (1) $\nu s > 0$;
- (2) $\nu s = 0$, $\beta E - (\alpha^2 - 2\beta)(\alpha F - E) > 0$;
- (3) $\nu s = 0$, $\beta E - (\alpha^2 - 2\beta)(\alpha F - E) = 0$, $\alpha F - E < 0$,

then the fluctuation spectrum of $\{Z(\xi_t)\}$ is nonmonotonic on $[0, +\infty)$.

Remark 1 When $\Delta \neq 0$, the numerator of $S'_Z(\omega)$ is a quintic function, so it is complicated to find the necessary and sufficient condition of existing at least a positive real solution for $S'_Z(\omega) = 0$.

2 Proofs of the theorems

Lemma 1 The unique stationary distribution (i. e. invariant probability distribution, limiting probabilities) of the process is $\mu_i = k_i/\beta, i = 1, 2, 3$.

The proof is given in many Refs. [7, 9, 10] and is omitted here.

Denote by $\{P(t), t \geq 0\}$ the transition probability matrix. Its (i, j) entry is written as $P_{ij}(t)$.

Lemma 2 If $\Delta \neq 0$, then

$$\begin{aligned} P_{11}(t) &= \mu_1 + \frac{1}{\lambda_1 - \lambda_2} [(a_1 - \mu_2\lambda_2 - \mu_3\lambda_2) \exp(-\lambda_1 t) - (a_1 - \mu_2\lambda_1 - \mu_3\lambda_1) \exp(-\lambda_2 t)], \\ P_{12}(t) &= \mu_2 + \frac{1}{\lambda_1 - \lambda_2} [(-a_2 + \mu_2\lambda_2) \exp(-\lambda_1 t) - (-a_2 + \mu_2\lambda_1) \exp(-\lambda_2 t)], \\ P_{13}(t) &= \mu_3 + \frac{1}{\lambda_1 - \lambda_2} [(-a_3 + \mu_3\lambda_2) \exp(-\lambda_1 t) - (-a_3 + \mu_3\lambda_1) \exp(-\lambda_2 t)], \\ P_{21}(t) &= \mu_1 + \frac{1}{\lambda_1 - \lambda_2} [(-b_1 + \mu_1\lambda_2) \exp(-\lambda_1 t) - (-b_1 + \mu_1\lambda_1) \exp(-\lambda_2 t)], \\ P_{22}(t) &= \mu_2 + \frac{1}{\lambda_1 - \lambda_2} [(b_2 - \mu_1\lambda_2 - \mu_3\lambda_2) \exp(-\lambda_1 t) - (b_2 - \mu_1\lambda_1 - \mu_3\lambda_1) \exp(-\lambda_2 t)], \\ P_{23}(t) &= \mu_3 + \frac{1}{\lambda_1 - \lambda_2} [(-b_3 + \mu_3\lambda_2) \exp(-\lambda_1 t) - (-b_3 + \mu_3\lambda_1) \exp(-\lambda_2 t)], \\ P_{31}(t) &= \mu_1 + \frac{1}{\lambda_1 - \lambda_2} [(-c_1 + \mu_1\lambda_2) \exp(-\lambda_1 t) - (-c_1 + \mu_1\lambda_1) \exp(-\lambda_2 t)], \\ P_{32}(t) &= \mu_2 + \frac{1}{\lambda_1 - \lambda_2} [(-c_2 + \mu_2\lambda_2) \exp(-\lambda_1 t) - (-c_2 + \mu_2\lambda_1) \exp(-\lambda_2 t)], \\ P_{33}(t) &= \mu_3 + \frac{1}{\lambda_1 - \lambda_2} [(c_3 - \mu_1\lambda_2 - \mu_2\lambda_2) \exp(-\lambda_1 t) - (c_3 - \mu_1\lambda_1 - \mu_2\lambda_1) \exp(-\lambda_2 t)], \end{aligned}$$

where $-\lambda_1, -\lambda_2$ are the nonzero eigenvalues of the transition rate matrix \mathbf{Q} .

Lemma 3 If $\Delta = 0$ and the process $\{\xi_t\}$ is irreversible, then

$$P_{11}(t) = \mu_1 + [(\mu_2 + \mu_3)(1 + \lambda t) - a_1 t] \exp(-\lambda t),$$

$$\begin{aligned}
P_{12}(t) &= \mu_2 + [-\mu_2(1 + \lambda t) + a_2 t] \exp(-\lambda t), \\
P_{13}(t) &= \mu_3 + [-\mu_3(1 + \lambda t) + a_3 t] \exp(-\lambda t), \\
P_{21}(t) &= \mu_1 + [-\mu_1(1 + \lambda t) + b_1 t] \exp(-\lambda t), \\
P_{22}(t) &= \mu_2 + [(\mu_1 + \mu_3)(1 + \lambda t) - b_2 t] \exp(-\lambda t), \\
P_{23}(t) &= \mu_3 + [-\mu_3(1 + \lambda t) + b_3 t] \exp(-\lambda t), \\
P_{31}(t) &= \mu_1 + [-\mu_1(1 + \lambda t) + c_1 t] \exp(-\lambda t), \\
P_{32}(t) &= \mu_2 + [-\mu_2(1 + \lambda t) + c_2 t] \exp(-\lambda t), \\
P_{33}(t) &= \mu_3 + [(\mu_1 + \mu_2)(1 + \lambda t) - c_3 t] \exp(-\lambda t).
\end{aligned}$$

Lemma 4 If $\Delta = 0$ and the process $\{\xi_t\}$ is reversible, then

$$\mathbf{Q} = \begin{bmatrix} -(x+y) & x & y \\ z & -(y+z) & y \\ z & x & -(z+x) \end{bmatrix}.$$

In addition, the converse is also true.

Proofs of Lemma 2, Lemma 3 and Lemma 4 are given in Ref. [8] and are omitted here.

Denote the cubic function $f(x) = ax^3 + bx^2 + cx + d$ with $a \neq 0$, then $f'(x) = 3ax^2 + 2bx + c$. Let $\Delta'_2 = 4(b^2 - 3ac)$. When $\Delta'_2 \geq 0$, there exist two real numbers $x_1 = \frac{-b - \sqrt{b^2 - 3ac}}{3a}$, $x_2 = \frac{-b + \sqrt{b^2 - 3ac}}{3a}$, such that $x_1 \leq x_2$ and $f'(x_i) = 0$, ($i = 1, 2$). Clearly, one has

$$f(x_2) = \frac{2b^3 + 27a^2d - 9abc - 2\sqrt{(b^2 - 3ac)^3}}{27a^2}.$$

Denote $f(x_2)$ by A' . It is not hard to show the following Lemmas.

Lemma 5 For the cubic function $f(x) = ax^3 + bx^2 + cx + d$, ($a > 0$), there exists at least $x_0 > 0$ such that $f(x_0) = 0$, if and only if

- (1) $d < 0$; or
- (2) $d = 0$, $\Delta'_3 \geq 0$ and $\sqrt{\Delta'_3} > b$; or
- (3) $d > 0$, $\Delta'_2 \geq 0$, $A' \leq 0$ and $\sqrt{\Delta'_2} > 2b$,

where $\Delta'_3 = b^2 - 4ac$.

Lemma 6 For the quintic function $g(x) = a_5x^5 + a_4x^4 + a_3x^3 + a_2x^2 + a_1x + a_0$, ($a_5 > 0$), the sufficient conditions of existing positive real roots for $g(x)$ are one of the following five conditions holds.

- (1) $a_0 < 0$;
- (2) $a_0 = 0$, $a_1 < 0$;
- (3) $a_0 = 0$, $a_1 = 0$, $a_2 < 0$;
- (4) $a_0 = 0$, $a_1 = 0$, $a_2 = 0$, $\Delta'_4 \geq 0$ and $\sqrt{\Delta'_4} > a_4$;
- (5) $a_0 = 0$, $a_1 = 0$, $a_2 > 0$, $\Delta'_5 \geq 0$, $B' \leq 0$ and $\sqrt{\Delta'_5} > 2a_4$,

where $\Delta'_4 = a_4^2 - 4a_5a_3$, $\Delta'_5 = 4(a_4^2 - 3a_5a_3)$, $B' = \frac{2a_4^3 + 27a_5^2a_2 - 9a_5a_4a_3 - 2\sqrt{(a_4^2 - 3a_5a_3)^3}}{27a_5^2}$.

Proof of Theorem 1 We only prove the first part. The others can be shown similarly by Lemma 3 and Lemma 4, respectively. When $t \geq 0$, by the definition of autocorrelation,

$$B_Z(t) = \mathbf{E}[(Z(\xi_t) - \mu(Z))\overline{(Z(\xi_0) - \mu(Z))}] = \sum_{i,j=1}^3 \mu_i \overline{Z_i} P_{ij}(t) Z_j - \left| \sum_{i=1}^3 \mu_i Z_i \right|^2.$$

In $B_Z(t)$, by Lemma 2, the coefficient of $\frac{1}{\lambda_1 - \lambda_2} \exp\{-\lambda_1 t\}$ is

$$\begin{aligned} & \mu_1 \overline{Z_1} (a_1 - \mu_2 \lambda_2 - \mu_3 \lambda_2) Z_1 + \mu_1 \overline{Z_1} (-a_2 + \mu_2 \lambda_2) Z_2 + \mu_1 \overline{Z_1} (-a_3 + \mu_3 \lambda_2) Z_3 \\ & + \mu_2 \overline{Z_2} (-b_1 + \mu_1 \lambda_2) Z_1 + \mu_2 \overline{Z_2} (b_2 - \mu_1 \lambda_2 - \mu_3 \lambda_2) Z_2 + \mu_2 \overline{Z_2} (-b_3 + \mu_3 \lambda_2) Z_3 \\ & + \mu_3 \overline{Z_3} (-c_1 + \mu_1 \lambda_2) Z_1 + \mu_3 \overline{Z_3} (-c_2 + \mu_2 \lambda_2) Z_2 + \mu_3 \overline{Z_3} (c_3 - \mu_1 \lambda_2 - \mu_2 \lambda_2) Z_3 \\ & = \mu_1 (a_1 - \mu_2 \lambda_2 - \mu_3 \lambda_2) (\varphi_1^2 + \psi_1^2) + \mu_2 (b_2 - \mu_1 \lambda_2 - \mu_3 \lambda_2) (\varphi_2^2 + \psi_2^2) \\ & + \mu_3 (c_3 - \mu_1 \lambda_2 - \mu_2 \lambda_2) (\varphi_3^2 + \psi_3^2) \\ & + (\varphi_1 \varphi_2 + \psi_1 \psi_2) (-2\gamma + 2\mu_1 \mu_2 \lambda_2) - 2\nu (\varphi_1 \psi_2 - \varphi_2 \psi_1) \mathbf{i} \\ & + (\varphi_2 \varphi_3 + \psi_2 \psi_3) (-2\delta + 2\mu_2 \mu_3 \lambda_2) - 2\nu (\varphi_2 \psi_3 - \varphi_3 \psi_2) \mathbf{i} \\ & + (\varphi_3 \varphi_1 + \psi_3 \psi_1) (-2\kappa + 2\mu_3 \mu_1 \lambda_2) - 2\nu (\varphi_3 \psi_1 - \varphi_1 \psi_3) \mathbf{i}. \end{aligned}$$

In the above expression, the coefficient of λ_2 is

$$\begin{aligned} & -\mu_1 (\mu_2 + \mu_3) (\varphi_1^2 + \psi_1^2) - \mu_2 (\mu_1 + \mu_3) (\varphi_2^2 + \psi_2^2) - \mu_3 (\mu_1 + \mu_2) (\varphi_3^2 + \psi_3^2) \\ & + 2\mu_1 \mu_2 (\varphi_1 \varphi_2 + \psi_1 \psi_2) + 2\mu_2 \mu_3 (\varphi_2 \varphi_3 + \psi_2 \psi_3) + 2\mu_3 \mu_1 (\varphi_3 \varphi_1 + \psi_3 \psi_1) \\ & = -\mu_1 \mu_2 [(\varphi_1 - \varphi_2)^2 + (\psi_1 - \psi_2)^2] - \mu_2 \mu_3 [(\varphi_2 - \varphi_3)^2 + (\psi_2 - \psi_3)^2] \\ & - \mu_3 \mu_1 [(\varphi_3 - \varphi_1)^2 + (\psi_3 - \psi_1)^2] = -\mu_1 \mu_2 |y_1|^2 - \mu_2 \mu_3 |y_2|^2 - \mu_3 \mu_1 |y_3|^2 = -F; \end{aligned}$$

the constant term is

$$\begin{aligned} & \mu_1 a_1 (\varphi_1^2 + \psi_1^2) + \mu_2 b_2 (\varphi_2^2 + \psi_2^2) + \mu_3 c_3 (\varphi_3^2 + \psi_3^2) \\ & - 2\gamma (\varphi_1 \varphi_2 + \psi_1 \psi_2) - 2\delta (\varphi_2 \varphi_3 + \psi_2 \psi_3) - 2\kappa (\varphi_3 \varphi_1 + \psi_3 \psi_1) \\ & - 2\nu [(\varphi_1 \psi_2 - \varphi_2 \psi_1) + (\varphi_2 \psi_3 - \varphi_3 \psi_2) + (\varphi_3 \psi_1 - \varphi_1 \psi_3)] \mathbf{i} \\ & = (\gamma + \kappa) (\varphi_1^2 + \psi_1^2) + (\delta + \gamma) (\varphi_2^2 + \psi_2^2) + (\kappa + \delta) (\varphi_3^2 + \psi_3^2) \\ & - 2\gamma (\varphi_1 \varphi_2 + \psi_1 \psi_2) - 2\delta (\varphi_2 \varphi_3 + \psi_2 \psi_3) - 2\kappa (\varphi_3 \varphi_1 + \psi_3 \psi_1) - (2\nu s) \mathbf{i} \\ & = \gamma [(\varphi_1 - \varphi_2)^2 + (\psi_1 - \psi_2)^2] + \delta [(\varphi_2 - \varphi_3)^2 + (\psi_2 - \psi_3)^2] \\ & + \kappa [(\varphi_3 - \varphi_1)^2 + (\psi_3 - \psi_1)^2] - (2\nu s) \mathbf{i} \\ & = \gamma |y_1|^2 + \delta |y_2|^2 + \kappa |y_3|^2 - (2\nu s) \mathbf{i} = E - (2\nu s) \mathbf{i}. \end{aligned}$$

Thus the coefficient of $\frac{1}{\lambda_1 - \lambda_2} \exp\{-\lambda_1 t\}$ is $E - (2\nu s) \mathbf{i} - F \lambda_2$, and similarly the coefficient of $\frac{1}{\lambda_2 - \lambda_1} \exp\{-\lambda_2 t\}$ is $E - (2\nu s) \mathbf{i} - F \lambda_1$. This ends the proof.

Proof of Theorem 2 We only prove the first case, and the others can be shown similarly by (2) and (3) of Theorem 1. In fact we only prove the case $\Delta < 0$. When $\Delta > 0$, the proof is similar. Without loss of generality, let $-\lambda_1 = -p + \mathbf{i}q$ and $-\lambda_2 = -p - \mathbf{i}q$ be a pair of conjugate

complex eigenvalues of the matrix \mathbf{Q} . By the definition of fluctuation spectrum,

$$S_Z(\omega) = \frac{1}{2\pi} \left[\int_0^{+\infty} \exp\{-i\omega t\} B_Z(t) dt + \int_{-\infty}^0 \exp\{-i\omega t\} B_Z(t) dt \right] = \frac{1}{2\pi} (I_1 + I_2),$$

where

$$\begin{aligned} I_1 &= \int_0^{+\infty} \exp\{-i\omega t\} B_Z(t) dt \\ &= \int_0^{+\infty} \exp\{-i\omega t\} \left[\frac{E - (2\nu s)\mathbf{i} - F\lambda_2}{\lambda_1 - \lambda_2} \exp(-\lambda_1 t) + \frac{E - (2\nu s)\mathbf{i} - F\lambda_1}{\lambda_2 - \lambda_1} \exp(-\lambda_2 t) \right] dt \\ &= \frac{E - (2\nu s)\mathbf{i} + F(-p - \mathbf{i}q)}{-2\mathbf{i}q} \int_0^{+\infty} \exp\{-i(\omega - q)t\} \exp\{-pt\} dt \\ &\quad + \frac{E - (2\nu s)\mathbf{i} + F(-p + \mathbf{i}q)}{2\mathbf{i}q} \int_0^{+\infty} \exp\{-i(\omega + q)t\} \exp\{-pt\} dt \\ &= \frac{E - (2\nu s)\mathbf{i} + F(-p - \mathbf{i}q)}{-2\mathbf{i}q} \cdot \frac{p - (\omega - q)\mathbf{i}}{(\omega - q)^2 + p^2} + \frac{E - (2\nu s)\mathbf{i} + F(-p + \mathbf{i}q)}{2\mathbf{i}q} \cdot \frac{p + (\omega + q)\mathbf{i}}{(\omega + q)^2 + p^2}, \end{aligned}$$

similarly,

$$\begin{aligned} I_2 &= \int_{-\infty}^0 \exp\{-i\omega t\} B_Z(t) dt \\ &= \int_0^{+\infty} \exp\{\mathbf{i}\omega t\} \left[\frac{E + (2\nu s)\mathbf{i} - F\bar{\lambda}_2}{\bar{\lambda}_1 - \bar{\lambda}_2} \exp(-\bar{\lambda}_1 t) + \frac{E + (2\nu s)\mathbf{i} - F\bar{\lambda}_1}{\bar{\lambda}_2 - \bar{\lambda}_1} \exp(-\bar{\lambda}_2 t) \right] dt \\ &= \frac{E + (2\nu s)\mathbf{i} + F(-p + \mathbf{i}q)}{2\mathbf{i}q} \cdot \frac{p + (\omega - q)\mathbf{i}}{(\omega - q)^2 + p^2} + \frac{E + (2\nu s)\mathbf{i} + F(-p - \mathbf{i}q)}{-2\mathbf{i}q} \cdot \frac{p + (\omega + q)\mathbf{i}}{(\omega + q)^2 + p^2}. \end{aligned}$$

Note that $p^2 + q^2 = \beta$, $p = \frac{\alpha}{2}$, we obtain

$$S_Z(\omega) = \frac{1}{\pi} \frac{\omega^2 E + (2\alpha\nu s)\omega + \beta(\alpha F - E)}{\omega^4 + (\alpha^2 - 2\beta)\omega^2 + \beta^2}.$$

This ends the proof.

Proof of Theorem 3 Since

$$S'_Z(\omega) = -\frac{2[E\omega^3 + (3\alpha\nu s)\omega^2 + \beta(2\alpha F - 3E)\omega - (\alpha\beta\nu s)]}{\pi(\omega^2 + \beta)^3},$$

it can be shown directly by Lemma 5.

Proof of Theorem 4 Since

$$\begin{aligned} S'_Z(\omega) &= -\frac{2}{\pi[\omega^4 + (\alpha^2 - 2\beta)\omega^2 + \beta^2]^2} \{E\omega^5 + (3\alpha\nu s)\omega^4 + 2\beta(\alpha F - E)\omega^3 \\ &\quad + (\alpha\nu s)(\alpha^2 - 2\beta)\omega^2 - \beta[\beta E - (\alpha^2 - 2\beta)(\alpha F - E)]\omega - (\alpha\nu s\beta^2)\}, \end{aligned}$$

it can be also shown directly by Lemma 6.

3 Applications

Example 1

$$\mathbf{Q} = \begin{bmatrix} -4a & 4a & 0 \\ 0 & -a & a \\ a & 0 & -a \end{bmatrix}, \quad (a > 0).$$

Clearly, $\Delta = 0$ and the process $\{\xi_t\}$ is irreversible. For the complex function $Z(1) = 1 + \mathbf{i}$, $Z(2) = -1 - \mathbf{i}$, $Z(3) = 1 - \mathbf{i}$, it is easy to show $\nu s > 0$. By Theorem 3, the fluctuation spectrum with respect to the above complex function is nonmonotonic on $[0, +\infty)$. However, the fluctuation spectrum with respect to the complex function $Z(1) = 1 - \mathbf{i}$, $Z(2) = -1 - \mathbf{i}$, $Z(3) = 1 + \mathbf{i}$, is monotonic on $[0, +\infty)$, since $\nu s < 0$, $\Delta_2 < 0$.

Example 2

$$\mathbf{Q} = \begin{bmatrix} -2a & a & a \\ a & -3a & 2a \\ 2a & 2a & -4a \end{bmatrix}, \quad (a > 0).$$

Clearly, $\Delta \neq 0$. For the complex function $Z(1) = 1 + \mathbf{i}$, $Z(2) = -1 - \mathbf{i}$, $Z(3) = 1 - \mathbf{i}$, it is easy to show $\nu s > 0$. By Theorem 4, the fluctuation spectrum with respect to the above complex function is nonmonotonic on $[0, +\infty)$.

Acknowledgements The authors are grateful to the anonymous referees for their helpful comments and for pointing out several mistakes, which helped considerably in improving the final form of this paper.

[References]

- [1] VANKAMPEN N G. Stochastic Processes in Physics and Chemistry[M]. New York: North-Holland Publishing Co,1992.
- [2] QIAN M, QIAN M P, ZHANG X J. Fundamental facts concerning reversible master equations[J]. Phys Lett A 2003, 309: 371-376.
- [3] JIANG D Q, ZHANG F X. The Green-Kubo formula and power spectrum of reversible Markov processes[J]. J Math Phys, 2003, 44: 4681-4689.
- [4] CHEN Y, CHEN X, QIAN M P. The Green-Kubo formula, autocorrelation function and fluctuation spectrum for finite Markov chains with continuous time[J]. J Phys, A: Math Gen, 2006, 39: 2539-2550.
- [5] CHEN Y, QIAN M P, XIE J S. On characterization of reversible Markov processes by monotonicity of the fluctuation spectral density[J]. J Math Phys, 2006, 47: 103301-103309.
- [6] CHEN Y, QIAN M P, XIE J S. Irreversibility Implies the Occurrence of Non-monotonic Power Spectra[J]. J Math Phys, 2007, 48: 073301-073313.
- [7] JIANG D Q, QIAN M, QIAN M P. Mathematical Theory of Nonequilibrium Steady States[M]. Berlin: Springer, 2004.
- [8] CHEN Y. On the monotonicity of fluctuation spectra for three-state Markov processes[J]. Fluctuation and Noise Lett, 2007, 7(3): 181-192.
- [9] ROSS S M. Introduction to Probability Models[M]. Amsterdam: Academic Press, 2007.
- [10] CHIANG C L. An Introduction to Stochastic Processes and Their Applications[M]. Huntington, N Y: Robert E Krieger Publishing Co, 1980.