Effects of weak disorder on the thermalization of Fermi–Pasta–Ulam–Tsingou model

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Keywords: energy equipartition, weak disorder, nonlinearity, Fermi–Pasta–Ulam–Tsingou model

Abstract

We study the effects of two kinds of weak disorders on the thermalization of the Fermi–Pasta–Ulam–Tsingou model by extensive numerical simulations. The disorders are introduced to the mass of atom or coefficient of the quadratic term of potential energy. The initial energy is distributed equally among some lowest frequency modes. We find that the energy transports to high-frequency modes with time and eventually approaches energy equipartition faster with either weak disorder than that in the homogeneous case. That means weak disorders accelerate the process of thermalization. We further study the effects of two kinds of disorders on the scaling law of equipartition time \( T_{eq} \). We find that \( T_{eq} \) satisfies the following scaling law: \( T_{eq} \sim (\varepsilon)^{a} |\alpha|^{-b} \) for different disorder strengths in the thermodynamic limit. It is found that the exponent \( a \approx 1.0 \) while \( b \) depends on the strength of disorder, which are different from \( b = 2a \) in the homogeneous case.

1. Introduction

Generally, the thermalization refers to the energy equipartition among all the normal modes. Equipartition and thermalization have been fundamental research topics in dynamic and statistical behaviors of classical many-body systems over the years, initiating to a great deal of works in different systems [1–26], among which the most typical system is the Fermi–Pasta–Ulam–Tsingou (FPUT) chain. The numerous numerical simulations showed that the FPUT model overcame the metastable state and achieved the energy equipartition through two dynamic stages [27–35]. Furthermore, the dependence of equipartition time \( T_{eq} \) on parameters satisfies the general scaling law for the FPUT model: \( T_{eq} \sim (|\alpha| \sqrt{\varepsilon})^{-9/2} \) in the thermodynamic limit. The \( \alpha, \varepsilon \) are the coefficient of cubic term and energy density, respectively [17]. Recently, for short chains with weak nonlinearity, the analytical results show that nontrivial six-wave resonance leads to thermalization, and the equipartition time \( T_{eq} \) satisfies the following scaling law: \( T_{eq} \sim (\alpha \varepsilon^{1/2})^{-8} \) for FPUT-\( \alpha \) and \( T_{eq} \sim (\beta \varepsilon)^{-4} \) for FPUT-\( \beta \), respectively [36, 37]. In addition, Fu et al have deduced that generalized FPUT systems with polynomial potential \( V(x) = \frac{x^2}{2} + \lambda x^n \) for \( n \geq 4 \), the universal scaling law follows: \( T_{eq} \sim \lambda^{-2} \varepsilon^{-(n-2)} \) [38]. Besides, thermalization has also been studied in other systems. For example, the Frenkel–Kontorova (FK) chain with a periodic on-site potential energy [25, 26], the Bose–Einstein condensation system described by Gross–Pitaevskii (GP) equation at mean field level [21, 22], and the Klein–Gordon (KG) model with linear dispersion term and nonlinear quartic term [23, 24].

All of the above works are carried out in homogeneous systems. However, it is well known that disorders will localize the eigenmodes of the system, i.e., Anderson localization. Therefore, how localized modes affect the thermalization of the nonlinear system is an interesting question. Recently, it is been found that the disordered on-site potential energy can destroy the integrability of the Toda model and induce the thermalization in the thermodynamic limit [39]. Moreover, for the disordered chain with the polynomial potential \( V(x) = \frac{x^2}{2} + \lambda x^n \), Wang et al find that the scaling law mentioned above, \( T_{eq} \sim \lambda^{-2} \varepsilon^{-(n-2)} \), still
holds but \( n \) can be extended to \( n \geq 3 \) [40]. However, how disorders affect the thermalization of the FPUT system remains to be clearly understood.

Therefore, in this work, we study the effects of two kinds of weak disorders on the process of thermalization of the FPUT system. The disorder is introduced either on the mass of atom or on the coefficient of the quadratic term of potential energy. In addition, we also study the effects of disorder strengths on the scaling law of equilibrium time \( T_{eq} \) with the system parameter \( \varepsilon \) and \( \alpha \) in the thermodynamic limit. The structure of this paper is as follows. The model is given in section 2. Section 3 mainly introduces the method and numerical results followed by the conclusion in section 4.

2. Dynamical model and numerical method

Generally, the Hamiltonian of the generalized FPUT model is:

\[
H = \sum_{n=1}^{N} \frac{p_n^2}{2m_n} + \sum_{n=0}^{N} \frac{\gamma_n}{2}(q_{n+1} - q_n)^2 + \frac{\alpha}{3}(q_{n+1} - q_n)^3 + \frac{\beta}{4}(q_{n+1} - q_n)^4,
\]

(1)

where \( m_n, q_n, p_n \) are the mass, displacement and momentum of the \( n \)th atom, and \( \gamma_n, \alpha, \beta \) are the coefficient of second, cubic and fourth terms of potential energy between \( n \)th and \( (n + 1) \)th atoms, respectively. When \( m_n = m \) and \( \gamma_n = \gamma \) are independent of the position, the above Hamiltonian corresponds to the homogeneous case (original FPUT model). We consider two kinds of disorders, one is \( m_n = m \), while \( \gamma_n \) takes randomly \( \gamma_1 \) or \( \gamma_2 \) with the same probability, and the other is \( \gamma_n = \gamma \), while \( m_n \) is chosen in a similar way as \( \gamma_n \).

Without the nonlinear terms, the eigenmodes \( A \) of the system (1) satisfy the following equations

\[
m_n \omega_n^2 A_n^k = -\gamma_n A_n^k_{n+1} - \gamma_{n+1} A_n^k_{n-1} + (\gamma_n + \gamma_{n-1}) A_n^k \quad (n = 1, 2, \ldots, N),
\]

(2)

or \( \omega^2 C A = SA \) in the form of matrix, with \( C, S \) a diagonal matrix and tridiagonal matrix,

\[
C = \begin{pmatrix} m_1 & 0 & \cdots & 0 \\ m_2 & m_1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & m_2 & m_1 \end{pmatrix}_{N \times N}, \quad \text{and} \quad S = \begin{pmatrix} \gamma_0 + \gamma_1 & -\gamma_1 & \cdots & 0 \\ -\gamma_1 & \gamma_1 + \gamma_2 & \cdots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & -\gamma_{N-1} & \gamma_{N-1} + \gamma_N \end{pmatrix}_{N \times N},
\]

respectively.

2.1. Quadratic potential disorder

In this case, \( m_n = m, \gamma_n \) takes randomly \( \gamma_1 \) or \( \gamma_2 \) with the same probability. \( C = m \times I \) (\( I \) is the unit matrix). The eigenvalue equation (2) becomes:

\[
\omega_n^2 A_n^k = \frac{S}{m} A_n^k.
\]

(3)

\( \omega_n, A_n^k \) are the \( k \)th eigenfrequency and eigenmode. Therefore, the coordinate and momentum of the \( k \)th normal mode are

\[
Q_k = \sum_n A_n^k q_n \quad \text{and} \quad P_k = \sum_n A_n^k p_n,
\]

(4)

respectively. Here, the \( A_n^k \) is the \( n \)th component of \( A^k \).

2.2. Mass disorder

In this case, \( \gamma_n = \gamma, m_n \) takes randomly \( m_1 \) or \( m_2 \) with the same probability. The linear eigenvalue problem becomes a generalized eigenvalue problem, i.e.,

\[
\omega_n^2 CA_k^k = SA_k^k.
\]

(5)

The matrix \( C \) can be decomposed into two matrices

\[
C = LL^T,
\]

where \( L \) is a lower triangular matrix [41]. Therefore, we can retrieve a symmetric eigenvalue equation in the following form:

\[
\sum_m \left[ L^{-1} S(L^{-1})^T \right]_{nm} Y_m^k = \omega_k Y_n^k.
\]

(6)
here, \( Y_n^k = \sum_{m=1}^{N} L_m T_n A_m^k \). Then the generalized coordinate and momentum are

\[
Q_k = \sum_{n=1}^{N} Y_{n}^k q_n \sqrt{m_n} \quad \text{and} \quad P_k = \sum_{n=1}^{N} Y_{n}^k p_n / \sqrt{m_n}
\]

respectively.

Therefore, according to the expressions (4) or (7), the harmonic energy of \( k \) mode becomes

\[
E_k = \frac{1}{2}(P_k^2 + \omega_k^2 Q_k^2),
\]

the average energy of \( k \) normal mode in long time \( t \) is:

\[
\overline{E_k}(t) = \frac{1}{t} \int_0^t E_k(P(t), Q(t))dt.
\]

If the value of \( \overline{E_k}(t) \) does not change with time \( t \) and \( \overline{E_k}(t) = \varepsilon = E/N \) \((E \text{ is the initial total energy of the system})\), the system gets to the thermalization. In order to describe the progress of thermalization, we introduce the following physical quantity \( \xi(t) \) similar to that in reference [17],

\[
\xi(t) = \frac{2\eta(t)}{N} \zeta(t),
\]

where \( \eta(t) = -\sum_{k>N/2} F_k(t) \log F_k(t), F_k(t) = \sum_{n>N/2} P_{n}^{(k)} / \overline{P}_{n}^{(k)}, \tilde{\zeta}(t) = \frac{2\sum_{k>N/2} P_{n}^{(k)}}{\sum_{k=1}^{N} \overline{P}_{n}^{(k)}} \). Then, \( \xi(t) = 1 \) corresponds to the energy equipartition\(^4\).

3. Method and numerical results

In this paper, we use the symplectic SABA method [42] to integrate numerically the canonical equations of the system (1), and we initially assign the total energy \( N\varepsilon \) to the lowest 10% of frequency modes [15]. Due to the presence of disorders, the numerical results of different samples will be different, so it is necessary to average the quantities. Therefore, we average 10 disordered samples to ensure the accuracy of results and use \( \langle A \rangle \) to denote an average value of \( A \). Averages on more than 10 different samples are also calculated. The variation on the result is negligible.

3.1. The effects of weak disorders on the process of thermalization

Firstly, we study the properties of \( \langle \xi(t) \rangle \) in two kinds of disordered FPUT systems to understand the effects of disorder strengths on the process of thermalization. For weak quadratic potential disorder, we take \( \overline{m} = \frac{1}{2}(\gamma_1 + \gamma_2) = 1 \) and \( m = 1 \) without loss of generality, then \( \delta_\gamma = |\gamma_1 - \gamma_2| \) reflects the strength of disorder. For the weak mass disorder, \( \overline{m} \) and \( \delta m \) are chosen in a similar way as \( \overline{m} \) and \( \delta_\gamma \). Figure 1 shows that the evolution of \( \langle \xi(t) \rangle \) with time \( t \) for different disorder strengths. Obviously, the value of \( \langle \xi(t) \rangle \) is approximately equal to 1.0 by the time \( t = 10^7 \) after the introduction of both kinds of disorders. Whereas, in the homogeneous case, \( \langle \xi(t) \rangle \) reaches about 0.2 around the time \( t \approx 10^8 \) that far from the thermalization (see figure 1). Therefore, compared with the homogeneous case, disorders accelerate the process of thermalization. Moreover, for the case of the two kinds of disorders, as can be seen in figure 1 that the larger the strength of disorders, the shorter the process of thermalization. Nevertheless, the behaviors of \( \langle \xi(t) \rangle \) with time \( t \) are slightly different for two kinds of disorders. As shown in figure 1, the value of \( \langle \xi(t) \rangle \) is equal to 0 at first for the weak quadratic potential disorder. Whereas, \( \langle \xi(t) \rangle \) soon take a non-zero value for the weak mass disorder.

To better understand the process of thermalization of the FPUT system, we further study the distribution of energy on the normal modes. Figure 2 shows that the evolution of energy of the normal modes \( \langle E_k \rangle \) for two kinds of disorders at different time \( t \). For the weak quadratic potential disorder, we find that the energy of the normal modes continuously transports to the high-frequency modes until thermalization (see figure 2(a)). Whereas, for the weak mass disorder, as presented in figure 2(b) that the energy transports to the high-frequency mode immediately at the beginning of evolution, and oscillates

\(^4\) The first factor \( \frac{2\eta(t)}{N} \) is bounded between \( 2/N \) and 1.0. The \( \frac{2\eta(t)}{N} = 1.0 \) corresponds to the energy equipartition of high modes \((k \geq N/2)\). The second factor \( \tilde{\zeta}(t) \) represents the ratio of twice the energy of high modes \((k > N/2)\) to the energy of the total modes. \( \xi(t) = 1.0 \) corresponds to the energy equipartition of system. However, if the overall energy of the high modes \((k > N/2)\) is greater than that of low modes \((k \leq N/2)\), \( \xi(t) \) is slightly greater than 1.0. Therefore, \( \xi(t) \) can be a little greater than 1.0. This situation mainly appears in mass disorder case that the mass disorder makes the energy transport quickly to the high modes.
Figure 1. The behaviors of $\langle \xi(t) \rangle$ for two kinds of disordered chains. (a) The case of quadratic potential disorder for $\delta \gamma = 0, 0.05, 0.1$ and $0.2$, respectively. (b) The case of mass disorder for $\delta m = 0, 0.05, 0.1$ and $0.15$, respectively. The other parameters are $N = 1024$, $\alpha = -1.0$, $\beta = 2.0$, $\varepsilon = 0.0001$ for both (a) and (b).

Figure 2. The evolutions of energies of normal modes at different time $t$. (a) The case of quadratic potential disorder. (b) The case of weak mass disorder. The parameters are $N = 1024$, $\alpha = -1.0$, $\beta = 2.0$, $\varepsilon = 0.0001$.

intensely on the high-frequency modes until thermalization. Those also correspond to the different evolution of $\langle \xi(t) \rangle$ in figure 1 for two kinds of disorders. Obviously, for the two kinds of disorders under consideration, the energy does not localize on some low-frequency modes during the process of thermalization. These are quite different from those in the homogeneous case. In the homogeneous system, the energy would be localized on some low-frequency modes for a long time due to the existence of a metastable state. Therefore, the disorders destroy the existence of the metastable state and then accelerate the process of thermalization.

3.2. The scaling law of equipartition time $T_{eq}$

In order to describe quantitatively the effects of disorder strengths on the scaling law of equipartition time $T_{eq}$, we define equipartition time $T_{eq}$ similar to that in reference [17]. Figure 3 shows the numerical results of $\langle \xi(t) \rangle$ over time $t$ at different energy densities for the same strength of disorder. For the weak quadratic potential disorder, it can be seen in figure 3(a) that $\langle \xi(t) \rangle$ as functions of time $t$ have similar S-shaped curves at different energy density $\varepsilon$. An appropriate rescaling of $\langle \xi(t) \rangle$ are shown in figure 3(b).

It can be seen that $\langle \xi(t) \rangle$ almost coincides with each other. Therefore, we take the time at which $\langle \xi(t) \rangle = 0.5$ as the equipartition time $T_{eq}$. Similarly, for the weak mass disorder, as shown in figure 3(c), the shapes of $\langle \xi(t) \rangle$ are also similar to sigmoids. The results of $\langle \xi(t) \rangle$ by a suitable rescaling are shown in figure 3(d).

Though the shapes of $\langle \xi(t) \rangle$ are not overlapping for small $\langle \xi(t) \rangle$ after rescaling for different energy densities $\varepsilon$, $\langle \xi(t) \rangle$ coincides well above 0.6. So we take the time of $\langle \xi(t) \rangle = 0.8$ as the equipartition time $T_{eq}$. 

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Figure 3. The evolutions of $\langle \xi(t) \rangle$ with time $t$ at fix energy density $\varepsilon$ for typical weak disorders. (a) The case of quadratic potential disorder. (b) The case of mass disorder. Panels (c) and (d) represent the results by a suitable rescaling of $\langle \xi(t) \rangle$ in (a) and (c), respectively. The parameters are $N = 2048$, $\alpha = -1.0$, $\beta = 2.0$ at $\varepsilon = 0.00005$, 0.0005 and 0.005, respectively.

Figure 4. The numerical data of $T_{eq}$ as function of $\varepsilon$ for different $\alpha$. (a) The fitting results for weak quadratic potential disorder. (b) The fitting results for weak mass disorder. The parameters are $N = 2048$, $\beta = 2.0$, $\alpha = -1.0$ and $\alpha = -1.6$, respectively.

Now, we turn to study the scaling law between equipartition time $T_{eq}$ and energy densities $\varepsilon$ for the same strength of disorder. For the consideration of computing time, we take chain length $N = 2048$. The systems with larger chain length (such as $N = 4096$) are also studied and the results are almost the same. Figure 4 shows the numerical results of $T_{eq}$ as functions of $\varepsilon$ in the same strength of disorder for two different $\alpha$. From the figure 4, for the two kinds of weak disorders, we can get the following scaling law for $T_{eq}$ and $\varepsilon$: $T_{eq} \sim \varepsilon^{-a}$, where $a \approx 1.0$ and is nearly independent of the $\alpha$.

We further study the scaling law between equipartition time $T_{eq}$ and coefficient of cubic terms of potential energy $\alpha$ for the same strength of disorder. The behaviors of $T_{eq}$ as functions of $\alpha$ are plotted in figure 5 in the same strength of disorder for two different $\varepsilon$. For the two kinds of weak disorders, $T_{eq}$ and $\alpha$ has a scaling law: $T_{eq} \sim (|\alpha|)^{-b}$ (see figures 5(a) and (b)). Combining the scaling law of $T_{eq}$ and $\varepsilon$, we can get the following scaling law of equipartition time $T_{eq}$ with $\varepsilon$ and $\alpha$: $T_{eq} \sim (\varepsilon)^{-a}(|\alpha|)^{-b}$ for the same strength of disorder, where $a \approx 1.0$ and $b \neq 2a$, which is different from the $T_{eq} \sim (|\alpha|\sqrt{\varepsilon})^{-9/2}$ in the homogeneous FPUT system.

Finally, we study the effects of different disorder strengths on scaling law mentioned above. Figure 6 shows that the dependence of $T_{eq}$ on $\varepsilon$ and $\alpha$ for different disorder strengths of two kinds of disorders. It is
Figure 5. The numerical data of $T_{eq}$ as function of $\alpha$ for different $\varepsilon$. (a) The fitting results for weak quadratic potential disorder. (b) The fitting results for weak mass disorder. The parameters are $N = 2048$, $\beta = 2.0$, $\varepsilon = 0.0005$ and $\varepsilon = 0.001$, respectively.

Figure 6. The fitting results of $T_{eq}$ for different disorder strengths. (a) $T_{eq}$ as a function of $\varepsilon$ for the case of weak quadratic potential disorder. (b) $T_{eq}$ as a function of $\varepsilon$ for the case of weak mass disorder. (c) $T_{eq}$ as a function of $\alpha$ for the case of weak quadratic potential disorder. (d) $T_{eq}$ as a function of $\alpha$ for the case of weak mass disorder. The other parameters are $N = 2048$, $\beta = 2.0$, respectively.

found that $T_{eq}$, $\varepsilon$ and $\alpha$ still satisfies the following scaling law: $T_{eq} \sim (\varepsilon)^{-a}(|\alpha|)^{-b}$, but the effects of disorder strengths on $a$ and $b$ is different (see figure 6). In summary, the dependence of equipartition time $T_{eq}$ on $\varepsilon$ and $\alpha$ satisfies the following scaling law: $T_{eq} \sim (\varepsilon)^{-a}(|\alpha|)^{-b}$ for different disorder strengths, where $a \approx 1.0$ and is nearly independent of the disorder strengths, while $b$ depends on the disorder strengths and $b \neq 2a$ either, which differs from those of the homogeneous FPUT system.

4. Conclusion

In this paper, we study the effects of two kinds of weak disorders on the process of thermalization of the FPUT system. Our numerical results show that disorders accelerate the process of thermalization and the larger the strength of disorders, the shorter the process of thermalization. At the same time, we also find that the energy is not concentrated on some low-frequency modes during the process of thermalization after introducing the two kinds of weak disorders. This means that the disorders destroy the existence of metastability and then accelerate the process of thermalization. Finally, we have also studied the effects of disorder strengths on the scaling law of the equipartition time $T_{eq}$. We find that the dependence of $T_{eq}$ on energy density $\varepsilon$ and the coefficient of cubic terms of potential energy $\alpha$ satisfies the following scaling law: $T_{eq} \sim (\varepsilon)^{-a}(|\alpha|)^{-b}$ with $b \neq 2a$, which differs from $T_{eq} \sim (|\alpha|\sqrt{\varepsilon})^{9/2}$ in the homogeneous FPUT system.
It should be noted that all the above results are obtained in the case of weak disorders. In addition, we also find that strong disorder will lead to the system unable to thermalize, which is quite different from that in weak disorder. It is an interesting question of why the strong and weak disorders have different effects on the thermalization of the FPUT model, more details about the effects of strong disorder on the thermalization of the FPUT model deserve to study in the future.

Acknowledgments

The work is supported by the National Natural Science Foundation of China (Grant Nos. 11575087 and 11975126) and the Fundamental Research Funds for the Central Universities of China (Grant No. 2017B17114). We are grateful to the High Performance Computing Center (HPCC) of Nanjing University and Jiangsu Key Laboratory for Numerical Simulation of Large Scale Complex Systems for doing the numerical calculations in this paper on its blade cluster system. In addition, we also thank Wei Wang for her insightful contributions to the preliminary work.

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