Equilibrium and nonequilibrium states in thermostated Gledzer-Ohkitani-Yamada shell models

Hidetsugu Sakaguchi
Department of Applied Science for Electronics and Materials, Interdisciplinary Graduate School of Engineering Sciences, Kyushu University, Kasuga, Fukuoka 816-8580, Japan
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We study Gledzer-Ohkitani-Yamada shell models with heat reservoirs. Time-reversible Nosé-Hoover dynamics are used for the heat reservoirs. Both equilibrium and nonequilibrium cascade states are obtained by changing the heat reservoirs.

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Gledzer-Ohkitani-Yamada (GOY) shell models were proposed as simple dynamical models of the energy cascade in well-developed turbulence [1,2]. The models have been studied to understand the intermittency and multifractal behaviors of energy dissipation [3–6]. A GOY shell model has the form

$$\left(\frac{d}{dt}+\nu k_i^2\right)u_i=i(a_ik_iu_{i+1}^*u_{i+2}^*+b_ik_{i-1}u_{i-1}^*u_{i+1}^*+c_ik_{i-2}u_{i-1}^*u_{i-2}^*)+f\delta_{i,4}, \tag{1}$$

where $i=1,\ldots,N, k_i=k_02^i$, f is an external forcing, and ν is the viscosity. The boundary conditions are $b_1=b_N=c_1=c_2=a_{N-1}=a_N=0$. The coefficients of the nonlinear terms must satisfy

$$a_i+b_{i+1}+c_{i+2}=0$$

in order to satisfy the conservation of energy $\Sigma_i|u_i|^2$ when $f=\nu=0$. If $a_i=1, b_i=2b$, and $c_i=4c$ are assumed, Eq. (1) becomes

$$\left(\frac{d}{dt}+\nu k_i^2\right)u_i=ik_i(u_{i+1}^*u_{i+2}^*+bu_{i-1}^*u_{i+1}^*+cu_{i-1}^*u_{i-2}^*)+f\delta_{i,4}, \tag{2}$$

where the parameters b and c are chosen as $b=-\delta/2$ and $c=-(1-\delta)/4$ owing to the conservation of energy, and δ is a parameter that changes the interaction among the neighboring shells.

On the other hand, Nosé-Hoover dynamical systems have been studied to understand nonequilibrium states from the viewpoint of chaotic dynamical systems [7,8]. Lepri, Livi, and Politi studied heat transport in the Fermi-Past-Ulam chain with time-reversible thermostats [9].

The GOY shell model has the form of a chain with a nonlinear interaction and the energy is transported as a forward cascade. We study a GOY shell model with time-reversible thermostats to study the equilibrium and nonequilibrium states from the viewpoint of chaotic dynamical systems. The model equation is

$$\frac{du_i}{dt}=ik_i(u_{i+1}^*u_{i+2}^*+bu_{i-1}^*u_{i+1}^*+cu_{i-1}^*u_{i-2}^*),$$

for

$$i=n+1,\ldots,N-n \tag{3}$$

and

$$\frac{du_i}{dt}=ik_i(u_{i+1}^*u_{i+2}^*+bu_{i-1}^*u_{i+1}^*+cu_{i-1}^*u_{i-2}^*)-z_iu_i,$$

$$\frac{dz_i}{dt}=dk_i(|u_i|^2-T_i)\quad \text{for}\quad i=1,\ldots,n \quad\text{and}\quad N-n+1,\ldots,N, \tag{4}$$

where the z_i's are the thermal variables, T_i's are variables that can be interpreted as the temperature of the ith shell, and d expresses the response time. The first n shells and the last n shells interact with heat reservoirs. The equations for the intermediate shells have neither external forcing terms nor energy dissipation terms. The equations of motion have time-reversal symmetry with respect to $t\to -t, u_i\to -u_i, z_i\to -z_i$. The entropy production rate is the summation of z_i. If the temperature T_i of all the heat reservoirs is T, the Maxwell distribution

$$P(u,z)\propto \exp\left(-\sum_i |u_i|^2/T\right)\exp\left(-\sum_i (z_i^2/dk_iT)\right) \tag{5}$$

is a stationary distribution for time evolution by Eqs. (3) and (4), since

$$\sum_i \frac{\partial}{\partial u_i}(\dot{u}_iP)+\sum_i \frac{\partial}{\partial u_i^*}(\dot{u}_i^*P)+\sum_i \frac{\partial}{\partial z_i}(\dot{z}_iP)=0, \tag{6}$$

where the overdot denotes the time derivative. We have performed a numerical simulation to find a statistically stationary state of the thermostated GOY model. Figure 1 is the result of a numerical simulation for $N=16$, $\delta=0.05$, $k_0=2^{-4}$, $n=3$, $T=0.01$, and $d=20$. We have assumed that the first and last three shells interact with heat reservoirs in order to reduce the influence of the period-3 structure for the GOY shell model. Figure 1(a) displays the plot of the averaged energy $\langle|u_i|^2\rangle$ for each shell vs $\ln(k_i)=\ln(k_02^i)$. The dashed line denotes $\langle|u_i|^2\rangle=T$. Equipartition of energy is approximately attained. Figure 1(b) displays a semilogarithmic plot of the numerically obtained histogram $P(|u_i|^2)$ for $i=10$ and it is compared with the Gaussian distribution $P(|u_i|^2)=\exp(-|u_i|^2/T)/T$. This numerical result shows that

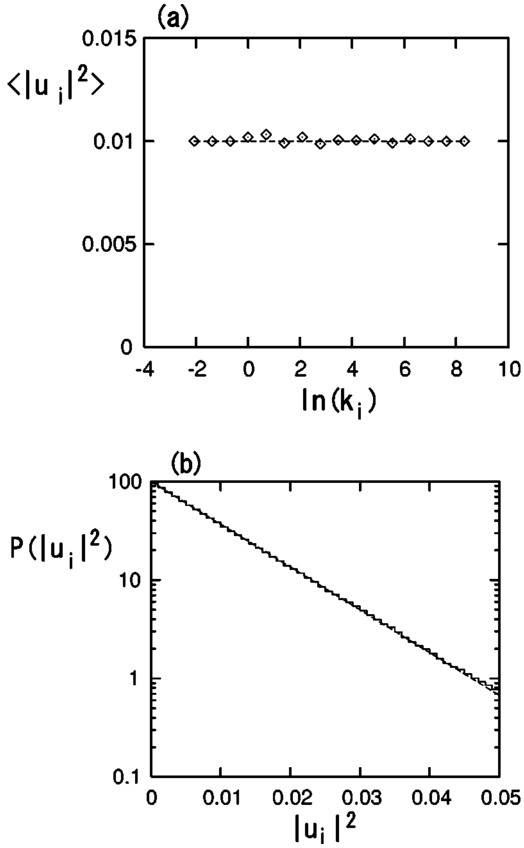

FIG. 1. (a) Averaged energy $\langle |u_i|^2\rangle$ vs $\ln(k_i)$ for Eqs.(3) and (4) with $N=16,\delta=0.05,n=3,T_i=0.01$, and $d=20$. (b) Semilogarithmic plot of the histogram $P(|u_i|^2)$ for $i=10$ and the Gaussian distribution $P(|u_i|^2)=\exp(-|u_i|^2/T_i)/T_i$.

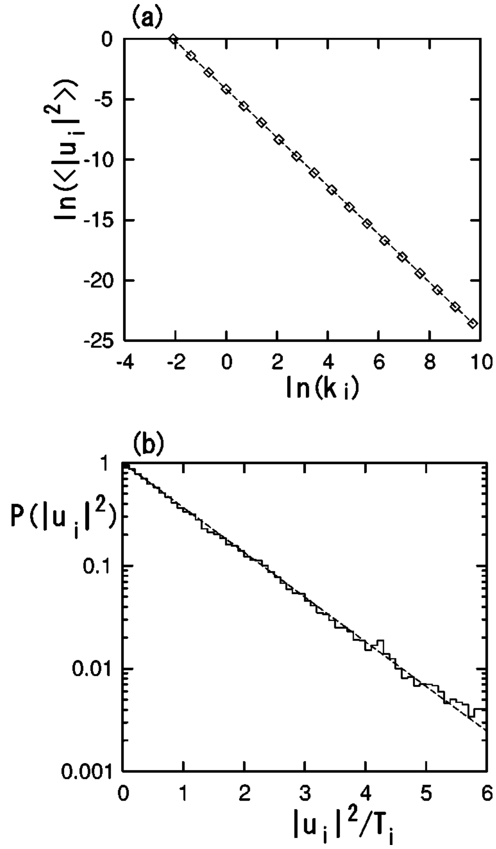

FIG. 2. (a) Averaged energy $\ln(\langle |u_i|^2\rangle)$ vs $\ln(k_i)$ for Eqs. (3) and (4) with $N=18,\delta=1.25,n=3,T_i=2^{-2(i-1)}$, and $d=20$. (b) Semilogarithmic plot of the histogram $P(|u_i|^2)$ for $i=10$ and the Gaussian distribution $P(|u_i|^2)=\exp(-|u_i|^2/T_i)/T_i$ with $T_i=2^{-18}$.

the Maxwell distribution is realized as a stationary state in deterministic time evolution according to Eqs. (3) and (4).

For $\delta>1$, Eq. (3) has another positive-definite conserved quantity $\Sigma_i k_i^2|u_i|^2$ called the enstrophy in addition to the energy. A distribution of the form

$$P(u)\propto\exp\left(-\sum_i k_i^2|u_i|^2/T\right) \tag{7}$$

is a stationary distribution of Eqs. (3) and (4), if the reservoir temperatures are assumed to be $T_i=T/k_i^2$. We have performed a numerical simulation to check whether this distribution is realized in the time evolution of Eqs. (3) and (4). Figure 2 shows a numerical result for $N=18$, $\delta=1.25$, $k_0=2^{-4}$, $n=3$, $T_i=2^{-2(i-1)}$, and $d=20$. Figure 2(a) displays a logarithmic plot of the averaged energy vs k_i. The dashed line denotes $\langle|u_i|^2\rangle=2^{-2(i-1)}$. The averaged energy obeys $\langle|u_i|^2\rangle\sim k_i^{-2}$, that is, the equipartition of enstrophy $\langle k_i^2|u_i|^2\rangle$ is satisfied. The relation $\langle|u_i|^2\rangle\sim k_i^{-2}$ implies that the normal energy spectrum satisfies $\langle E(k)\rangle\sim\langle|u_i|^2\rangle/k_i\propto k^{-3}$, which corresponds to the Batchelor-Kraichnan spectrum. Figure 2(b) displays a semilogarithmic plot of a numerically obtained histogram of $P(|u_i|^2)$ vs $|u_i|^2/T_i$ for $i=10$ with $T_i=2^{-18}$. The Maxwell distribution is approximately obtained in this simulation.

The stationary distributions (5) and (7) express equilibrium states, in which the average rate of entropy production is zero. We have checked numerically that the averaged entropy production rate is nearly zero for the equilibrium states. For our dynamical system, this means that the average expansion rate of the phase space volume is zero. We can obtain nonequilibrium states by changing the temperature distribution of the heat reservoirs. This corresponds to the situation where a chain with a nonlinear interaction is in contact with thermal reservoirs of different temperatures at both ends of the chain. Figure 3 shows a numerical result for $N=21$, $\delta=1.5$, $n=3$, $d=10$, and temperature $T_i=2^{-4(i-1)/3}$. Equation (3) has two types of static solution (fixed points) characterized by scaling exponents: (1) the Kolmogorov-like solution $u_i\sim k_i^{-1/3}$ and (2) $u_i\sim k_i^{-\alpha}$ with $\alpha=[-\log_2(\delta-1)+1]/3$. For $\delta=1.5$, $\alpha=2/3$. The reservoir temperature $T_i\propto 2^{-2\alpha(i-1)}$ is consistent with the averaged energy of the second scaling solution. Figure 3(a) displays a logarithmic plot of the numerically obtained averaged energy vs k_i. The dashed line denotes $\langle|u_i|^2\rangle=2^{-4(i-1)/3}$. The averaged energy obeys $\langle|u_i|^2\rangle\propto k_i^{-4/3}$, which implies that the enstrophy-type cascading solution is approximately realized. The averaged entropy production rate $\langle\Sigma z_i\rangle\sim 28.7$ is definitely positive, which implies that the system is in a nonequilibrium stationary state. That is, the distribution is stationary, but there is a flow of enstrophy. Figure 3(b) displays a semilogarithmic plot of a numerically obtained histogram of $P(|u_i|^2)$ vs $|u_i|^2/T_i$ for $i=16$ with $T_i=2^{-20}$. This distribution is also approximated at the Gaussian distribution $P(|u_i|^2)\propto\exp(-|u_i|^2/T_i)/T_i$ with $T_i=2^{-4(i-1)/3}$. This non-

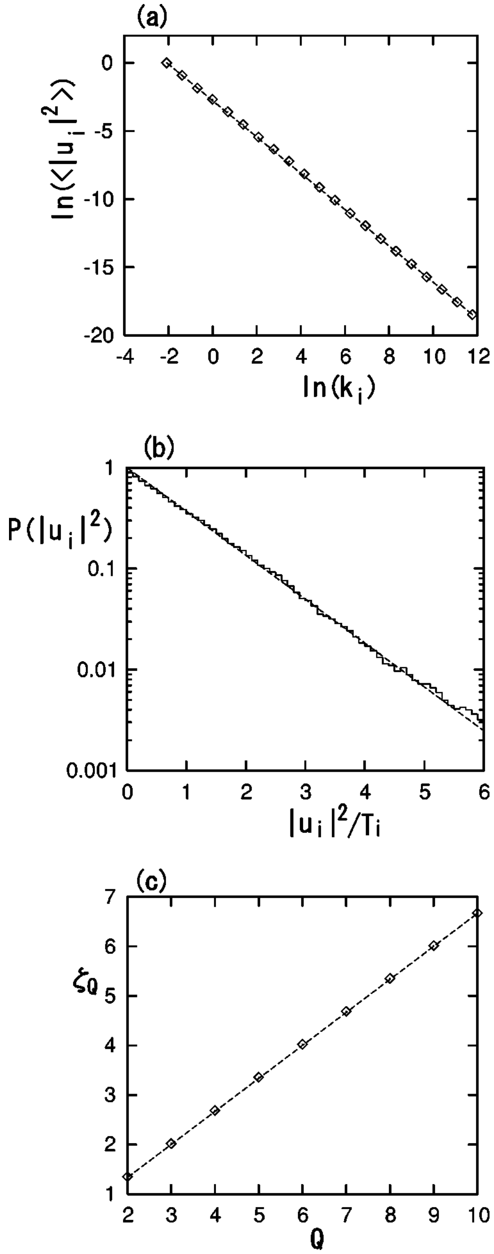

FIG. 3. (a) Averaged energy $\ln(\langle|u_i|^2\rangle)$ vs $\ln(k_i)$ for Eqs. (3) and (4) with $N=21,\delta=1.5,n=3,T_i=2^{-4(i-1)/3}$, and $d=10$. (b) Semilogarithmic plot of the histogram $P(|u_i|^2)$ for $i=16$ and the Gaussian distribution $P(|u_i|^2)=\exp(-|u_i|^2/T_i)/T_i$ with $T_i=2^{-20}$. (c) Exponent ζ_Q for the structure functions. The dashed line denotes $\zeta_Q=2Q/3$.

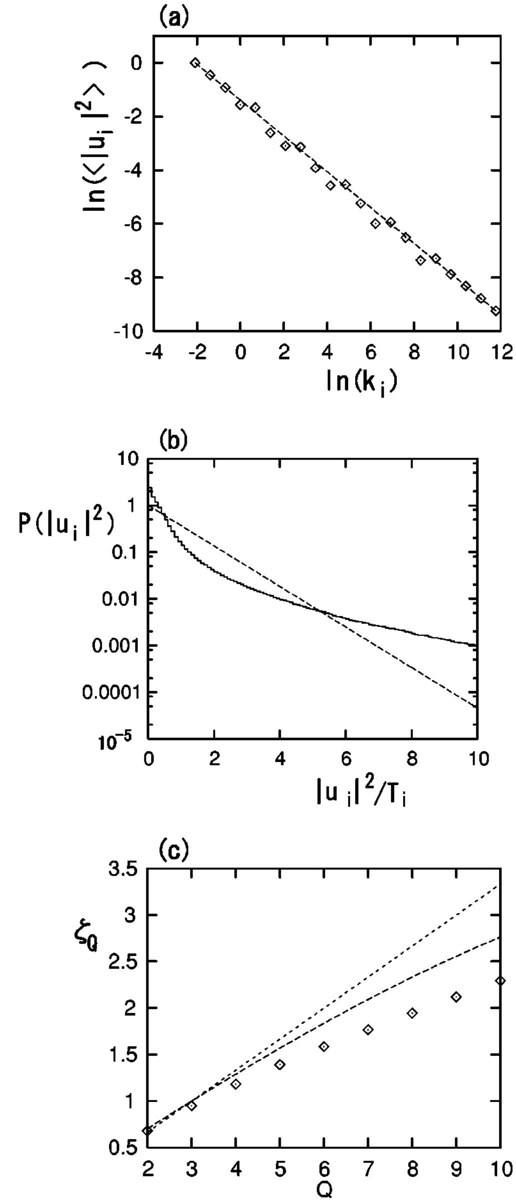

FIG. 4. (a) Averaged energy $\ln(\langle|u_i|^2\rangle)$ vs $\ln(k_i)$ for Eqs. (3) and (4) with $N=21,\delta=0.5,n=3,T_i=2^{-2(i-1)/3}$, and $d=0.1$. (b) Semilogarithmic plot of the histogram $P(|u_i|^2)$ for $i=16$ and the Gaussian distribution $P(|u_i|^2)=\exp(-|u_i|^2/T_i)/T_i$ with $T_i=2^{-10}$. (c) Exponent ζ_Q for the structure functions. The dashed line denotes the random β model $\zeta_Q=Q/3-\log_2\{1-x+x(1/2)^{1-Q/3}\}$ with $x=0.12$ and the dotted line denotes $\zeta_Q=Q/3$.

equilibrium state may be interpreted as a local equilibrium state, since the probability distribution of each shell has the form of the Maxwell distribution. We have calculated the velocity structure functions $\langle|u_i|^Q\rangle\sim k_i^{-\zeta_Q}$ for $Q=2,3,\ldots,10$. Figure 3(c) displays the numerically obtained exponent ζ_Q vs Q. The exponent obeys $\zeta_Q\sim(2/3)Q$ and this implies that there are no multifractal characteristics. The Maxwell distribution is a good approximation for the stationary distribution.

Figure 4 shows a numerical result for $N=21$, $\delta=0.5$, $n=3$, $d=0.1$, and temperature $T_i=2^{-2(i-1)/3}$. The temperature profile of the heat reservoirs is consistent with the Kolmogorov-like solution. Figure 4(a) displays a logarithmic plot of the numerically obtained averaged energy vs k_i. The dashed line denotes $\langle|u_i|^2\rangle=2^{-2(i-1)/3}$. The averaged energy obeys $\langle|u_i|^2\rangle\propto k_i^{-2/3}$. The corresponding energy spectrum is $E(k)\propto\langle|u_i|^2\rangle/k_i\sim k^{-5/3}$. That is, the Kolmogorov spectrum is approximately realized in this numerical simulation. Figure 4(b) displays a semilogarithmic plot of a numerically obtained histogram of $P(|u_i|^2)$ vs $|u_i|^2/T_i$ for $i=16$ with $T_i=2^{-10}$ and it is compared with the Gaussian distribution $P(|u_i|^2)\propto\exp(-|u_i|^2/T_i)/T_i$ with $T_i=2^{-2(i-1)/3}$. For these parameter values, the nonequilibrium stationary distribution is far from the Maxwell distribution and has a long tail. Therefore, the nonequilibrium stationary state cannot be interpreted as a local equilibrium state. The average entropy production rate is 419.5, which is considerably larger than in the case of Fig. 3. Figure 4(c) displays the numerically obtained exponent ζ_Q vs Q. The exponent ζ_Q deviates from $Q/3$ and this indicates a multifractal property of the energy cascading solution. Our exponent ζ_Q is slightly different from that of the random β model $\zeta_Q = Q/3 - \log_2\{1-x + x(1/2)^{1-Q/3}\}$ with $x = 0.12$ (shown by the dashed curve), which was obtained by Jensen, Paladin, and Vulpiani [3] for the original GOY model (1).

To summarize, we have proposed a thermostated GOY shell model and performed numerical simulations. We have obtained an equilibrium state satisfying energy equipartition and an equilibrium state satisfying enstrophy equipartition. By changing the temperature profile of the heat reservoirs, we have obtained nonequilibrium states, one of which may be interpreted as a local equilibrium state and the other as a nonequilibrium state far from equilibrium. Cascading states are realized in the nonequilibrium states. For temperature profiles inconsistent with static cascading solutions, we have obtained various results, which we have not understood well. For example, if the temperature profile of the heat reservoirs is assumed to be $T_i = 2^{-2(i-1)/3}$ for the parameter values of Fig. 3, we have not obtained the averaged energy $\langle |u_i|^2 \rangle \sim 2^{-2(i-1)/3}$, but the logarithmic plot of the averaged energy vs k_i is curved and has a steeper slope for $i > 10$.

The thermostated model gives a statistical-mechanical viewpoint to the GOY model for turbulence. It may also be another useful model for understanding nonlinear and nonequilibrium energy transport from the viewpoint of chaotic dynamical systems.

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