Thermalization of high-dimensional classical lattices

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The energy equipartition hypothesis is one of the dynamical foundations of the statistical mechanics. It has been established a general consensus that typical one-dimensional classical lattices in the thermal dynamical limit can be thermalized by arbitrarily small nonlinear perturbations. In this Letter we show analytically and numerically that the thermalization time of typical two-dimensional and three-dimensional lattices follows also the universal scaling of $T_{eq} \sim \tilde{g}^{-2}$ for sufficient large systems with either homogeneous or disordered masses, where $\tilde{g}$ is the perturbation strength. Comparing to the one-dimensional counterparts, high-dimensional lattices can be thermalized quickly, since the three-wave resonance usually dominate the relaxation time scaling and the interconnection network over all normal modes can be easily formed due to the existence of multiple branches of phonons. This result means that the energy equipartition hypothesis applies in general for typical lattice systems, and the thermalization obeys qualitatively the same law.

The energy equipartition hypothesis (EEH) states that in the thermodynamic limit, arbitrarily weak nonlinear interactions can result in energy equipartition among all degrees of freedom. The EEH is at the basis of statistical mechanics, but suspicions are raised due to the establishment of the Kolmogorov-Arnold-Moser (KAM) theorem and the finding of the Fermi-Pasta-Ulam-Tsingou (FPUT) recurrence [1] in the 1950s. The former proof rigorously that there exist a positive-measure set of invariant tori in a weakly perturbed integral Hamiltonian system, and the latter indicates directly by numerical simulation that the energy has been initially assigned on a normal mode of a lattice chain may return to it after a certain time of evolution, both violating the EEH. Intensive studies are then excited and continued to this day. [2–17]. These studies restore the confidence of the EEH to a large extent. Rigorously, the Poincare-Fermi theorem gives that, for nonlinearly perturbed high-dimensional systems (with degrees of freedom $n_i=3$) smooth invariant manifolds separating the phase space into disjoint regions cannot exist, which allows the trajectories diffuse in the whole space by the Arnold diffusion. Several approximate analytical results as well as a large amount of numerical simulations confirm that the EEH applies for at least typical one-dimensional (1D) lattice models. Recently, it is shown that even for the small-size chains studied originally by Fermi et.al. the equipartition can reached with sufficient small perturbations [10, 12, 13, 16], as long as the evolution time is long enough. Moreover, even introducing the disorder to the lattice models can not alter the law of thermalization [17]. Therefore, it has become a general consensus that the equipartition is always attained in the thermodynamic limit for 1D chains at finite temperature.

Furthermore, the relaxation time, $T_{eq}$, is found, especially for large systems, to follow a power-law like scaling, $T_{eq} \sim \varepsilon^{-\delta}$, where $\varepsilon$ represents the specific energy (energy per particle). The exponent $\delta$ has not been generally fixed till the introduce of the wave turbulence theory [10, 12, 13, 16]. Following the wave turbulence approach, for a quasi-integrable Hamiltonian $H = H_0 + gV^n$, where $V^n$ represents the $n$th-order polynomial potential, i.e., $V^n \sim x^n$, and $g$ controls the strength of the perturbation, M. Onorato et.al present that if the $n$-wave nontrivial resonance sets exist and interconnected, the relaxation of the energy fluctuation of the system follows the relaxation time scaling of the $n$-wave resonance, i.e., $T_{eq} \sim \varepsilon^{-(n-2)}$. Later, it is shown that for large enough 1D lattices if applying the integrable Hamiltonian that is closest to the quasi-integrable one as the reference, and adopting a proper perturbation parameter $\tilde{g}$, the $n$-wave resonance sets must exist and form a interconnected network. Consequently, the energy relaxation in typical 1D lattices obey the universal scaling of $T_{eq} \sim \tilde{g}^{-2}$.

The questions remained are then how and in precisely what way a high-dimensional nonlinear lattice is thermalised, and on what time scales the thermalization, or equipartition, is reached. These questions are essential for a full verification of the EEH and for a general understanding of the thermalization time scaling, since high-dimensional systems having more realistic importance. However, few studies have been devoted to them. For two-dimensional (2D) lattices, Benettin has studied a hexagonal lattice with interaction potentials of Lennard-Jones type [18, 19], and speculate that the energy equipartition can occur in the thermodynamic limit. Huang et.al have studied the energy equipartition process among normal modes perpendicular to the plane [20, 21] of a graphene sheet. For three-dimensional (3D) case, we can only able to find a paper by Carati et. al [22], who study an ionic-crystal model and infers that the energy equipartition may not occur at low temperatures [4]. In this Letter, we report our studies for several typical high-Dimensional lattice models, i.e., the 2D hexagonal lattice, 2D square lattice, 3D face-centered cubic lattice, and 3D simple cubic lattice. We first derive the $n$-wave.

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kinetic equation for a norm mode following the perturbation theory approach. For this aim, a key point is that we introduce the generalized Gibbs ensemble (GGE) ansatz which has been applied in studying the thermalization of quantum systems. In addition, we show that the condition of interconnected resonant wave sets can be much easily established in the high-dimensional lattices due to the existence of the multiple branches of the linear dispersion relation. The rigorous analysis enable us to predict that the thermalization of these models obey also the same universal law of 1D lattices, which is verified by numerical simulations.

These lattices can be described by the Hamiltonian

\[ H = \sum_l \frac{1}{2} M(l) u_n^2(l) + \frac{1}{2} \sum_{l'} \sum_{\alpha \beta} \Phi_{\alpha \beta}(l, l') u_n(l) u_n(l') + \sum_{n=3}^{\infty} \frac{1}{n} \sum_{l'} \sum_{\alpha_1 ... \alpha_n} \Psi_{1 ... n}(l, l') \prod_{j=1}^{n} [u_{\beta_j}(l) - u_{\beta_j}(l')] , \]

where the coefficients are given by

\[ \Phi_{\alpha \beta}(l, l') = \frac{\partial^2 V}{\partial u_\alpha(l) \partial u_\beta(l')} \bigg|_0 , \]

and

\[ \Psi_{1 ... n}(l, l') = \left( \prod_{s=1}^{n} \frac{\partial}{\partial u_{s}(l)} \right) V \bigg|_0 . \]

Here \( \alpha \) and \( \beta \) labels the direction of the coordinate \( x, y \)-and \( z \)-axis; \( u_\alpha(l) \) represents the displacement of the particle at site \( l \) along the \( \alpha \) direction; and \( M(l) \) represents the mass.

In Eq. (2) the first two terms are \( H_0 \), the other terms can be considered as the perturbation Hamiltonian, denoted by \( H' \), by assuming that particles perform small vibrations around their equilibrium positions. Supposing that \( H_0 \) has a set of integral of motion with totally \( N_c \) members, \( I_k \) with \( k = 1, 2, 3, ..., N_c \), then according to the dynamical system theory these integrals of motion commute with \( H_0 \) under the Poisson bracket, i.e., \( \{ H_0, I_k \} = 0 \). In the present of the perturbation, the system evolves following the Liouville equation [23],

\[ \frac{\partial}{\partial t} I_k = L_0 I_k + L' I_k , \]

where \( L_0 \) and \( L' \) are Liouville operators, i.e., \( L_0 I_k = \{ H_0, I_k \} \) and \( L' I_k = \{ H', I_k \} \).

The kinetic equation up to the second-order perturbation for \( I_k \) (the first-order term vanishes always) is described by

\[ \langle I_k(t) \rangle \approx - \langle L'(t) f(t) | I_k(t) \rangle - \int_0^\infty \langle L'(\tau) f(t) | L' I_k(t) \rangle d\tau , \]

where \( L'(\tau) = e^{-L_0 \tau} L' e^{L_0 \tau} \), \( f(t) \) is the distribution function of the system (1), and the average is taken over the initial distribution function \( f(0) \). With the weak enough perturbation, the dynamics of the system is still dominated by \( H_0 \). In other words, the deformed \( I_k(t) \) can still be considered as the integral of motion of \( H_0 \) during the evolution process. In this case, according to the GGE ansatz [24], the distribution obeys the GGE, i.e.,

\[ f_{\text{GGE}}(t) = C \exp \left( - \sum_k \lambda_k(t) I_k(t) \right) , \]

approximately all the time, and leads to the Wick’s theorem applies and gives \( \langle I_k(t) I_k(t') \rangle = \delta_{kk'} \). Here \( C \) is a normalization factor. The role of the perturbation is to drive \( I_k \) evolving in the space of integrals of motion.

For a lattice system, introducing the normal modes \( P_s(k) \) and \( Q_s(k) \) and defining the complex amplitude of a normal mode as \( a_s(k) = (P_s(k) + i \omega_s(k) Q_s(k)) \), the integral part of Hamiltonian can be written as

\[ H_0 = \sum_s \sum_k \omega_s^k a_s(k) a_s^*(k) , \]

where the frequency \( \omega_s^k \) obeys the linear dispersion relation, \( s \) enumerates the set of cardinality \( \{ s \} \) of frequencies associated with wave vector \( k \), corresponding to the number of branches of the linear dispersion relation. Similarly, the \( n \)-th order perturbation terms (i.e., the \( n \)-th order terms in the Taylor expansion in Eq. (2)), can be rewritten as

\[ V^n = g \sum_{\ell=0}^{n} \binom{n}{\ell} \sum_{\Gamma_{\ell+1 ... n}^{\ell}} W_{\ell+1 ... n}^{1 ... \ell} \Gamma_{\ell+1 ... n}^{1 ... \ell} , \]

where \( \Gamma_{\ell+1 ... n}^{1 ... \ell} = \prod_{j=1}^{\ell} a_{s_j}(k_j) \prod_{j'=\ell+1}^{n} a_{s_j}(k_{j'}) \). Also, the integral of motion of \( H_0 \) turns to be \( I_k^n = a_s(k) a_s^*(k) \).

Then with this perturbation potential we can solve Eq. (4) and obtain the \( n \)-wave kinetic equation for a specific
integral of motion, $I_{k_1}^{s_1}$ for example, as
\[
\langle \dot{I}_{k_1}^{s_1}(t) \rangle = \gamma_{k_1}^{s_1} (f_{k_1}^{s_1}(t)),
\]
where $\eta_{k_1}^{s_1}$ and $\gamma_{k_1}^{s_1}$ are $f_{k_1}^{s_1}$-independent constants proportional to $g^2$. As long as $\gamma_{k_1}^{s_1}$ is non-vanishing, we obtain that $\langle \dot{I}_{k_1}^{s_1}(t) \rangle$ relaxes with the time scaling $\simeq 1/\gamma_{k_1}^{s_1}$. Please see the SM for the detailed derivation. We would like to point out that the same kinetic equation can also be obtained based on the wave turbulence theory (see SM) as well as possibly by other approximate analytical approaches with several different assumptions.

To guarantee $\gamma_{k_1}^{s_1}$ non-vanishing, the $n$-wave resonant condition,
\[
\omega_{k_1}^{s_1} + \ldots + \omega_{k_\ell}^{s_\ell} = \omega_{k_{\ell+1}}^{s_{\ell+1}} + \ldots + \omega_{k_n}^{s_n},
\]
should be satisfied. For an infinite large lattice, the satisfying of this condition can be easily shown. As $H_0$ represents the harmonic oscillators, the frequencies of normal modes lie in a bounded interval of $\omega_k \in (0, \omega_{\text{max}})$. In the thermodynamic limit, the frequencies are dense in this interval. In such a case, for a given mode one can always construct an infinite sets of modes satisfy the resonance condition. Let’s take the case of $n = 3$ as an example. For a fixed mode of $\omega_{k_1}^{s_1}$, we can always find solutions $\omega_{k_2}^{s_2}$ and $\omega_{k_3}^{s_3}$ satisfying $\omega_{k_1}^{s_1} = \omega_{k_2}^{s_2} + \omega_{k_3}^{s_3}$ in the interval of $(0, \omega_{\text{max}})$ due to the continuity. We thus obtain a series of solution with infinite sets of normal modes connected by $\omega_{k_1}^{s_1}$. Similarly, for a fixed $\omega_{k_2}^{s_2}$ there is also an infinite three-wave resonance sets. These two series are connected by $\omega_{k_3}^{s_3}$. In this way all of the modes can be involved into a connected network. Therefore, in the interconnected network, each normal mode disperses its energy simultaneously to a infinite sets of normal modes by the three-wave resonance, and thus the equipartition time of the system can be characterized by the time scaling of the three-wave resonance.

For a finite-size system, since frequency peaks would be broadened by the nonlinearity, such that a frequency peak will have a finite width proportional to $\gamma_{k_1}^{s_1}$. As a result, the resonance condition can be replaced by the quasi-resonance condition,
\[
\left| \omega_{k_1}^{s_1} + \ldots + \omega_{k_\ell}^{s_\ell} - \omega_{k_{\ell+1}}^{s_{\ell+1}} - \ldots - \omega_{k_n}^{s_n} \right| \lesssim \gamma_{k_1}^{s_1^2}.
\]
Since the space between frequency peaks of neighbour modes is about $1/N$, this condition can be satisfied for a fixed $g$ (i.e., with a fixed nonlinearity) as long as $N$ is large enough.

The constant $\gamma_{k_1}^{s_1}$ is also determined by the interaction matrix element $W_{1,1}^{s_1^2}$. For lattices with disordered mass, this term is generally nonzero. Therefore, a sufficient large disordered lattice can always satisfy the resonance and interconnection conditions of $n$-waves, as long as there exist $n$-th-order polynomial term in the perturbation potential.
that in the case of mass; the solid and dot lines connected symbols are for simple cubic, and face-centered cubic lattices; the solid and angles, circles, squares, and stars are for the square, hexagonal, and ε we check the predicted scaling law of Eq. (12) in the low-energy region for the four models with either homogeneous mass(solid symbols) or disordered mass (open symbols), for n = 3 (solid line connected symbols) and n = 4 (dashed line connected symbols), respectively, excepting for the square lattice and the simple cubic lattice in the case of n=4. The scaling for the square lattice with n = 3 has also not perfectly close to the universal law yet. In our simulations, the mass of particles in the homogeneous models is set to m = 1, and in the disordered model takes random values of m = 1.2 and m = 0.8. We see that the disorder induces no obvious difference in the thermalization time for either models. In Fig. 2(d) we extend the simulation to region with much weak perturbation strength for the square lattice model with n = 3, 4 and for the simple cubic lattice model with n = 4. We see that the square lattice with n = 3 converges to the universal scaling. But with n = 4, both models can be considered as following the universal law roughly in the weak-perturbation limit.

Comparing to the hexagonal lattice and the face-centered cubic lattice, the convergence for the square lattice model and the simple cubic lattice model is rather ambiguous. Even for the simple cubic lattice with n = 3, there is qualitative difference. From Fig. 2(b)-(c) we see that $T_{eq}$ shows a cross over transition with the decrease of $\tilde{g}$ or $\varepsilon$. In the strong perturbation region, it has $T_{eq} \propto \tilde{g}^{-1}$ ($T_{eq} \propto \varepsilon^{-1/2}$ in terms of the specific energy), while turns to the universal law of 2 in the weak perturbation region. On the contrary, the universal law applies in a wide parameter region with relatively law energy for the hexagonal lattice and face-centered cubic lattice; The divergences from the universal law are not significant even in the high-energy region. In addition, it can be seen that the thermalization time at a given $\tilde{g}$ is much shorter in the simple cubic lattice than in the face-centered cubic lattice, and in the square lattice than in the hexagonal lattice, respectively.

The difference should be due to the energy degeneracy. In the hexagonal lattice and the face-centered cubic lattice, normal modes have no degeneracy. On the contrary, the square lattice and the simple cubic lattice have a large degrees of degeneracy. According to their linear dispersion relations, there are 2N and 3N wave vectors take the same frequency $|\omega_k^s|$ for these two models, respectively. The energy would rapidly distribute among the degenerated modes, which is responsible for the fast thermalization. The transformation for energy among degenerate modes may be also the reason leading to the universal scaling law not been satisfied perfectly for these models. In Fig. 3(a) and 3(b) we show the evolution process of the energy distribution spectrum of normal modes at three times when we initially excite the lowest-energy mode for the hexagonal and the square lattices, respec-

![FIG. 2. Finite-size effect of the thermalization time $T_{eq}$ for the hexagonal lattice (a) and simple cubic lattice (b), and the universal time scaling of thermalization (c). The last plot (d) extends the numerical verification to the weak-perturbation limit region for the square lattice with perturbation potential of n = 3 (triangle top) and n = 4 (triangle bottom), and the simple cubic lattice with perturbation potential of n = 4 (square). The meanings of symbols in (c) are: triangles, circles, squares, and stars are for the square, hexagonal, simple cubic, and face-centered cubic lattices; the solid and open symbols are for lattices with homogenous and disordered mass; the solid and dot lines connected symbols are for n = 3 and n = 4, respectively.](image-url)
tively. The specific energy is fixed at $\varepsilon \sim 10^{-2}$?. We see that their spectra have obvious difference. In the first model, the spectrum show same platforms, indicating that the degenerated modes possess approximately the same energy and evolve synchronously. While in the last model there is no platform structure.

For realistic systems, the interaction potential involves all of the polynomial potential in the sense of the Taylor expansion. One can thus predict that the three-phonon resonance should dominate the energy relaxation property in the region with weak perturbations since the cubic polynomial term is the first nonlinear term of the Taylor expansion. To confirm this prediction, in Fig. (4) we show $T_{eq}$ as a function of $\varepsilon$ for the four lattices with the Lennard-Jones potential (i.e., $V(\mathbf{u}(l) - \mathbf{u}(l'))$ with $V(r) = r^{-12} - 2r^{-6}$) to be the inter-particle potential. Here only the results for homogenous models are shown: it can be verified that introducing the disordered masses to particles does not change the scaling behavior, as in the case of Fig. 2. We see that $T_{eq}$ converges to the law of three-wave resonance prediction for all the models in the region of low energy, confirming that three-wave process should be dominate the energy relaxation in high-dimensional real-world lattices. In addition, we see that there is a strong finite-size effect in the low-energy region for the simple cubic lattice and the face-centered cubic lattice. If the system size is not large enough, one gains the scaling law of $T_{eq} \propto \varepsilon^{-2}$, which represents a four-wave-resonance-dominated relaxation process. The strong finite-size effect explains why a $T_{eq} \propto \varepsilon^{-2}$ scaling is reported previously [18, 19] (?FU). Therefore, large-scale simulations of lattices with sufficient large sizes are essential for concreting the thermalization law of high-dimensional lattices.

In summary, the EEE applies in general for typical classical lattice models described by near integrable Hamiltonian. The way of thermalization is as follows. Supposing that the perturbation potential involves the $n$-th-order polynomial interaction terms, then for a large enough lattice normal modes manifested themselves into a connected network of $n$-wave resonance sets, and energy thus can be dispersed to any normal modes from a specific one. Since each normal mode in the network is connected by a large number (infinite number in the thermodynamic limit) of $n$-wave resonance sets and disperses energy through them simultaneously, the relax time scaling, $T_{eq} \sim \tilde{g}^{-2} = g^{-2}e^{-(n-2)}$, of the $n$-wave resonance would characterize the energy relax on the network.

For a real-world lattice, the inter-particle potential usually involves all the polynomials, such as in the case with the Lennard-Jones potential, in its Taylor expansion. In this case, a cascade of networks of $n = 3, 4, 5...$ exist if the system is large enough, and energy is dispersed along such a sup-network. Note that with dimensionless Hamiltonian we employed in our simulation, it has $T \sim \varepsilon \sim r^2$. Therefore, $\varepsilon \sim 10^{-2}$ ($r \sim 0.1$) is around about the melting temperature according to the Lindemann criterion of melting which stats that fluctuations over about $\sim 10\%$ to the lattice constant may lead to the solid melt. Therefore, in the room temperature region around about $\varepsilon \sim 10^{-4}$, the network of three-wave resonances should dominate the dispersion of energy, which gives $T_{eq} \sim \tilde{g}^{-2} \sim e^{-1}$, as confirmed by our direct simulations of Fig. 4. This law thus should be the universal law of thermalization of typical real-world classical lattices around room temperature. Furthermore, in the thermalization of quantum systems it has been found that the thermalization time constantly scales as $T_{eq} \sim \lambda^{-2}$, where $\lambda$ is a constant related to the perturbation strength [25]. We expect that the thermalization may follow the same universal scaling.

The degeneracy may influence the thermalization behavior not only quantitatively but also qualitatively. It is found that the the square lattice and simple cubic lattice have much fast thermalization rate comparing to the
hexagonal lattice and the face-centered cubic lattice, respectively. We attribute the reason to that energy can disperse much quickly among degenerated normal modes. As this way of dispersing energy is beyond the framework of $n$-wave resonances, it may leads to the time scaling of energy relaxation divergences to the universal thermalization law more or less. Nevertheless, remarkable divergences are observed for the square lattice and the cubic lattice with pure polynomial perturbation potential of $n = 4$, which could not lead to distinguishing effects for real-world lattices. The detail role of degeneracy, however, remains to be topics of further studies.

Finally, we would like to point out that comparing to the 1D lattices, high-dimensional lattices have a faster thermalization rate. Moreover, the resonance conditions as well as the interconnect condition of the $n$-wave resonance network can be more easily shown. In addition, mass disorder seems to do not dramatically influence the thermalization rate of the high-dimensional lattices.

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