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Citation: Chin. Phys. B, 2021, 30 (**6**): 060505. DOI: 10.1088/1674-1056/abd92f
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Behaviors of thermalization for the Fermi–Pasta–Ulam–Tsingou system with small number of particles*

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(Received 28 November 2020; revised manuscript received 31 December 2020; accepted manuscript online 7 January 2021)

We study the behaviors of thermalization in Fermi–Pasta–Ulam–Tsingou (FPUT) system with small number of particles using periodic boundary conditions. The total energy has initially equidistributed among some of the lowest frequency modes. The thermalization time t_{eq} depending on system's energy density ε scales as $t_{eq} \propto \varepsilon^{-4}$ only within a certain range of nonlinearity. In this range of nonlinearity, energies can interchange between the initial excited modes and other modes continuously with time until reaching the thermalized state. With a further decreasing nonlinearity, a steeper growth than ε^{-4} will appear. In the very weakly nonlinear regime, energies on low frequency modes are found to be frozen on large time scales. Redistribution of mode energies happens through the resonances of high frequency modes.

Keywords: FPUT system, thermalization, small number of particles

PACS: 05.45.–a, 05.60.Cd, 63.10.+a **DOI:** 10.1088/1674-1056/abd92f

1. Introduction

To confirm the connection between nonlinearity and ergodicity in a classical Hamiltonian system with many degrees of freedom, Fermi in collaboration with Pasta, Ulam, and Tsingou (FPUT) performed the first numerical experiment via a one-dimensional harmonic chain coupled with cubic or quartic potentials.[1] They expected that the nonlinearity would lead to a thermalized state, *i.e.*, a state in which the influence of the initial modes disappears and all modes are excited equally on average. Instead of the expected irreversible process of thermalization, the system exhibits a quasiperiodic recurrences to the initial state. Their work has stimulated prolific activities for several decades in the study of the temporal evolution of an initially localized energy excitation in various nonlinear systems.[2–38]

Izraielev and Chirikov predicted there is an energy threshold, above which the FPUT system can reach thermalization.[3] Such concept, also known as the Chirikov overlap criterion, is based on the fact that the nonlinearity changes the linear dispersion relation, and the resonant condition in frequency is then modified. When the nonlinearity becomes large enough, a mechanism of "overlap of frequencies" may happen. Fast thermalization has been subsequently confirmed by different numerical studies.[4,8,9,14,15] However, whether the FPUT system can be thermalized for arbitrary small nonlinearity has not been settled clearly. Recently, resonant wave–wave interaction theory has been applied to discuss this problem.[39–47] According to this theory, the long time dynamics is ruled by exact resonances in weak nonlinear regime. Thermalization is achieved by the nontrivial resonances. In the thermodynamic limit, if the nontrivial n-wave resonances exist and dominate the thermalization, the thermalization time-scale should be the derivation of the corresponding n-wave kinetic equation, which lead to the thermalization time t_{eq} depending on system's energy density ε scales as $t_{eq} \propto \varepsilon^{-(n-2)}$.[41,45] For the FPUT system in the thermodynamic limit, the lowest order nontrivial resonances are four-wave resonances, which result in $t_{eq} \propto \varepsilon^{-2}$. Numerical simulations for large number of particles show that the results are mostly consistent with theoretical predictions.[45,46] Besides, the thermalization behaviors for one-dimensional disordered lattices systems in the thermodynamic limit have been studied recently.[48,49] For the FPUT system with small number of particles using periodic boundary conditions, the lowest order nontrivial resonances were found to be six-wave resonances.[42,43,46] However, the n-wave kinetic equation can be rigorously derived only in the thermodynamic limit. For the FPUT system with small number of particles, deriving a discrete version of the kinetic equation poses significant mathematical problems.[46] Therefore, they made the conjecture that the time scale of thermalization corresponding to the six-wave interaction for small number of particles is equivalent to that for the thermodynamic limit, which leads to $t_{eq} \propto \varepsilon^{-4}$. This scaling law has been verified by their numerical simulations in the range of nonlinearity they studied.[42,43,46] Obviously, the discrete case stands on a less rigorous ground and further work is definitely needed.

In this paper, we study the behaviors of thermalization for the FPUT system in a wider range of weak nonlinearity compared with previous studies.[42,43] We find the scaling $t_{eq} \propto \varepsilon^{-4}$ observed in Refs. [42,43] is only established within a certain range of nonlinearity. In this range of non-

*Project supported by the Fundamental Research Funds for the Central Universities, China (Grant Nos. 2017B17114 and B210202152).

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linearity, energies can transfer from the initial excited modes to other modes continuously. This energy transport process happens via the nontrivial six-wave resonances,[42,43] which hence lead to $t_{\rm eq} \propto \varepsilon^{-4}$. With a further decreasing nonlinearity, a crossover from $t_{\rm eq} \propto \varepsilon^{-4}$ to a steeper growth will appear. In the very weakly nonlinear regime, energy transport process becomes obviously different. Energies on low frequency modes are found to be frozen on large time scales. It indicates that these low frequency modes cannot take part in the energy sharing for a long time. Therefore, resonant wave–wave interaction theory no longer works for energy transport in the very weakly nonlinear regime. In this case, redistribution of mode energies happens through the resonances of high frequency modes, which lead to the deviation from $t_{\rm eq} \propto \varepsilon^{-4}$.

2. Model and method of numerical experiments

The Hamiltonian of the FPUT model is

$$H = H_{\rm lin} + H_{\rm nonlin} \tag{1}$$

with

$$H_{\rm lin} = \sum_{j=0}^{N-1} \left[\frac{p_j^2}{2} + \frac{1}{2}(q_{j+1} - q_j)^2 \right], \tag{2}$$

$$H_{\rm nonlin} = \sum_{j=0}^{N-1} \left[\frac{\alpha}{3}(q_{j+1} - q_j)^3 + \frac{\beta}{4}(q_{j+1} - q_j)^4 \right]. \tag{3}$$

Here q_j is the displacement of the particle j from its equilibrium position and p_j is the associated momentum. N is the particle number of the system. α and β are positive constants. $\alpha \neq 0$, $\beta = 0$ and $\alpha = 0$, $\beta \neq 0$ correspond to the α-FPUT model and β-FPUT model, respectively. The relevant quantities determining the dynamics are $\alpha^2\varepsilon$[30] and $\beta\varepsilon$[31] for α-FPUT model and β-FPUT model, respectively. A more systematic definition of nonlinearity strength for one-dimensional lattices can be found in Ref. [50]. In the linear case ($\alpha = 0$, $\beta = 0$) with periodic boundaries ($q_N = q_0$), the normal modes are given by

$$P_k = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} \left(\sin\frac{2\pi kj}{N} + \cos\frac{2\pi kj}{N} \right) p_j, \tag{4}$$

$$Q_k = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} \left(\sin\frac{2\pi kj}{N} + \cos\frac{2\pi kj}{N} \right) q_j, \tag{5}$$

where P_k and Q_k are the momentum and amplitude of the k-th normal mode, respectively.

The dispersion relation (frequency *versus* mode index k) is

$$\omega_k = 2\sin\frac{\pi k}{N}, \quad k = 0, \ldots, N-1. \tag{6}$$

To each mode k one can associate a harmonic energy

$$E_k = \frac{1}{2}(P_k^2 + \omega_k^2 Q_k^2). \tag{7}$$

A phase φ is defined by

$$P_k = \sqrt{2E_k}\cos\varphi, \quad Q_k = \sqrt{\frac{2E_k}{\omega_k^2}}\sin\varphi. \tag{8}$$

The average of E_k up to time t is

$$\overline{E}_k(t) = \frac{1}{t}\int_0^t E_k(P(s), Q(s))\,{\rm d}s. \tag{9}$$

We introduce the following quantity as an indicator of thermalization[8]

$$\xi(t) = \frac{{\rm e}^{\eta(t)}}{N-1}, \tag{10}$$

where

$$\eta(t) = -\sum_{k=0}^{N-1} F_k(t)\log F_k(t), \tag{11}$$

in which

$$F_k(t) = \frac{\overline{E}_k(t)}{\sum_{j=0}^{N-1}\overline{E}_j(t)}. \tag{12}$$

In definition (10), we have used $N-1$ instead of N, because with periodic boundary conditions, the modes that can thermalize are $N-1$ (the first mode $k=0$ is not involved in the dynamics). For a thermalized state, the values of $\overline{E}_k(t)$ is theoretically equal to the energy density $\varepsilon = E/(N-1)$, where E denoting the total energy of the system, and the value of ξ is theoretically 1.0.

We use an SABA$_2$C symplectic algorithm[51] to integrate the equations of motion derived by the Hamiltonian (1). Energy is initially equidistributed among some of the lowest frequency linear modes. The time step was set to 0.1 in all simulations, and it was checked that from beginning to the end of the simulation the relative energy error keeps smaller than 10^{-5}. Note that the relevant quantities determining the strength of nonlinearity are $\alpha^2\varepsilon$[30] and $\beta\varepsilon$[31] for α-FPUT model and β-FPUT model, respectively. Therefore, it is equivalent to study the scaling of α (β) by fixing ε or that of ε by fixing α (β). Here, without loss of generality, we vary the energy density ε and fix $\alpha = 0.33$[30] and $\beta = 1.0$ for α-FPUT model and β-FPUT model, respectively. Particle number of the system is $N = 32$. In order to suppress fluctuations, the result of $\xi(t)$ is averaged on 50 different random phases for each ε. We use $\langle\xi(t)\rangle$ to denote the averaging results.

3. Numerical results

In Fig. 1(a), we show the results of $\langle\xi(t)\rangle$ for different energy density ε for α-FPUT model in semilog scale. Modes $k = 1, 2, 30, 31$ are initially excited for all ε. The curves start at the value $4/(N-1)$ then settle to intermediate values for

a transient interval of time that increases as the energy density ε decreases. After that, the curves grow gradually and finally tend to 1.0 with the time increasing. In order to obtain the scaling law of thermalization time $t_{\rm eq}$ depending on ε, we introduce a threshold $\langle\xi\rangle_{\rm eq}$ to estimate the time it takes for the system to reach thermalization. Specifically, we have defined the time as $t_{\rm eq}$ in which $\langle\xi(t)\rangle$ reaches the value of $\langle\xi\rangle_{\rm eq} = 0.99$. We find the scaling law of $t_{\rm eq}$ depending on ε is quite insensitive to the choice of the value of $\langle\xi\rangle_{\rm eq}$. This can be seen from the rescaled results of $\langle\xi(t)\rangle$ for different ε shown in Fig. 1(b). We rescale $\langle\xi(t)\rangle$ for different ε as the time is divided by a suitable factor so that they superpose at $\langle\xi(t)\rangle = 0.9$. One can see that all curves nearly collapse to a single one when $\langle\xi(t)\rangle$ is greater than 0.7.

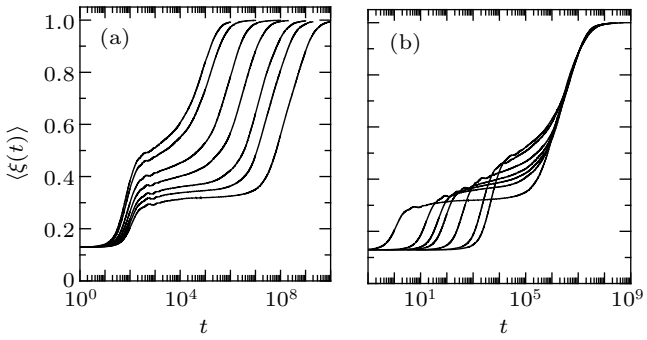


Fig. 1. (a) The dependence of $\langle\xi(t)\rangle$ on time t for different energy density ε for α-FPUT model in semilog scale. The curves from left to right at $\langle\xi(t)\rangle = 0.8$ are for $\varepsilon = 0.1$, 0.08, 0.05, 0.035, 0.025, 0.02, and 0.015, respectively. Modes $k = 1$, 2, 30, 31 are initially excited for each ε. (b) The curve of $\varepsilon = 0.035$ is kept fixed. The other curves are rescaled as the time is divided by a suitable factor so that they superpose at $\langle\xi(t)\rangle = 0.9$.

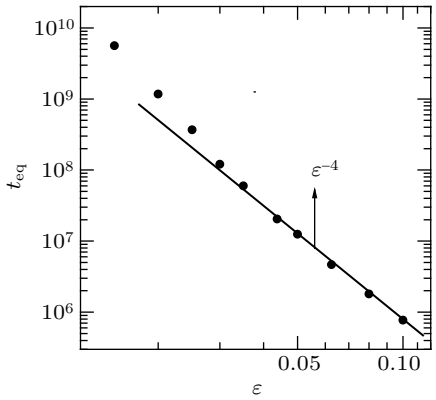


Fig. 2. The results of thermalization time $t_{\rm eq}$ depending on ε in log–log scale for α-FPUT model.

The results of $t_{\rm eq}$ depending on ε for α-FPUT model are shown in Fig. 2. One can see that a power law scaling $t_{\rm eq} \propto \varepsilon^{-4}$ is observed within a certain range of ε. This scaling has been found in Ref. [42]. However, a deviation from $t_{\rm eq} \propto \varepsilon^{-4}$ will appear with a further decreasing ε. This deviation has not been observed in Ref. [42] because the strength of nonlinearity they studied is not small enough. One can see from Fig. 2 that an obvious deviation from $t_{\rm eq} \propto \varepsilon^{-4}$ appears at $\varepsilon_{\rm c} \approx 0.025$. Therefore, $\alpha^2\varepsilon_{\rm c} \approx (0.33)^2 \times 0.025 \approx 0.0027$. A deviation from $t_{\rm eq} \propto \varepsilon^{-4}$ can be observed only when the value of $\alpha^2\varepsilon$ is less than 0.0027. However, one can see from Ref. [42] that the smallest value of $\alpha^2\varepsilon \approx (0.06)^2 \times 1.0 = 0.0036$, above which only the scaling $t_{\rm eq} \propto \varepsilon^{-4}$ can be observed. The deviation from $t_{\rm eq} \propto \varepsilon^{-4}$ is found to be independent of the number of the initially excited modes.

The results of $t_{\rm eq}$ depending on ε for β-FPUT model in log–log scale are shown in Fig. 3. The scaling $t_{\rm eq} \propto \varepsilon^{-4}$, which has been found in Ref. [43], is observed only when the value of ε is grater than $\varepsilon_{\rm c} \approx 0.014$. With a further decreasing ε, a deviation from $t_{\rm eq} \propto \varepsilon^{-4}$ appears. Therefore, this deviation can be observed only when the value of $\beta\varepsilon$ is less than 0.014. In Ref. [43], the smallest value of $\beta\varepsilon \approx 0.02$, above which only the scaling $t_{\rm eq} \propto \varepsilon^{-4}$ can be observed.

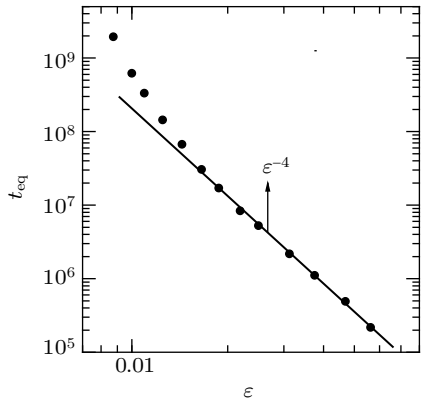


Fig. 3. The results of thermalization time $t_{\rm eq}$ depending on ε in log–log scale for β-FPUT model.

According to the resonant wave–wave interaction theory,[41] all modes of the FPUT system with small number of particles for periodic boundary conditions are interconnected via the nontrivial six-wave resonances.[42,43] Therefore, energies can exchange among all modes continuously through the nontrivial wave–wave interaction until reaching the thermalized state. In other words, energy on each mode should varies continuously with time until reaching the thermalized state if energy can spread via the nontrivial wave–wave interaction. Figure 4(a) gives the results of $\overline{E}_k(t)$ depending on t with different k for α-FPUT model at $\varepsilon = 0.05$. It is seen that the energy on each mode varies continuously with time, and finally approaches to the expected value 0.05, which means thermalization has reached. Figure 4(b) gives the results of $\overline{E}_k(t)$ *versus* k for $\varepsilon = 0.05$ at different time t for α-FPUT model. One can see that each mode at different time owns different energy. The above results indicate that energies can interchange among all modes continuously. This energy transfer behavior is consistent with the resonant wave–wave interaction theory. Therefore, resonant wave–wave interaction theory works well in this range of nonlinearity. The lowest order nontrivial resonances have been found to be six-wave resonances,[42,43] which hence lead to the power law scaling $t_{\rm eq} \propto \varepsilon^{-4}$. However, energy transport process becomes obviously different in

the very weakly nonlinear regime. Figure 5(a) gives the results of $\overline{E}_k(t)$ depending on t with different k for α-FPUT model at $\varepsilon = 0.01$. One can see that except the energies on high frequency modes vary continuously with time, energies on low frequency modes are almost unchanged on large time scales. Figure 5(b) gives the results of $\overline{E}_k(t)$ *versus* k for $\varepsilon = 0.01$ and different time t for α-FPUT model. The profile of energy at different time almost perfectly superposes on low frequency modes. It indicates that these low frequency modes cannot take part in the energy sharing for a long time. Therefore, resonant wave–wave interaction theory no longer works for energy transport in the very weakly nonlinear regime. Besides, one can see from Fig. 5(b) that energies on high frequency modes grow gradually with time. It demonstrates that energy transport process in the very weakly nonlinear regime happens due to the resonances of high frequency modes, which result in the deviation from the scaling law $t_{\rm eq} \propto \varepsilon^{-4}$.

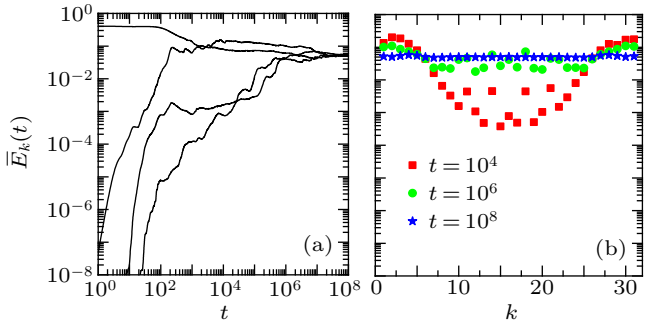


Fig. 4. (a) The results of $\overline{E}_k(t)$ depending on t with different k for α-FPUT model at $\varepsilon = 0.05$. The curves from top to bottom at $t = 10^4$ are for $k = 1$, 5, 10, and 16, respectively. Modes $k = 1$, 2, 30, 31 are initially excited. (b) Parameters are the same as those in panel (a), but now for the results of $\overline{E}_k(t)$ *versus* k at different time t.

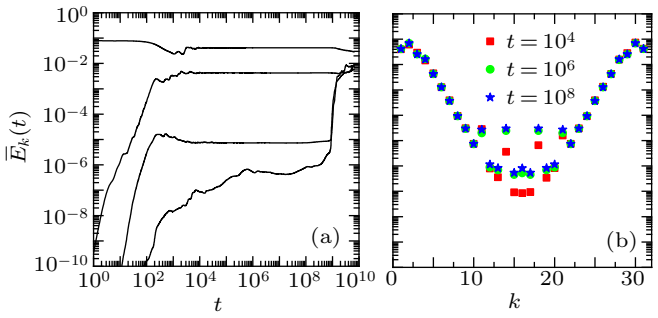


Fig. 5. (a) The results of $\overline{E}_k(t)$ depending on t with different k for α-FPUT model at $\varepsilon = 0.01$. The curves from top to bottom at $t = 10^4$ are for $k = 1$, 5, 10, and 16, respectively. Modes $k = 1$, 2, 30, 31 have been initially excited. (b) Parameters are the same as those in panel (a), but now for the results of $\overline{E}_k(t)$ *versus* k at different time t.

In order to obtain the scaling law in the very weakly nonlinear regime, we study the normalized high frequency energy $\sigma(t) = \sum_{k=11}^{21} F_k(t)$, as has been studied in Ref. [30] for the α-FPUT system with fixed boundary conditions. For the α-FPUT system with fixed boundary conditions, the results of $\sigma(t)$ for different ε are found to be fitted by a power law $\sigma(t) \propto Dt^{\gamma}$.[30] Both the exponent γ and the coefficient D depend on ε. According to this power law, the values of $t_{\rm eq}$ can be obtained only via relatively short time scales even in the very weakly nonlinear regime. The thermalization time $t_{\rm eq}$ depending on ε is found to be $t_{\rm eq} \propto 10^{c/\varepsilon b}$, with suitable constants c and b, in the very weakly nonlinear regime.[30] However, the dynamical results of $\sigma(t)$ for the FPUT system with periodic boundary conditions are different from those with fixed boundary conditions. In Fig. 6, we plot the results of $\sigma(t)$ *versus* t for two values of $\varepsilon = 0.008$, 0.004. For $\varepsilon = 0.008$, one can see that $\sigma(t)$ does not grow with time with a period of time. It suggests that even the high frequency modes are frozen for a period of time. Afterwards, $\sigma(t)$ grows continuously with time. For $\varepsilon = 0.004$, $\sigma(t)$ keeps unchanged even up to $t = 10^{10}$. $\sigma(t)$ no longer displays a power law for the FPUT system with periodic boundary conditions in the very weakly nonlinear regime. Therefore, we cannot obtain the values of $t_{\rm eq}$ through relatively short time scales for very weak nonlinearity through $\sigma(t)$. The scaling law for the FPUT system with small number of particles for periodic boundary conditions in the very weakly nonlinear regime remains a very difficult problem.

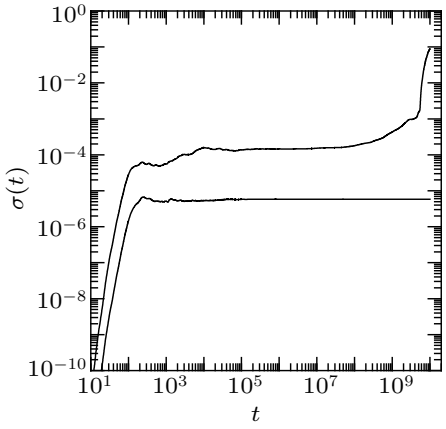


Fig. 6. The results of $\sigma(t)$ depending on t in log–log scale for α-FPUT model. The curves from top to bottom at $t = 10^6$ are for $\varepsilon = 0.008$, and 0.004, respectively.

4. Conclusion

In this paper, we studied numerically the behaviors of thermalization in the range of weak nonlinearity for α-FPUT model and β-FPUT model with $N = 32$. We find the scaling $t_{\rm eq} \propto \varepsilon^{-4}$, which has been observed in Refs. [42,43], is only established within a certain range of nonlinearity for both models. In this range of nonlinearity, energies can transfer from the initial excited modes to other modes continuously. This energy transport process happens via the nontrivial six-wave resonances, which hence lead to $t_{\rm eq} \propto \varepsilon^{-4}$. With a further decreasing nonlinearity, a crossover from $t_{\rm eq} \propto \varepsilon^{-4}$ to a steeper growth will appear. Energies are found to be frozen on low frequency modes for large time scales in the very weakly nonlinear regime, which indicates that the resonant wave–wave interaction theory no longer works in the very weakly nonlinear regime. In this case, redistribution of mode energies

happens through the resonances of the high frequency modes, which lead to the deviation from the scaling law $t_{\rm eq} \propto \varepsilon^{-4}$. Finally, we stress that the scaling law for the FPUT system with small number of particles for periodic boundary conditions in the very weakly nonlinear regime remains a very difficult problem. We hope our work can be useful in motivating more studies in this direction.

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