Dynamical energy equipartition of the Toda model with additional on-site potentials*

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We study the dynamical energy equipartition properties in the integrable Toda model with additional uniform or disordered on-site energies by extensive numerical simulations. The total energy is initially equidistributed among some of the lowest frequency linear modes. For the Toda model with uniform on-site potentials, the energy spectrum keeps its profile nearly unchanged in a relatively short time scale. On a much longer time scale, the energies of tail modes increase slowly with time. Energy equipartition is far away from being attached in our studied time scale. For the Toda model with disordered on-site potentials, the energy transfers continuously to the high frequency modes and eventually towards energy equipartition. We further perform a systematic study of the equipartition time t_{eq} depending on the energy density ε and the nonlinear parameter α in the thermodynamic limit for the Toda model with disordered on-site potentials. We find $t_{\rm eq} \propto (1/\varepsilon)^a (1/\alpha)^b$, where $b \approx 2a$. The values of a and b are increased when increasing the strengths of disordered on-site potentials or decreasing the number of initially excited modes.

Keywords: energy transport behaviors, Toda model, uniform or disordered on-site potentials

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1. Introduction

Since the pioneering work of Fermi, Pasta and Ulam (FPU)[1] revealed that recurrence of the energy on the initial excited modes prevented energy equipartition in the FPU model, there have been large activities for many years in the study of the temporal evolution of an initially localized energy excitation in various nonlinear systems.[2–27] For the FPU-α model, two stage dynamics are found at weak nonlinearity.[23] At the first stage of the dynamics, the energies of the unexcited modes grow with time for a certain time scale. After that, the energy spectrum keeps its profile nearly unchanged. At the second stage of the dynamics, the energies of tail modes increase and eventually move towards energy equipartition. Further studies find that the equipartition time $t_{\rm eq}$ depends on the energy density ε and nonlinear parameter α in the thermodynamic limit satisfies a power law behavior, $t_{\rm eq} \sim \varepsilon^{-9/4}\alpha^{-9/2}$.[22] Energy equipartition is also found in other nonlinear lattices such as the φ^4 model[6] and the Frenkel–Kontorova model.[27] For the integrable Toda model, the short time dynamic is found to be very similar to that of the FPU-α model.[23,25] However, energy equipartition is sure to not be reached due to the consequence of the system's complete integrability.[28]

The question we focus on in this paper is whether the effect of on-site potentials may cause the dynamical energy equipartition of the integrable Toda model. Therefore, we investigate the energy transport properties of the integrable Toda model with additional uniform or disordered on-site potentials. We organize the paper as follows. The model, and the method of numerical experiments are introduced in Section 2. In Section 3, we give the main numerical results. The conclusions are shown in Section 4.

2. Model and method of numerical experiments

The Hamiltonian we discuss here is

$$H = \sum_{n=1}^{N} \frac{p_n^2}{2} + \sum_{n=0}^{N} H_T(q_{n+1} - q_n) + \frac{1}{2}\sum_{n=1}^{N} V_n q_n^2, \qquad (1)$$

where p_n is the momentum of the n-th particle. q_n is the displacement that corresponds to the equilibrium position of the n-th particle. The number of particles of the system is $N+2$. For uniform on-site potentials, V_n are identical constants for all n. For disordered on-site potentials, V_n are randomly chosen values in some field. The boundary condition is $q_0 = q_{N+1} = 0$. The Toda energy $H_{\rm T}$ is

$$H_{\rm T}(q_{n+1} - q_n) = \frac{{\rm e}^{2\alpha(q_{n+1}-q_n)} - 1 - 2\alpha(q_{n+1} - q_n)}{4\alpha^2}. \qquad (2)$$

Expanding the exponential in Eq. (2), one can write

$$V_{\rm T}(q_{n+1} - q_n) = \frac{1}{2}(q_{n+1} - q_n)^2 + \frac{1}{3}\alpha(q_{n+1} - q_n)^3 + \frac{1}{6}\alpha^2(q_{n+1} - q_n)^4 + \cdots,$$

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where α is the nonlinearity parameter. The Toda energy is identical to the FPU-α model up to third order. If $V_n = 0$ for all n and $\alpha \neq 0$, equation (1) is reduced to the integrable Toda model.[29]

In the linear case ($\alpha = 0$), equation (1) can be reduced to the linear eigenvalues problem with $-A_{n+1} - A_{n-1} + (2 + V_n)A_n = \lambda A_n$ using $q_n = A_n e^{i\omega t}$. The eigenstates A_n^k are extended modes for uniform V_n and are exponentially localized normal modes[30] for disordered V_n. The frequencies $\omega_k = \sqrt{\lambda_k}$. The harmonic energy of mode k is $E_k = (1/2)(P_k^2 + \omega_k^2 Q_k^2)$, where P_k and Q_k are the momentum and amplitude of the k-th normal modes.

We define the time averaged energy spectrum $\overline{E}_k(t)$ up to time t as

$$\overline{E}_k(t) = \frac{1}{t}\int_0^t E_k(P(t), Q(t))\,\mathrm{d}t.$$

If energy equipartition is achieved, $\overline{E}_k(t)$ converges to the energy density $\varepsilon = E/N$, where E is the total energy of the chain. Based on $\overline{E}_k$'s, we now can define a physical quantity $\xi(t)$ which describes a distance to energy equipartition. The definition of $\xi(t)$ is

$$\xi(t) = \frac{e^{\eta(t)}}{N}. \tag{3}$$

The definition of $\eta(t)$ is

$$\eta(t) = -\sum_{k=1}^{N} \rho_k(t)\log\rho_k(t), \rho_k(t) = \frac{\overline{E}_k(t)}{\sum_{j=1}^{N}\overline{E}_j(t)}. \tag{4}$$

If the system approaches energy equipartition completely, then the value of ξ reaches 1.0.

At first, some of the lowest frequency normal modes are excited, with identical energy. The Hamilton equation of motion is solved numerically with the help of the $SABA_2C$ symplectic algorithm.[31] The $SABA_2C$ integration scheme preserves the energy of the system quite well. For example, the relative error of the energy keeps smaller than 10^{-5} for all our studies here with the typical integration time step $\Delta t = 0.1$. Because of the disorder nature, the evolution of $\xi(t)$ differs slightly from one disorder realization to another realization. For this reason, $\xi(t)$ are averaged over 10 different disorder realizations. The averaged results of $\xi(t)$ are denoted by $\langle\xi(t)\rangle$. $\xi(t)$ are also averaged over more than 10 different disorder realizations. We find the differences of $\langle\xi(t)\rangle$ can be negligible.

3. Main results

3.1. Energy transport results

The results of the time averaged energy spectrum $\overline{E}_k(t)$ at different times t for the Toda model are shown in Fig. 1(a). One can see that except the initial excited modes, only a little of new low frequency modes are excited. The energy of high frequency modes remains very small and keeps unchanged all the time. When uniform on-site energies are added to the Toda model, the energy transport behavior becomes very different. The results of the time averaged energy spectrum $\overline{E}_k(t)$ at different times t for the Toda model with uniform on-site energies are shown in Fig. 1(b). In a relatively short time, the energy spectrum keeps its profile nearly unchanged. However, this state is only quasi-stationary. On a much longer time scale, the energies of tail modes increase with time. The process of energy transfer to high frequency modes is very slow and energy equipartition is far away from being attached in our studied time scale. The process of energy transfer to high frequency modes becomes slower as the values of V_n are increased. The results of the time averaged energy spectrum $\overline{E}_k(t)$ at different times t for the Toda model with disordered on-site energies are shown in Fig. 1(c). One can see that the energy of the high frequency modes grows continuously with time. Especially, the energy of the modes around $k/N = 0.6$ grows faster than others. When the time goes up to $t = 10^7$, an energy equipartition state is nearly attached. Therefore, the integrable property of the Toda model is destroyed and the energy transfers to the high frequency modes with the effect of uniform or disordered on-site energies. The results of $\xi(t)$ are shown in Fig. 1(d).

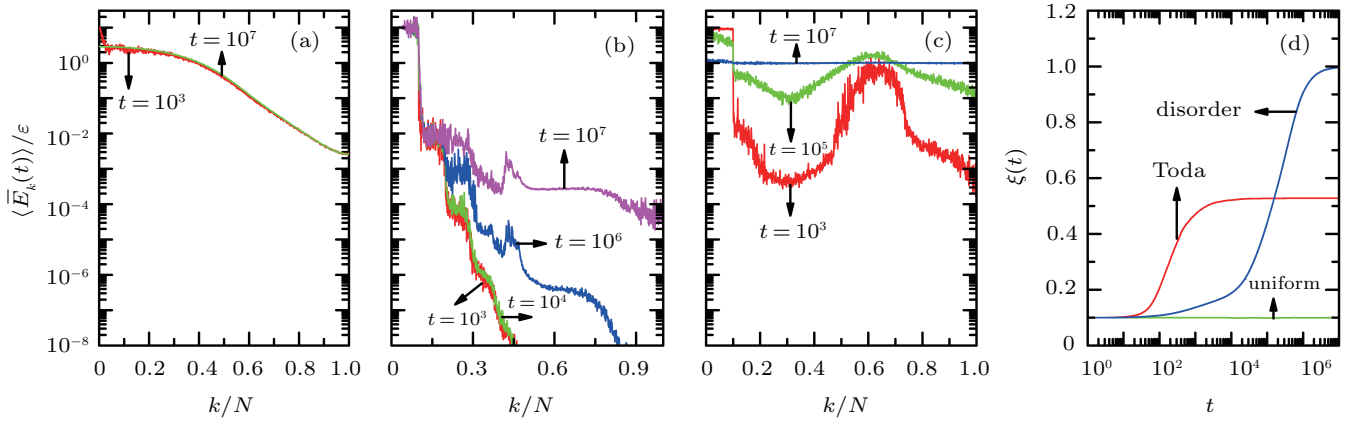


Fig. 1. (color online) (a) $\overline{E}_k(t)/\varepsilon$ versus k/N for the Toda model at different times t with $N = 1024$, $\varepsilon = 0.01$, and $\alpha = 1.0$. (b) $\overline{E}_k(t)/\varepsilon$ vs. k/N for the Toda model with uniform on-site energies at different times t for N=1024, $\varepsilon = 0.01$, $\alpha = 1.0$. $V_n = 0.1$ for all n. (c) $\overline{E}_k(t)/\varepsilon$ versus k/N for the Toda model with disordered on-site energies at different times t for N=1024, $\varepsilon = 0.01$, and $\alpha = 1.0$. V_n are chosen randomly from the interval $(0.5, 1.5)$. (d) The red curve is the result of $\xi(t)$ with the same parameters as those in panel (a). The green curve is the result of $\xi(t)$ with the same parameters as those in panel (b). The blue curve is the result of $\xi(t)$ with the same parameters as those in panel (c). For all cases, the lowest 10% of frequency modes are initially excited.

One can see from Fig. 1(d) that the quantity $\xi(t)$ asymptotically approaches a constant which is less than 0.6 as the time is increased for the Toda model. For the Toda model with uniform on-site energies, $\xi(t)$ nearly keeps the initial value 0.1 and does not grow with time in our studied time scale. The reason is that although the energies of high frequency modes grow with time, these energies are much smaller than those of the initial excited modes and the contribution of these energies to $\xi(t)$ is thereby negligible. For the Toda model with disordered on-site energies, $\xi(t)$ grows gradually from 0.1 to 1.0. Therefore, the process of the energy transport is much faster for the Toda model with disordered on-site energies than that with uniform on-site energies.

3.2. Energy equipartition properties for the Toda model with disordered on-site energies

Figure 2(a) shows the dependencies of $\langle\xi(t)\rangle$ on time t for different values of ε. One can see that the profiles of all curves are very similar to each other. We rescale $\langle\xi(t)\rangle$ for different ε as the time is divided by a suitable factor so that they superpose at $\langle\xi(t)\rangle = 0.5$. The rescaled results are shown in Fig. 2(b). One can see that all curves nearly coincide with each other. Now, we can define the equipartition time $t_{\rm eq}$. Generally speaking, one should define the time when the value of $\langle\xi(t)\rangle$ reaches a value $\xi_{\rm eq}$ that is very close to 1.0 as the equipartition time $t_{\rm eq}$. However, $t_{\rm eq}$ is quite insensitive to the value of $\xi_{\rm eq}$ here due to the profiles of $\langle\xi(t)\rangle$ being very similar to each other. Therefore, we choose $\xi_{\rm eq} = 0.5$ as the equipartition time $t_{\rm eq}$ in this paper.

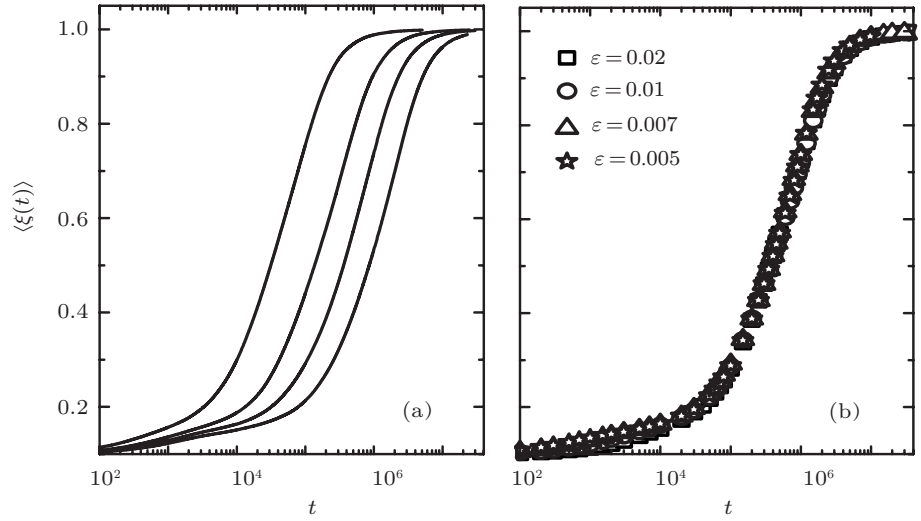


Fig. 2. (a) The results of $\langle\xi(t)\rangle$ for $N = 1024$, $\alpha = 1.0$, and different ε. From right to left, the curves are for $\varepsilon = 0.005$, 0.007, 0.01, and 0.02, respectively. For all cases, V_n are chosen randomly from the interval $(0.5, 1.5)$ and the lowest 10% of frequency modes are initially excited. (b) The curve of $\varepsilon = 0.007$ is kept fixed. The other curves are rescaled as the time is divided by a suitable factor so that they superpose at $\langle\xi(t)\rangle = 0.5$.

In the following, we turn to clarify the equipartition time $t_{\rm eq}$ depending on the energy density ε and the nonlinear parameter α in the thermodynamic limit.

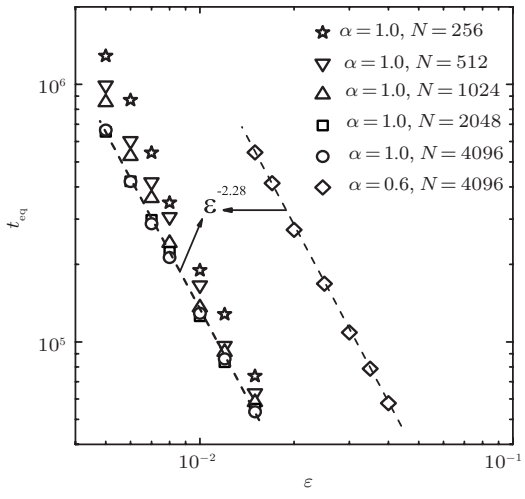


Fig. 3. The dependencies of $t_{\rm eq}$ on ε for different N and α. For all cases, V_n are chosen randomly from the interval $(0.5, 1.5)$ and the lowest 10% of frequency modes are initially excited.

Firstly, we study the dependence of $t_{\rm eq}$ on ε for fixed α. The results are shown in Fig. 3. One can see that $t_{\rm eq}$ is increased when decreasing ε. It indicates more time is needed to reach energy equipartition for smaller ε. The reason is as follows. The strength of nonlinearity is the key factor affecting the process of thermalization. More time is needed to achieve energy equipartition for weaker nonlinearity. When decreasing ε, both the energies in linear and nonlinear parts are decreased. While the linear terms are quadratic, the nonlinear terms are greater than quadratic. Therefore, the proportion of the energy in nonlinear parts decreases; i.e., the strength of nonlinearity decreases as ε is decreased. Therefore, it needs more time to approach energy equipartition for smaller ε. From Fig. 3, we also find that $t_{\rm eq}$ depends on the length N when N is small for fixed α. $t_{\rm eq}$ decreases as N is increased until N reaches 2048. Therefore, the thermodynamics limit is attached when the length N is no less than 2048 in our studied range of ε. Moreover, $t_{\rm eq}$ depends on ε in the thermodynamics limit and satisfies a power law behavior, $t_{\rm eq} \sim (1/\varepsilon)^a$. The

exponent a is found to be 2.28. We also study the dependence of $t_{\rm eq}$ on ε for different α. It is clearly seen that the value of a is independent of α in the thermodynamics limit.

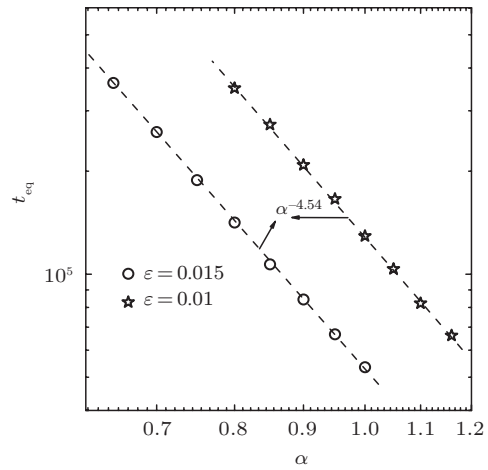


Fig. 4. The dependence of $t_{\rm eq}$ on α in log–log scale with $N = 4096$, and different values of ε. For all cases, V_n are chosen randomly from the interval $(0.5, 1.5)$ and the lowest 10% of frequency modes are initially excited.

Secondly, we study the dependence of $t_{\rm eq}$ on α for fixed ε. Figure 4 shows the results of $t_{\rm eq}$ versus α for different values of ε. One can see that $t_{\rm eq}$ is increased when decreasing α for fixed ε. Thus, it needs more time to reach energy equipartition for smaller α. The reason is that α is the nonlinear parameter and represents the strength of nonlinearity directly. When decreasing α, the nonlinearity becomes weaker and the time needed to achieve energy equipartition is thereby increased. We also find that $t_{\rm eq}$ versus α for fixed ε in the thermodynamics limit shows a power law behavior, $t_{\rm eq} \sim (1/\alpha)^b$. The exponent b is found to be 4.54, and is nearly independent of the value ε. Therefore, the dependence of equipartition time $t_{\rm eq}$ on energy density ε and nonlinear parameter α in the thermodynamics limit, is

$$t_{\rm eq} \sim \left(\frac{1}{\varepsilon}\right)^a \left(\frac{1}{\alpha}\right)^b. \tag{5}$$

When V_n are chosen randomly from the interval $(0.5, 1.5)$, the values of exponents are $a = 2.28$ and $b = 4.54$. We find $b \approx 2a$. This relationship is very similar to that of the FPU-α model.[22] For that model, it is found that $t_{\rm eq} \sim \varepsilon^{-9/4}\alpha^{-9/2}$.

Thirdly, we study the values of a and b depending on the strengths of disordered on-site potentials. Figure 5(a) gives the results of t_{eq} as functions of ε at $\alpha = 1.0$ for different values of N and different strengths of disorder. One can see that $t_{\rm eq}$ versus ε for different strengths of disorder in the thermodynamics limit all display power law behaviors. When V_n are chosen randomly from the interval $(0.7, 1.3)$ and $(0.3, 1.7)$, the values of exponent a are found to be 1.71 and 2.50, respectively. It indicates that the value of a increases as the strength of disordered on-site potential is increased. Figure 5(b) gives the results of $t_{\rm eq}$ as functions of α at $\varepsilon = 0.015$ for different values of N and different strengths of disorder. Also, $t_{\rm eq}$ versus α for different strengths of disorder in the thermodynamics limit display power law behaviors. When V_n are chosen randomly from the interval $(0.7, 1.3)$, the value of exponent b is found to be 3.44. When V_n are chosen randomly from the interval $(0.3, 1.7)$, the value of exponent b is found to be 4.99. Therefore, the relationship $b \approx 2a$ is still satisfied for different strengths of disorder.

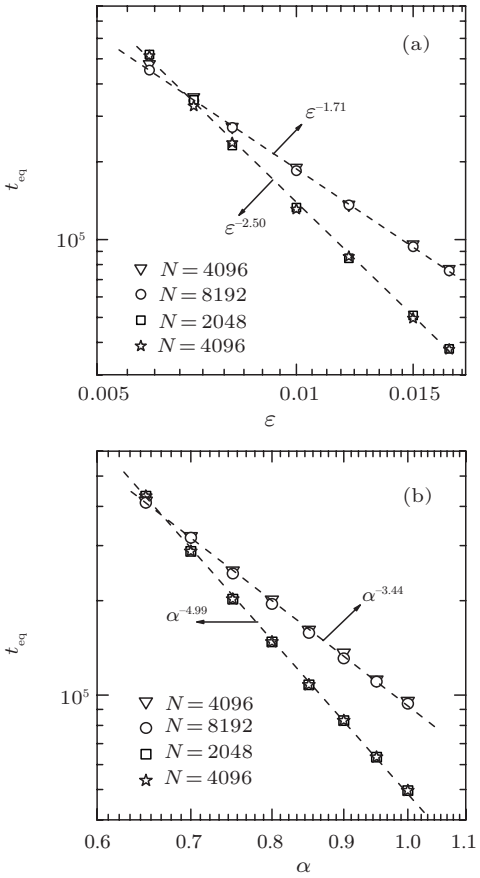


Fig. 5. (a) The dependence of $t_{\rm eq}$ on ε with $N = 4096$, and 8192 for V_n chosen randomly from the interval $(0.7, 1.3)$ and with $N = 2048$, and 4096 for V_n chosen randomly from the interval $(0.3, 1.7)$. For all cases, the lowest 10% of frequency modes are initially excited and the nonlinear parameter $\alpha = 1.0$. (b) The dependence of $t_{\rm eq}$ on α with $N = 4096$, and 8192 for V_n chosen randomly from the interval $(0.7, 1.3)$ and with $N = 2048$, and 4096 for V_n chosen randomly from the interval $(0.3, 1.7)$. For all cases, the lowest 10% of frequency modes are initially excited and the energy density $\varepsilon = 0.015$.

Finally, we study the values of a and b depending on different initial conditions in the thermodynamics limit. The results of $t_{\rm eq}$ as functions of ε for different initial conditions are shown in Fig. 6(a). One can see that when the lowest 20%, 10%, and 5% of modes are initially excited, the exponent a is found to be 1.99, 2.28, and 2.55, respectively. It indicates that the value of a increases as the number of initially excited modes is decreased. The results of $t_{\rm eq}$ as functions of α for different initial conditions are shown in Fig. 6(b). When the lowest 20%, 10%, and 5% of modes are initially excited, the

value of exponent b is found to be 3.92, 4.54, and 5.16, respectively. Also, the relationship $b \approx 2a$ is satisfied for different initial conditions.

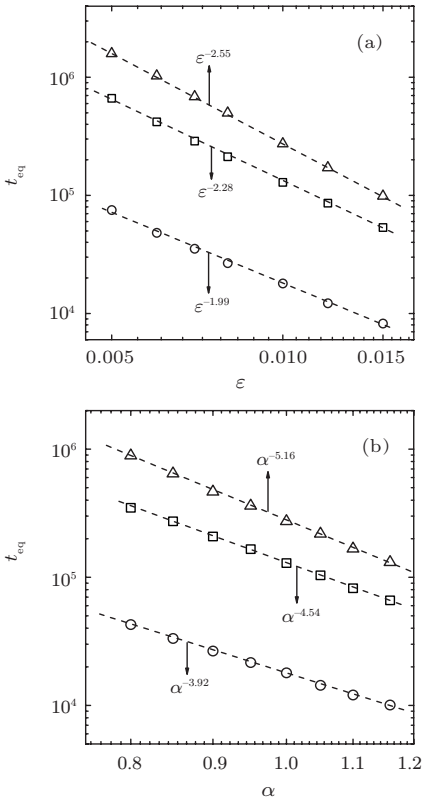


Fig. 6. (a) The dependence of t_{eq} on ε with $N = 4096$, $\alpha = 1.0$, and different initial conditions. The circles, squares, and triangles are the results for the lowest 20%, 10%, and 5% of modes initially excited. For all cases, V_n are chosen randomly from the interval $(0.5, 1.5)$. (b) The dependence of t_{eq} on α with $N = 4096$, $\varepsilon = 0.01$, and different initial conditions. The circles, squares, and triangles are the results for the lowest 20%, 10%, and 5% of modes initially excited, respectively. For all cases, V_n are chosen randomly from the interval $(0.5, 1.5)$.

4. Conclusion

In summary, we studied the energy equipartition properties in the integrable Toda model with additional uniform or disordered on-site energies by extensive numerical simulations. Some of the lowest frequency normal modes are initially excited, with identical energy. Due to the integrable property of the Toda model, the energy of high frequency modes remains very small and does not grow with time. The energy equipartition state is sure to not be attached. However, the energy transport behavior becomes very different for the Toda model with uniform or disordered on-site energies. For the Toda model with uniform on-site energies, the energy spectrum keeps its profile nearly unchanged for a certain time scale. After that, the energies of tail modes increase with time. The process of energy transfer to high frequency modes is very slow and energy equipartition is far away from being attached in our studied time scale. For the Toda model with disordered on-site energies, the energy of the high frequency modes grows continuously with time and eventually towards energy equipartition. Therefore, the integrable property of the Toda model is destroyed and the energy transfers to the high frequency modes with uniform or disordered on-site energies. Moreover, the process of energy transport is much faster for the Toda model with disordered on-site energies than that with uniform on-site energies. We further studied the equipartition time t_{eq} that depends on the energy density ε and the nonlinear parameter α in the thermodynamic limit for the Toda model with disordered on-site potentials. We found that t_{eq} versus ε and α in the thermodynamics limit is $t_{eq} \propto (1/\varepsilon)^a (1/\alpha)^b$. The values of a and b are increased when increasing the strengths of disordered on-site potentials or decreasing the number of initially excited modes. For all cases, we find $b \approx 2a$. This relationship is very similar to that of the FPU-α model.

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