Universal Time Scale for Thermalization in Two-dimensional Systems

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The Fermi-Pasta-Ulam-Tsingou problem, i.e., the problem of energy equipartition among normal modes in a weakly nonlinear lattice, is here studied in two types of two-dimensional (2D) lattices, more precisely in lattices with square cell and triangular cell. We apply the wave-turbulence approach to describe the dynamics and find multi-wave resonances play a major role in the transfer of energy among the normal modes. We show that, in general, the thermalization time in 2D systems is inversely proportional to the squared perturbation strength in the thermodynamic limit. Numerical simulations confirm that the results are consistent with the theoretical prediction no matter systems are translation-invariant or not.

I. INTRODUCTION

The numerical study of the equipartition was initiated by the seminar work of Fermi, Pasta, Ulam, and Tsingou in the 1950s [1], which investigated on a chain of nonlinear oscillators and showed the very little tendency towards thermalization/equipartition, known as the FPUT paradox. Since then, much effort has been devoted to one-dimensional (1D) systems [2–13]. Nowadays, there is a rather general agreement that thermalization can be attained after a suitably long relaxation time [9–18]. Along with this progress of numerical studies of thermalization, however, there is increasing concern over whether a system can be thermalized for arbitrarily small nonlinearity.

In few-particle classical systems, the Kolmogorov-Arnold-Moser theorem ensures that chaotic motion does not appear immediately after one breaks integrability. It is not known whether a similar scenario is realized in extended systems in the thermodynamic limit. Recently, the wave-turbulence approach [19, 20] has been applied to attack this problem [14–18], and suggests the following picture: in weak-nonlinearity limit, multi-wave resonances constitute the effective mechanism of relaxation to equilibrium, as a result the thermalization time \( T_{eq} \) scales as a power-law of the perturbation strength. More importantly, in the thermodynamic limit, the thermalization time is inversely proportional to the squared perturbation strength. Most recent works [17, 18] point out that this inverse square law is universal for thermalization of translation-invariant FPUT-like systems. In addition, our group has also reported the universal scaling in the perturbed Toda chain [21] and the diatomic chain [22]. Our recently work further generalizes this universal law to the disordered system, whose translation-invariance is broken [23]. The universal law implies that the equipartition can always be reached for arbitrarily small nonlinearity in the thermodynamic limit.

It is obviously interesting to know whether the 1D picture persists in higher-dimension, or instead changes in some essential way. In fact, a few papers on the equipartition problem in two-dimensional (2D) systems already exist, namely, to our knowledge, Refs. [24–31]. However, some results [24–27] are performed on small-size systems compared to nowadays possibilities. More recent studies by G. Benettin et al [28, 29] in 2D systems are carried on the Lennard-Jones lattice with a triangular cell. The results of numerical experiments show that the thermalization time scales as \( T_{eq} \propto \varepsilon^{-\alpha} \) in the thermodynamic limit and the exponent \( \alpha \) is relevant with boundary condition. Asymptotic analyses suggest a possible exponent \( \alpha = 5/4 \) for the periodic boundary condition, while \( \alpha = 1 \) for fixed, free and periodic with obstacle boundary conditions. Most recent studies [30, 31] carried on the graphene have identified energy flow pathway of the out-of-plane flexural modes during the equipartition process and revealed the dynamical organization and the route to equipartition of the flexural modes. However, the existing studies on 2D systems do not give a generic mechanism of equipartition like that given in 1D systems.

In this manuscript, based on the wave-turbulence approach, we show that the mechanism of equipartition attributed to multi-wave resonances persists in 2D systems. The kinetic equation of the multi-wave resonance predicts that the universal scaling law for the thermalization time, i.e., \( T_{eq} \propto \lambda^{-2} \), applies to 2D systems. Our extensive numerical simulations performed on lattices with square and triangular cell confirm that this scaling is accurate no matter systems are translation-invariant/ordered or not.

II. THEORETICAL ANALYSIS

The model adopted here is the 2D lattice of size \((N + 2) \times (N + 2)\) and with fixed boundary condition, and the Hamiltonian of the system is

\[
H = H_0 + H'(\lambda),
\]

where \(H_0\) is the integrable Hamiltonian, corresponding to a linear dispersive dynamics; \(H'\) contains the nonlinearity of the potential and \(\lambda\) is a nonlinear parameter. More in
particular we will deal with
\[ H_0 = \frac{1}{2} \sum_{\alpha} m(\alpha) \dot{u}_\alpha^2 (I) + \frac{1}{2} \sum_{\alpha, \beta} \phi_{\alpha \beta}(I, I') u_\alpha(I) u_\beta(I'), \] (2)
and
\[ H' = \frac{\lambda}{n!} \sum_{\beta_1, ..., \beta_n} \gamma_{\beta_1, ..., \beta_n} (l - I') \prod_{s=1}^{n} \left[ u_{\beta_s}(I) - u_{\beta_s}(I') \right], \] (3)
which is a direct result of expanding the interaction potential in terms of small displacements from lattice sites, and the coefficient is given by
\[ \phi_{\alpha \beta}(I, I') = \left. \frac{\partial^2 V}{\partial u_\alpha(I) \partial u_\beta(I')} \right|_0, \]
and
\[ \lambda \gamma_{\beta_1, ..., \beta_n} (l - I') = \left( \prod_{s=1}^{n} \left. \frac{\partial}{\partial u_{\beta_s}(I)} \right|_0 \right) V, \]
where \( V \) represents the interaction potential. Here the Greek alphabet labels the direction of the coordinate axis, \( x \) or \( y \); \( u_\alpha(I) \) represents the displacement of the atom at site \( I \) along the \( \alpha \) direction; and \( m(I) \) the mass. For convenience below, we rescale Hamiltonian (1) by energy density \( \varepsilon \): \( u_\alpha(I) = \tilde{u}_\alpha(I) \varepsilon^{1/2} \) and \( H = \varepsilon \tilde{H} \), so that the parameter \( \lambda \) and \( \varepsilon \) has a scaling relation \( \tilde{\lambda} = \lambda \varepsilon^{(n-2)/2} \). Here \( \tilde{\lambda} \) represents the perturbation strength. We adopt this model for three reasons. First, any generic interaction potential \( V(r) \) can be expanded as the a power series in \( r \) and thus are expected to give, at low energy density, the same qualitative results. The theoretical prediction based on this model thus applies to generic 2D lattices. For instance, we will see in the following that the numerical results for the 2D Lennard-Jones lattice [28] falls on our prediction. Second, one can separately study the influence of different-order nonlinearity on the dynamic behavior. Third, the power potentials allow us to deal with the issue analytically by use of the wave-turbulence approach. Thanks to this advantage, we are able to obtain our key result, i.e, the thermalization time \( T_{\text{eq}} \) is inversely proportional to the squared perturbation strength, \( T_{\text{eq}} \propto \tilde{\lambda}^{-2} \), in the thermodynamic limit. Most importantly, it will be seen that this conclusion applies whether the system is translation-invariant or not.

In general, normal modes of systems can be obtained by diagonalizing the Hessian matrix, which is defined as
\[ \Phi = \Phi_{\alpha \beta}(I, I') = \frac{\phi_{\alpha \beta}(I, I')}{\sqrt{m(I)m(I')}}. \]
There exists a unitary transformation matrix \( U \), whose entries are the components of normal modes \( \tilde{e}(k) \), such that the linear part of the Hamiltonian (2) can be diagonalized by an orthogonal transformation
\[ U^\dagger \Phi U = \Omega^2, \]
where \( \Omega \) is a matrix whose elements are related to frequencies of normal modes, namely \( \Omega_{\alpha \beta}(k) = \omega_{\alpha}(k) \delta_{kk} \delta_{\alpha \beta} \). Here \( \alpha \) and \( \beta \) represents the polarization direction.

We introduce the direct and inverse discrete transformation of the \( u(I) \) variables
\[ \{ Q(k) \} = \sum_{I} \sqrt{m(I)} u(I) \tilde{e}(kI), \]
\[ \{ u(I) \} = \sum_{k} Q(k) \tilde{e}(k) / \sqrt{m(I)}. \] (4)
For convenience, we sort all the components of \( Q(k) \) in the order of increasing frequency, and use \( Q(k_i) \) for these components with a total number of \( M = 2k^2 \). The Hamiltonian (1) in terms of normal coordinates \( Q(k_i) \) gets the form
\[ \tilde{H} = \frac{1}{2} \sum_{i=1}^{M} \left[ P^2(k_i) + \omega^2(k_i) Q^2(k_i) \right] + \tilde{\lambda} V_n(Q), \] (5)
where \( V_n \) is a homogeneous polynomial of degree \( n \) in \( Q(k_i) \) and \( P(k_i) = Q(k_i) \). Any difference in the dynamical behavior of the systems should come from many-body interaction \( V_n \). Continuing with Eq. (5), we can further facilitate the problem by introducing the complex amplitude of a normal mode
\[ a(k_i, t) = \frac{1}{\sqrt{2\omega(k_i)}} \left[ P(k_i, t) - i \omega(k_i) Q(k_i, t) \right]. \] (6)
Substituting Eqs. (4) and (6) into Eq. (1), we obtain, in general, the Hamiltonian in the following form,
\[ \tilde{H} = \sum_{i=1}^{M} \omega(k_i) a(k_i) a^*(k_i) + \tilde{\lambda} \sum_{k_1, ..., k_n} W_{k_1, ..., k_n} \sum_{s=1}^{n} a(k_1) \cdots a(k_s) a^*(k_{s+1}) \cdots a^*(k_n) + c. c., \] (7)
where the matrix \( W_{k_1, ..., k_n} \) weights the transfer of energy among modes \( k_1, ..., k_n \) and relates to \( \gamma_{\beta_1, ..., \beta_n} \), and
waves and producing

Following the wave-resonance approach [19, 20], we then obtain the \( n \)-wave kinetic equation in the thermodynamic limit and in the weak-nonlinearity limit,

\[
\dot{D}_1 = \eta(k_1) - \tau^{-1}(k_1) D_1
\]

with

\[
\eta(k_1) = \hat{\lambda}^2 \sum_{k_2, \ldots, k_n} \left| W_{1, \ldots, s}^{s+1, \ldots, n} \right|^2 \delta(\omega_{s+1, \ldots, n}) D_2 \cdots D_s D_{s+1} \cdots D_n,
\]

and

\[
\tau^{-1}(k_1) = \hat{\lambda}^2 \sum_{k_1, \ldots, k_n} \left| W_{1, \ldots, s}^{s+1, \ldots, n} \right|^2 \delta(\omega_{s+1, \ldots, n}) D_1 \cdots D_s D_{s+1} \cdots D_n \left( \frac{1}{D_n} + \cdots + \frac{1}{D_{s+1}} - \frac{1}{D_s} - \frac{1}{D_2} \right),
\]

where \( \delta(\omega_{s+1, \ldots, n}) \) is the shorthand notation of delta function \( \delta(\sum_i \omega(k_i) - \sum_i \omega(k_{s+i})) \), and gives a resonance condition

\[
\omega(k_1) + \cdots + \omega(k_s) = \omega(k_{s+1}) + \cdots + \omega(k_n),
\]

which represents the \( n \)-wave resonances of eliminating \( s \) waves and producing \( n-s \) waves. The occurrence of a delta function in the kinetic equation always seems strange at first. It suggests that only energy transfer is nonzero only when

\[
k_1 + \cdots + k_s - k_{s+1} - \cdots - k_n \equiv 0,
\]

which, as result of spatial translation invariance, gives another \( n \)-wave resonance condition, a constraint on wave vector. But, since our formalism applies even if translational-invariance is broken, we keep \( W_{1, \ldots, s}^{s+1, \ldots, n} \) in the most general form.

### III. NUMERICAL EXPERIMENTS

#### A. Preparations

The transformation matrix \( U \), as well as the frequency of the normal mode \( \omega_n(k) \) can be computed numerically by diagonalizing the Hessian matrix \( \Phi \). Two lattice systems, namely lattices with square cell and triangular cell, are considered in this work. It is easy to see that the frequencies of the lattice with square cell are the same that of a 1D chain of length \( N + 2 \), each frequency having multiplicity \( 2N \), which comes from the fact that \( \phi_{xx} = 0 \) in Eq. (2). Such a situation looks somehow unnatural. To weaken the degeneracy, we set \( \phi_{xy} \) artificially to be nonzero such that \( \phi_{xy} = \phi_{xx} = \phi_{yy} = 1 \). For the lattice with triangular cell, everything becomes very natural, and there is no need for artificial modification. Figures 1(a) and 1(b) provide the three-dimensional graph of the dispersion relation for the 2D lattice, respectively, with square cell and triangular cell. For the lattice with square cell, each frequency is double degenerate at least. There are two branches, i.e., longitudinal and transverse acoustic branch, for the lattice with triangular cell.

We come now to the thermalization time, i.e., the times needed for attaining energy equipartition among the normal modes, starting from an initial condition in which just a few modes of frequencies are excited. Precisely, we excite only the 10% of modes of the lowest frequency. All the computations have been performed on 2D lattices.
shows in the semi-log scale the ratio $(E(k, t))/\varepsilon$ versus $t/M$ for the 2D lattice, respectively with square cell ($\varepsilon = 0.005$) and triangular cell ($\varepsilon = 0.001$). Our focus here is on the case of $n = 3$, while results of the models with higher-order nonlinearity are not presented, since the scenarios in these models are quite similar. It is seen from Fig. 2 that the energy of the initial excited modes and that of other modes change continuously in contrary direction. Despite details in the process of energy equipartition are different, we see that in both cases the equipartition almost occurs. The meta-stable state, in which the $(E(k, t))/\varepsilon$ keeps its profile nearly unchanged in a very long range of initial time scale with weak non-linearity and has been found in 1D systems, is not found here.

FIG. 2. The function $(E(k, t))/\varepsilon$ versus $t/M$ at various times for the 2D lattice (a) with square cell and $\varepsilon = 0.005$; and (b) with triangular cell and $\varepsilon = 0.001$. All results are obtained with $n = 3$ and $N = 31$. Energy is initially distributed among 10% modes of the lowest frequencies.

To obtain the thermalization time, we first study the properties of $n_{\text{eff}}$ defined by Eq. (12). In Figs 3(a) and 3(b), we show the $n_{\text{eff}}$ vs. time scaled by the power of the energy density $\varepsilon$ (the values are indicated in the figure), namely $\varepsilon^{n-2}t$ for the lattices, respectively with square cell and triangular cell. We find numerically that there is good data collapse for different energy density, which suggests that the concrete threshold value does not affect the scaling exponent of $T_{\text{eq}}$. What’s more, on a sufficiently large time scale, all values of $n_{\text{eff}}(t)$ increases monotonically towards the value 1 with very similar sigmoidal profiles. It suggests that thermalization is finally achieved.

In Fig. 4(a), we show $T_{\text{eq}}$ as a function of $\tilde{\lambda}$ for different translation-invariant systems of $n = 3$ and 4. It can be seen that all data sets collapse on the lines with a slope of $-2$, suggesting $T_{\text{eq}} \propto \tilde{\lambda}^{-2}$ holds for all the cases.
The validity of the scaling law for \( n = 3 \) implies the existence of solution for the three-wave resonance conditions (9) and (11), while there is no such solution for 1D systems [14, 17]. We find that the already reported result, namely \( T_{\text{eq}} \propto \varepsilon^{-1} \) [28, 29], for the 2D Lennard-Jones lattice agrees with our prediction for \( n = 3 \). This follows from the fact that the lowest-order of nonlinearity in the Taylor expansion of its potential is the cubic term. In the low-energy density regime, the cubic term is much larger than higher-order terms and thus dominates the equipartition process. As for the exception from the periodic boundary condition [29], we would say that either the system size is not large enough, or the energy density is outside the weak-wave regime. Figure 4(a) also indicates that the lattice with triangular cell (hexagonal) is more easily thermalized than that with square cell (square).

As we have mentioned above our formulas (4)-(10) applies even if translational-invariance is broken, we proceed to confirm this next. The translational-invariance is broken by the disorder which further enter the system (1) via random masses \( m(I) \), which fluctuate around \( \langle m(I) \rangle = 1 \). In the present work, \( m(I) \) is chosen independently and identically from a uniform distribution between \( 1 \pm \delta m \); thus \( \delta m \) characterizes the strength of disorder and is set to be 0.2 in simulation. Analogous to ordered systems, we investigate the evolution of \( \langle E(k_i) \rangle \) and \( \langle n_{\text{eff}} \rangle \) for the disordered counterparts, and find that there is no qualitative difference between two cases. Our focus is on the validity of scaling law (10) when translational-invariance is absent. As shown in Fig. 4(b), the scaling law of thermalization time, namely \( T_{\text{eq}} \propto \hat{\lambda}^{-2} \) still holds. Moreover, if we put the results of Fig. 4 into the same plot, we would see that the absence of translational-invariance has no noticeable effect on thermalization time. It is easy to understand if we regard \( H'(\hat{\lambda}) \) as perturbation on an integrable systems \( H_0 \), and thus under our parameters distance from the integrable limit is comparable for two cases. The interplay between disorder and nonlinear interaction is a complicated and outstanding problem. In this work we only focus our problem on the vicinity of an integrable limit.

IV. SUMMARY AND DISCUSSIONS

In summary, we have applied the wave-turbulence approach to the study of equipartition/thermalization of 2D systems and further verified in 2D systems that thermalization attributes to multi-wave resonances. Moreover, we show that the thermalization time is inversely proportional to the squared perturbation strength, i.e., \( T_{\text{eq}} \propto \lambda^{-2} \), in the thermodynamic limit. It leads to the conclusion that such systems can always be thermalized by the arbitrarily weak many-body interaction. It should be noted that these conclusions also hold in the presence of disorder, which implies that the localized states induced by disorder are unstable.

We emphasize that the weak-nonlinearity is a key premise of wave-turbulence analysis, therefore the interplay between strong interaction and disorder is excluded in our study, but deserves further investigation. Finally, combined with studies in 1D systems [14–18, 21, 23], we point out in the frame of wave-turbulence approach, that thermalization is dominated by multi-wave resonances, thus the scaling exponent of thermalization time is determined by the number of the waves and is independent of the spatial dimension. Therefore, thermalization can be expected in three-dimensional systems because the scaling law of the thermalization time we have obtained should also be valid.

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