Letter

Analytical approach to Lyapunov time: Universal scaling and thermalization

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Based on the geometrization of dynamics and self-consistent phonon theory, we develop an analytical approach to derive the Lyapunov time, the reciprocal of the largest Lyapunov exponent, for general nonlinear lattices of coupled oscillators. The Fermi-Pasta-Ulam-Tsingou-like lattices are exemplified by using the method, which agree well with molecular dynamical simulations for the cases of quartic and sextic interactions. A universal scaling behavior of the Lyapunov time with the nonintegrability strength is observed for the quasi-integrable regime. Interestingly, the scaling exponent of the Lyapunov time is the same as the thermalization time, which indicates a proportional relationship between the two timescales. This relation illustrates how the thermalization process is related to the intrinsic chaotic property.

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Lyapunov exponents, which quantify the average exponential rate of divergences of the initially neighboring trajectories in each direction of phase space, are powerful tools to provide quantitative characterization of chaotic dynamics [1]. Lyapunov exponents have been widely studied [2–19] to elucidate the relationship with the important physical phenomena, such as relaxation [5,8,9,20], transport [9,19,21–23], and phase transitions [5,8,11]. For Hamiltonian systems with symplectic structure, since the largest Lyapunov exponent is usually used for measuring the degree of chaos, how to estimate the largest Lyapunov exponent and its scaling properties are extremely important. An analytical method based on the geometrization of dynamics to calculate the largest Lyapunov exponent has been principally proposed [24,25]. However, it is generally difficult to quantify the largest Lyapunov exponent explicitly via this method due to the presence of nonlinearity in the Hamiltonian. Meanwhile, although various scaling laws of the largest Lyapunov exponent have been given for different models [17,26,27], whether there is a universal scaling law for the largest Lyapunov exponent has been undetermined, which requires the development of the analytical method for general nonlinear Hamiltonian systems.

The features of chaos have been generally shown in Hamiltonian systems that can relax to thermodynamic equilibrium from a nonequilibrium initial state, indicating the relevance between nonlinear dynamics and statistical mechanics. The relaxation process can be characterized by the property of equipartition that was first numerically investigated by Fermi, Pasta, Ulam, and Tsingou (FPUT) in 1955 [9,28]. During the past several decades, the delicate relationship between relaxation properties and chaos has drawn a lot of attention [20,26,29–32]. It has been shown in Refs. [26,29] that the behavior of relaxation time and the largest Lyapunov exponent change consistently in the strong-stochasticity threshold. The ergodization time defined in Refs. [30,31] shows that considerably different behavior in comparison with the Lyapunov time. Recently, numerical evidence suggests that a close relation exists between the equilibration time and the Lyapunov time [32]. For the quasi-integrable Hamiltonian systems, the thermalization time t_{eq} displays a universal power-law behavior with the nonintegrability strength in the thermodynamic limit, where the scaling exponent is -2 according to the wave-turbulence theory [33–37]. However, the relationship between two characteristic times, the Lyapunov time that represents how long we should wait until the chaotic system exhibits its chaotic features, and the thermalization time that indicates how fast the system can be thermalized, is still unclear.

In this Letter, we develop an analytical approach to calculate the Lyapunov time for nonlinear lattices of coupled oscillators in terms of the geometrization of dynamics and the self-consistent phonon theory (SCPT). In the quasi-integrable regime, a universal scaling behavior of the Lyapunov time is discovered, which is coincident with the universal scaling of the thermalization time. This fact indicates an interesting proportional relationship between the two timescales. The approach are verified by molecular dynamical simulations for the FPUT-like lattices. The numerical results agree well with the theoretical predictions.

The idea of looking at dynamics from the geometric point of view dates back to Poincaré, and qualitatively attempted to investigate dynamics and its connection with statistical mechanics in 1940s. Based on previous studies [8,20] that bridge the dynamical foundations of statistical mechanics with Riemannian differential geometry, the theory of geometrization of dynamics has been applied to study the chaos [24–27,38] and phase transition [11,39–44] in Hamiltonian systems. The key idea of geometrization of dynamics is connecting two functional extremes, the action functional for natural motions of system and the curve length functional for the geodesics of manifold via a suitable choice of metric. One can verify the geodesics of manifold with Jacobi or Eisenhart matric [45] are the trajectories of natural motions of Hamiltonian

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systems [5,8,45]. So that the stability for trajectories of natural motion corresponds to the stability of geodesics of manifold. In general, the evolution equation (called Jacobi equation) of the perturbation vector of geodesics, which is completely determined by the curvature properties of the underlying manifold, is too complex to be solved exactly. For simplifying the Jacobi equation to provide an average measure of the instability instead of the knowledge of dynamical trajectories, several assumptions are introduced. Two main assumptions are that the manifold is quasi-isotropic and the evolution of geodesics is chaotic, which are invalid for general cases but reasonable for the cases of large-N mechanics manifold. The final effective Jacobi equation is a stochastic oscillator equation

$$\frac{d^2\psi}{dt^2} + k(t)\psi = 0, \tag{1}$$

where ψ represents any of the components of perturbation vector, and the effective curvature $k(t)$ is regarded as a Gaussian and δ-correlated stochastic process on a convenient timescale τ. The mean and the variance of $k(t)$ are the average and fluctuations of the Ricci curvature per degree of freedom

$$k_0 = \frac{\langle K_R\rangle_\mu}{N}, \tag{2}$$

$$\sigma_k^2 = \frac{\langle (K_R - \langle K_R\rangle_\mu)^2\rangle_\mu}{N}, \tag{3}$$

respectively, where $\langle\cdot\rangle_\mu$ denotes microcanonical average. For Eisenhart metric and unit mass homogeneous chain, the Ricci curvature is given by

$$K_R = \Delta V, \tag{4}$$

where ΔV represents the Laplacian of the potential energy. According to the theory of stochastic oscillator equation developed by van Kampen [46], the largest Lyapunov exponent λ can be estimated by the exponential growth rate of the solutions of Eq. (1):

$$\lambda(k_0,\sigma_k,\tau) = \frac{1}{2}\left(\Lambda - \frac{4k_0}{3\Lambda}\right),$$
$$\Lambda = \left[\sigma_k^2\tau + \sqrt{\left(\frac{4k_0}{3}\right)^3 + \sigma_k^4\tau^2}\right]^{\frac{1}{3}}, \tag{5}$$

where $\tau = \pi\sqrt{k_0}/[2\sqrt{k_0(k_0+\sigma_k)} + \pi\sigma_k]$ is the characteristic correlation timescale of $k(t)$. Finally, the Lyapunov time is given by

$$t_L = \frac{1}{\lambda}. \tag{6}$$

The constant negative curvature or the fluctuations of the curvature can cause chaos rather than the constant positive curvature such as that for the harmonic or Toda lattices [47]. The theory of geometrization of dynamics not only explains the origin of chaos with the geometrical perspective, but also provides the quantitative measure of chaos, i.e., the largest Lyapunov exponent or the Lyapunov time.

As we can see in Eq. (5), how to analytically obtain k_0 and σ_k^2 is the key point for analytically calculating the Lyapunov time. However, due to the presence of nonlinear terms in Hamiltonian

$$H = \sum_i \frac{p_i^2}{2} + V(\mathbf{q}), \tag{7}$$

the exact evaluation of the microcanonical average and fluctuation, e.g., Eqs. (2) and (3), are generally difficult or even impossible.

To overcome the difficulty, we employ the self-consistent phonon theory (SCPT), which can be traced back to Feynman [48] and has been developed to study the properties of thermal conduction in low-dimensional nonlinear lattices [49–53] and the temperature of microcanonical ensemble [54]. The key idea of SCPT is replacing the original Hamiltonian by a trial Hamiltonian that allows an approximate evaluation of the exact partition function. For systems of only the two-body interaction, a reasonable choice of the trial Hamiltonian is a chain of N coupled harmonic oscillators chain in the form of

$$H_0 = \sum_i \frac{p_i^2}{2} + \frac{f}{2}(q_i - q_{i-1})^2 + \frac{f_c}{2}q_i^2. \tag{8}$$

The trial parameters f and f_c are obtained by minimizing the upper bound of the free energy, which is given by the Feynman-Jensen inequality [52,55]. Then the corresponding trial partition function can be calculated (see the Appendix for more details). In the thermodynamic limit $N \to \infty$, the microcanonical ensemble is generally equivalent to the canonical ensemble. For a physics quantity A, the microcanonical average $\langle A\rangle_\mu$ is equal to the canonical one

$$\langle A\rangle_\mu(\varepsilon) = \langle A\rangle_{\rm can}[T(\varepsilon)], \tag{9}$$

where $\langle\cdot\rangle_{\rm can}$ denotes canonical average. The temperature as a function of the energy density $T(\varepsilon)$ (caloric curve), as well as its inverse function $\varepsilon(T)$, can be analytically obtained by SCPT in general [54].

However, contrary to the average of physical quantity, the fluctuation $\langle\delta^2 A\rangle = (A - \langle A\rangle)^2$ is sensitive to the choice of probability measure, which means that canonical or microcanonical ensemble yields different values. The relationship between microcanonical and canonical fluctuation is given by the Lebowitz-Percus-Verlet formula [56]

$$\langle\delta^2 A\rangle_\mu(\varepsilon) = \langle\delta^2 A\rangle_{\rm can}(T) - \frac{T^2}{c_V(T)}\left\{\frac{\partial[\langle A\rangle_{\rm can}(T)]}{\partial T}\right\}^2, \tag{10}$$

where $c_V(T) = \frac{\partial\varepsilon(T)}{\partial T}$ is the specific heat capacity at constant volume. So the microcanonical average and fluctuation of the Ricci curvature per degree of freedom can be analytically evaluated by SCPT, and the Lyapunov time is explicitly available by Eqs. (5) and (6).

Here we consider one-dimensional FPUT-like lattices, of which the Hamiltonian is given by

$$H = \sum_i \frac{p_i^2}{2} + \frac{(q_{i+1} - q_i)^2}{2} + \frac{u}{n}(q_{i+1} - q_i)^n, \tag{11}$$

where $n \geqslant 4$ and u denotes the strength of nonlinearity. For the sake of simplicity, we only consider even n. We rescale the Hamiltonian (11) $H' = \varepsilon H$ by $q_i' = q_i\varepsilon^{1/2}$, so that the nonlinear parameter u and energy density ε has a rigid scaling

$u' = u\varepsilon^{\frac{n-2}{2}}$. Therefore, it is equivalent to study the effects of u by fixing ε or that of ε by fixing u [34,37]. For convenience, the nonintegrability strength of the FPUT-like lattices is defined by

$$\eta = u\varepsilon^{\frac{n-2}{2}}. \tag{12}$$

In our following numerical simulations, we fix $\varepsilon = 1$. For the case we consider, the self-consistent equation of f is written by (see the Appendix for more details)

$$f^{\frac{n}{2}} - f^{\frac{n}{2}-1} - u(n-1)(n-3)\cdots 1(k_BT)^{\frac{n}{2}-1} = 0, \tag{13}$$

and $f_c = 0$ due to the absence of the on-site potential in our model. The energy density can be evaluated by averaging the Hamiltonian (11) with the effective partition function basing on the effective Hamiltonian [54], which is given by

$$\varepsilon(u,T) = \frac{k_BT}{2} + \frac{k_BT}{2f} + \frac{u}{n}(n-1)(n-3)\cdots 1\left(\frac{k_BT}{f}\right)^{\frac{n}{2}}. \tag{14}$$

One can solve Eqs. (13) and (14) simultaneously to obtain f and T for given u and ε.

According to Eq. (4), the Ricci curvature for the FPUT-like system reads

$$K_R = 2N + 2u(n-1)\sum_i (q_{i+1} - q_i)^{n-2}. \tag{15}$$

The canonical average of the Ricci curvature per degree of freedom in terms of SCPT reads

$$\langle k_R\rangle_{\rm can}(u,T) = 2 + 2u(n-1)(n-3)\cdots 1\left(\frac{k_BT}{f}\right)^{\frac{n-2}{2}}. \tag{16}$$

In the thermodynamic limit $N \to \infty$, the microcanonical average of the Ricci curvature per degree of freedom $k_0(u,\varepsilon)$ can be obtained by changing the variable from T to ε by Eq. (14).

Similarly, the canonical fluctuation of the Ricci curvature per degree of freedom can be also calculated by SCPT and given by

$$\langle \delta^2 k_R\rangle_{\rm can}(u,T) = 4u^2(n-1)^2[(2n-5)(2n-7)\cdots 1 - (n-3)^2(n-5)^2\cdots 1^2]\left(\frac{k_BT}{f}\right)^{n-2}. \tag{17}$$

Then the microcanonical fluctuation $\sigma_k^2(u,\varepsilon)$ is evaluated by Eq. (10). Finally, the Lyapunov time is analytically given by Eqs. (5) and (6).

Taking the quasi-integrable regime $\eta \ll 1$ into account, one can easily find

$$k_0 \approx 2, \tag{18}$$

and

$$\sigma_k^2(u,\varepsilon) \approx C_1\eta^2. \tag{19}$$

With that the Lyapunov time can be approximately given by

$$t_L(u,\varepsilon) \approx C\eta^{-2}, \tag{20}$$

which indicates the universal scaling behavior of t_L in respect of u and ε with scaling exponents -2 and $-(n-2)$, respectively.

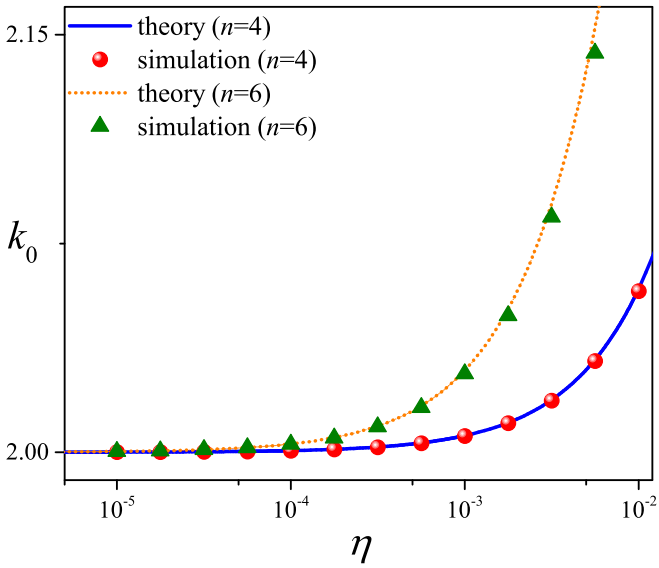

FIG. 1. The average Ricci curvature per degree of freedom as a function of the nonintegrability strength η, which is obtained by the presented analytical approach (solid line for $n = 4$ and dotted line for $n = 6$) and numerical simulations (solid ball for $n = 4$ and solid triangle for $n = 6$).

According to the results of Refs. [33–35,37] obtained by the wave-turbulence theory, the thermalization time follows the scaling law

$$t_{\rm eq} \sim \eta^{-2}, \tag{21}$$

whose scaling exponent coincides with the behavior of the Lyapunov time given by Eq. (20).

To verify the validity of our approach, molecular-dynamics simulations are applied for the $n = 4$ and $n = 6$ cases. The $SABA_2C$ symplectic algorithm [57] is employed to integrate the equations of motion derived from the Hamiltonian (7), with the fixed boundary conditions, i.e., $q_0 = 0$ and $q_{N+1} = 0$, and the system size $N = 1024$. In our simulations, the integration time step is $\Delta t = 0.1$ and the energy drift is kept less than 10^{-6}. The initial conditions follow by fixing the position to equilibrium position $q_i = 0$ and by choosing the moments p_i randomly. Then, we rescale $|p_i| \to b|p_i|$ to control the energy density to the desired value, which is fixed by $\varepsilon = 1$ in our simulations. We numerically compute the microcanonical average and fluctuation of the Ricci curvature per degree of freedom besides the Lyapunov time. Instead of ensemble average, the time average along numerical trajectory is employed in our numerical simulations thanks to the ergodic hypothesis. The average and fluctuation of the Ricci curvature are calculated by their definition (2) and (3). In our numerical simulations, the time steps is over 10^8 as to guarantee the system reaches the equilibrium state.

Figures 1 and 2 show the average and fluctuation of the Ricci curvature per degree of freedom as a function of η, respectively. One can see a nice agreement between theoretical prediction and numerical simulations. It has been shown in Fig. 2 that the fluctuation displays the power-law behavior $\sigma_k^2 \sim \eta^2$ for both $n = 4$ and $n = 6$ cases, which is consistent with the prediction of Eq. (19).

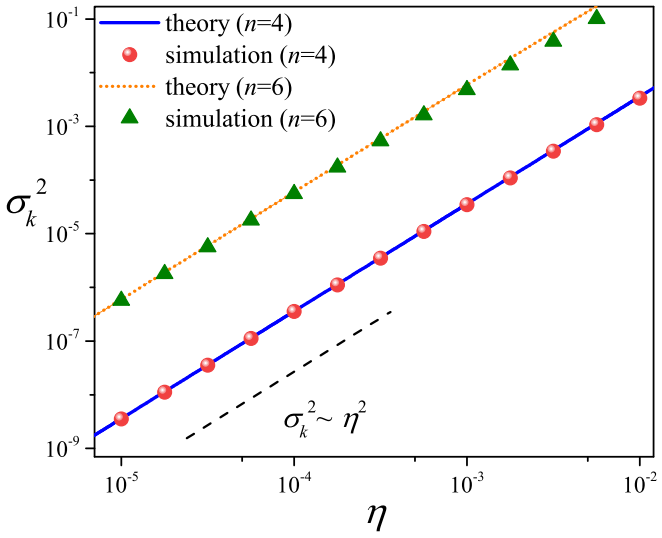

FIG. 2. The fluctuation of the Ricci curvature per degree of freedom as a function of the nonintegrability strength η, which is obtained by the presented analytical approach (solid line for $n = 4$ and dotted line for $n = 6$) and numerical simulations (solid ball for $n = 4$ and solid triangle for $n = 6$). The dashed line is drawn for $\sigma_k^2 \sim \eta^2$ as a reference.

The largest Lyapunov exponent is numerically computed via a standard technique [2,3] for over 10^9 time steps. It has been shown that the largest Lyapunov exponent does not depend on the initial condition of numerical simulation [58]. Then the Lyapunov time is given by Eq. (6). An excellent consistency between theoretical and numerical results of the Lyapunov time can be observed in Fig. 3. One can find that

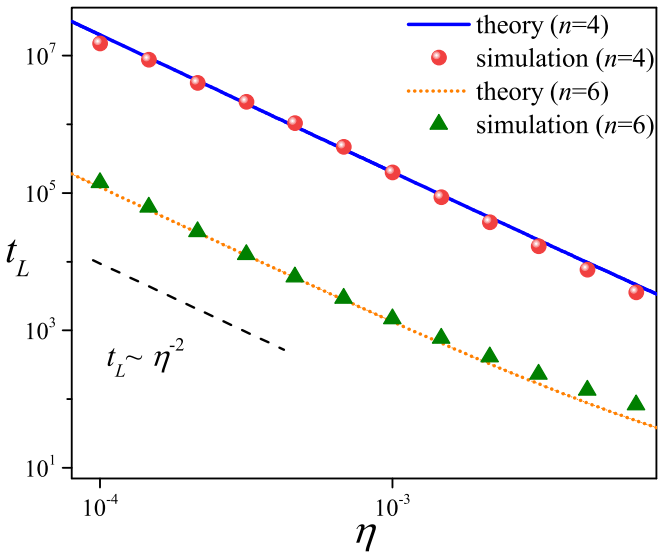

FIG. 3. The Lyapunov time as a function of the nonintegrability strength η, which is obtained by the presented analytical approach (solid line for $n = 4$ and dotted line for $n = 6$) and numerical simulations (solid ball for $n = 4$ and solid triangle for $n = 6$). The dashed line is drawn for $t_L \sim \eta^{-2}$ as a reference.

the Lyapunov time exhibits a universal scaling law

$$t_L \sim \eta^{-2} \tag{22}$$

for both the $n = 4$ and $n = 6$ cases in the regime of weak nonintegrability strength η, which agrees with the prediction by Eq. (20).

In summary, in terms of geometrization of dynamics and SCPT, we present an analytical approach to measure the degree of chaos, i.e., the Lyapunov exponent, in an explicit way. In the quasi-integrable regime, a universal scaling law of the Lyapunov time $t_L \sim \eta^{-2}$ is found. As the verification, the numerical results for the FPUT-like lattices with $n = 4$ and $n = 6$ are computed by molecular-dynamics simulations, which agree well with the analytical results.

It is noteworthy that the universal scaling exponent of the Lyapunov time and the thermalization time are the same. Thus the relation between the Lyapunov time and the thermalization time can be written by

$$t_{\rm eq}(u, \varepsilon) = \alpha t_L(u, \varepsilon), \tag{23}$$

where the proportional coefficient α depends on the initial state of the thermalization process and artificial cutoffs in numerical simulations, such as the global indicator of thermalization and the threshold of the indicator as to quantify the thermalization time. Numerical studies show the scaling law of thermalization remains unchanged with the variation of α [59]. The physical origin and the scope of validness of Eq. (23) are both interesting, which require further studies. In our preliminary opinion, the key for understanding Eq. (23) might be the phase mixing that could be a stronger dynamical property than ergodicity. Note that exponentially fast phase mixing implies exponential separation of trajectories, for which an obvious quantity to be examined is the largest Lyapunov exponent [9]. Accordingly, Eq. (23) implies a relationship between nonlinear dynamics and statistical mechanics.

Furthermore, we also obtain the same universal scaling law for Klein-Gordon-like (also called the ϕ^4-like) chains via this approach [60], which agree with the scaling exponent of the thermalization time [36,61]. As for heterogeneous cases, such as diatomic [35] and disorder [37] lattices, scaling of the thermalization time is the same as the homogeneous cases. Meanwhile, it has been numerically shown that the Lyapunov time does not obviously change in the impurity system [62], which indicates the scaling behavior of the Lyapunov time and Eq. (23) still holds.

Note that there are various ways to define the characteristic time to describe the thermalization process. Yet the Lyapunov time is uniquely defined as to describe the intrinsic property of chaotic systems. In this sense, the thermalization time $t_{\rm eq}$ defined in Ref. [63], which satisfies the proportional relation (23), might be a reasonable candidate. Similarly, we expect that there might also exist an appropriate candidate for the relaxation process in real space, which exhibits the same scaling behavior as the Lyapunov time.

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APPENDIX: SELF-CONSISTENT PHONON THEORY

In this Appendix, we give details on the self-consistent phonon theory. Without loss of generality, the Hamiltonian at Eq. (7) can be written in the following form:

$$H = \sum_i \frac{p_i^2}{2} + U(q_i) + W(q_i - q_{i-1}), \tag{A1}$$

where U and W donate the on-site potential and interaction potential energy. For such a system one can find the Feynman-Jensen inequality for the upper bound of the free energy [48]:

$$\mathcal{F} \leqslant \mathcal{F}_0 + \langle H - H_0 \rangle_0. \tag{A2}$$

The average $\langle\cdot\rangle_0$ is taken with respect to the trial system of free energy $\mathcal{F}_0 = -k_B T \ln Z_0$, where the trial partition function is written as

$$Z_0 = \int e^{-\frac{H_0}{k_B T}} d\mathbf{q} d\mathbf{p}. \tag{A3}$$

The average value of the on-site potential and interaction potential energies can be expressed by

$$\begin{aligned} U_\rho &= \int \frac{dy}{\sqrt{2\pi\rho^2}} e^{-\frac{y^2}{2\rho^2}} U(y), \\ W_\gamma &= \int \frac{dy}{\sqrt{2\pi\gamma^2}} e^{-\frac{y^2}{2\gamma^2}} W(y), \end{aligned} \tag{A4}$$

where ρ^2 and γ^2 correspond to the lattice displacement and two-point correlation function, i.e.,

$$\rho^2 \equiv \langle q_i^2 \rangle = \frac{k_B T}{N} \sum_k \widetilde{\omega}_k^{-2}, \tag{A5}$$

and

$$\gamma^2 \equiv \langle (q_i - q_{i-1})^2 \rangle = \frac{k_B T}{N} \sum_k \frac{4 \sin^2\left(\frac{k}{2}\right)}{\widetilde{\omega}_k^2}, \tag{A6}$$

respectively. By minimizing the right-hand side of Eq. (A2) with respect to $\widetilde{\omega}_k$, one can get the renormalized phonon frequency

$$\widetilde{\omega}_k^2 = 2\left\{ \frac{\partial U_\rho}{\partial \rho^2} + 4 \sin^2\left(\frac{k}{2}\right) \frac{\partial W_\gamma}{\partial \gamma^2} \right\}. \tag{A7}$$

The trial parameters f and f_c in Eq. (8) can be obtained by solving the self-consistent equations (A5)–(A7).

For the FPUT-like lattice described by Eq. (11), in terms of Eq. (A4), one immediately find that the average interaction potential

$$W_\gamma = \frac{1}{2}\gamma^2 + \frac{u(n-1)(n-3)\cdots 1}{n} \gamma^n, \tag{A8}$$

and the average on-site potential $U_\rho = 0$. Noting that the sinusoidal term in Eq. (A6) can be canceled since $U_\rho = 0$, one can get the two-point correlation function

$$u(n-1)(n-3)\cdots 1\gamma^n + \gamma^2 - k_B T = 0, \tag{A9}$$

and the effective force constant

$$f = 1 + u(n-1)(n-3)\cdots 1\gamma^{n-2}. \tag{A10}$$

With Eqs. (A9) and (A10), Eq. (13) can then be obtained.

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