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Analytical measure of temperature for nonlinear dynamical systems

Yue Liu and Dahai He[*]
Department of Physics and Jiujiang Research Institute, Xiamen University, Xiamen 361005, China

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We present an analytical approach for measuring the temperature of nonlinear dynamical systems in the microcanonical ensemble. Via the self-consistent phonon theory, one can analytically obtain the temperature with respect to the internal energy density in a canonical way. We show how that provides a measure of temperature in the microcanonical ensemble, under the hypothesis of ensemble equivalence. Two models, the FPU-β and ϕ^4 lattices, are studied obtaining results consistent with those derived from time averages along trajectories in the phase space. Furthermore, our approach is corroborated by the fact that temperature obtained in terms of the average energy density after thermalization agrees with the thermostat temperature. The hypothesis is validated via examining the energy distribution for different numbers of particles in the canonical ensemble. Further, we have quantified the corresponding finite size effects. Unlike other existing methods, which require time-consuming computations, our analytical approach performance improves with the number of particles.

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I. INTRODUCTION

Temperature, concerning the zero, second, and third laws of thermodynamics, is a cornerstone of thermodynamics and statistical mechanics [1–3]. The thermodynamic temperature T is defined as

$$\frac{1}{T} = \left(\frac{\partial S}{\partial E}\right)_M, \tag{1}$$

where S is entropy, E is the internal energy, and $M = \{M_1, M_2, \ldots\}$ are parameters, such as volume or external fields [4]. If a system is in contact with a heat bath, temperature is well defined as a parameter in the distribution function and as a measure of thermal fluctuations. However, if the system is isolated, the notion of temperature is subtle and must be derived from entropy in the microcanonical ensemble. Although there are many definitions of entropy [3] for dynamical systems, such as "surface" entropy obtained by Boltzmann and "volume" entropy derived by Gibbs, the temperatures obtained by these definitions in general approach the same value as the degrees of freedom tend to infinity. However, using Boltzmann entropy may lead to negative temperature for specific systems, such as spin system and classical pendulum [3,5–10]. The development of molecular dynamics simulations has further stimulated the interest for evaluating temperature in practical systems.

Considering the global geometric structure of the energy surface, Rugh [11,12] has proposed a dynamical expression for the temperature of Hamiltonian systems, which we denote T_R. Using Eq. (1) and the statistical physics definition of entropy, the temperature of isolated systems can be expressed by

$$\frac{1}{k_B T_R} = \lim_{t\to\infty} \frac{1}{t}\int_0^t \Psi(\mathbf{q}, \mathbf{p})d\tau, \tag{2}$$

where $\mathbf{q}$ and $\mathbf{p}$ are the canonical coordinates and momenta, respectively. Here one has [11,12]

$$\Psi = \nabla \cdot \left(\frac{\nabla H}{\|\nabla^2 H\|}\right), \tag{3}$$

where the gradient $\nabla = (\frac{\partial}{\partial \mathbf{q}}, \frac{\partial}{\partial \mathbf{p}})$ refers to the full phase space and H represents the Hamiltonian of the systems, and $\langle\cdot\rangle$ denotes the microcanonical average on the energy constant hypersurface. Jepps *et al.* [13], as well as Rickayzen and Powles [14], have generalized Rugh's formula as $\Psi = \nabla \cdot (\frac{\mathbf{B}}{\mathbf{B}\cdot\nabla H})$, where $\mathbf{B}$ is an arbitrary continuous and differentiable vector in phase space. Note that Eq. (3) is recovered when $\mathbf{B} = \nabla H$. When considering the choice $\mathbf{B} = \nabla V$, where V is the potential of the Hamiltonian, one obtains $\Psi = \nabla \cdot (\frac{\nabla V}{\|\nabla^2 V\|})$. This yields the configurational temperature [15–17], which provides a definition of the temperature only in terms of the coordinates and has been used for checking the algorithmic correctness of Monte Carlo programs as well as for designing new thermostats [13,18]. The above dynamical approaches have been widely used to study the temperature of spin systems [19–22], liquid [23], plasmas [24], and nonlinear lattice systems [12,18,25,26]. In particular, for one-dimensional lattice systems, Ψ can be written as [12,18]

$$\Psi = \frac{N-2}{\sum_{i=1}^N p_i^2}. \tag{4}$$

Note that the counting of degrees of freedom depends on the symmetry of the Hamiltonian. For systems conserving only energy, e.g., the ϕ^4 system, the numerator in Eq. (4) should be $N-1$. If the total momentum of systems is also conserved, e.g., the FPU-β system, the numerator should be $N-2$ instead [18].

All the above methods quantify temperature mainly in a numerical way. Yet analytical quantifications of temperature with respect to the energy of nonlinear systems seem unavailable so far. In this paper, using the self-consistent

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[*] dhe@xmu.edu.cn

phonon theory (SCPT), we propose an analytical approach to quantify the relation between temperature and energy for nonlinear Hamiltonian systems in the microcanonical ensemble. For illustrating the validity of our approach, we apply it to two popular models, namely, the FPU-β lattice and the ϕ^4 lattice. Meanwhile, the dynamical approach [11,12] and a thermalization method are also employed as for comparison, which shows that our approach is validated in the system of large size (see the discussion part). Note that our approach can be generalized to high-dimensional lattices of interacting oscillators [27,28].

The paper is organized as follows. In Sec. II, we briefly introduce the SCPT and derive the expression of temperature. In Sec. III, the temperature of two typical lattice models (FPU-β and ϕ^4) are studied. We then compare our analytical approach with Rugh's method and with the thermalization method. Finally, we summarize our main results and give a discussion in Sec. IV.

II. SELF-CONSISTENT PHONON THEORY

In this section, we use the self-consistent phonon theory for a one-dimensional Hamiltonian system to derive the temperature for dynamical systems in the microcanonical ensemble. In literature, SCPT, that can be traced back to Feynman [29], has been developed to study the properties of thermal conduction in low-dimensional nonlinear lattices [27,28,30,31].

Without loss of generality, we consider the Hamiltonian of a one-dimensional system in the form of

$$H = \sum_n \frac{p_n^2}{2m} + W(\delta q_n) + V(q_n), \tag{5}$$

where $\delta q_n = q_n - q_{n-1}$, $W(\delta q)$, and $V(q)$ are the nearest-neighbor interaction and on-site potentials, respectively. The partition function of systems in the canonical ensemble can be written by

$$Z = \int e^{-H/(k_B T)} d\mathbf{q}\, d\mathbf{p}. \tag{6}$$

An exact evaluation of the integral of the partition function Eq. (6) is generally impossible, due to the presence of nonlinearity in Eq. (5). The key idea of SCPT is replacing the original Hamiltonian by a trial Hamiltonian that allows an approximate evaluation of the exact partition function given by Eq. (6). A reasonable choice of the trial Hamiltonian is a chain of N coupled harmonic oscillators in the form of

$$H_0 = \sum_n \frac{p_n^2}{2m} + \frac{f_c}{2}(q_n - q_{n-1})^2 + \frac{f}{2} q_n^2, \tag{7}$$

where the trial parameters f_c and f are to be obtained by minimizing the right-hand side of the Feynman-Jensen inequality for free energies:

$$\mathcal{F} \leqslant \mathcal{F}_0 + \langle H - H_0 \rangle_0. \tag{8}$$

In Eq. (8) the average 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

$$Z_0 = \int e^{-H_0/(k_B T)} d\mathbf{q}\, d\mathbf{p}. \tag{9}$$

The average in Eq. (8) can be easily calculated because the integrand is of a quadratic form. Then one can obtain the renormalized phonon frequency

$$\omega_p^2 = \frac{2}{m}\left\{\frac{\partial V_\rho}{\partial \rho^2} + 4\sin^2\left(\frac{p\pi}{N}\right)\frac{\partial W_\gamma}{\partial \gamma^2}\right\}, \tag{10}$$

where V_ρ and W_γ are the average value of the on-site potential and interaction potential energies, respectively,

$$\begin{aligned} V_\rho &= \int \frac{dy}{\sqrt{2\pi\rho^2}} e^{-\frac{y^2}{2\rho^2}} V(y), \\ W_\gamma &= \int \frac{dy}{\sqrt{2\pi\gamma^2}} e^{-\frac{y^2}{2\gamma^2}} W(y). \end{aligned} \tag{11}$$

In Eq. (11), ρ^2 and γ^2 correspond to the lattice displacement and the two-point correlation function, i.e.,

$$\rho^2 \equiv \langle q_n^2 \rangle = \frac{k_B T}{Nm} \sum_p \omega_p^{-2} \tag{12}$$

and

$$\gamma^2 \equiv \langle (q_n - q_{n-1})^2 \rangle = \frac{k_B T}{Nm} \sum_p \frac{4\sin^2\left(\frac{p\pi}{N}\right)}{\omega_p^2}. \tag{13}$$

One can obtain the trial parameters f_c and f in Eq. (7) by solving the self-consistent equations (10)–(13).

Therefore, the self-consistent approach illustrated above yields the average internal energy density as

$$\langle \varepsilon \rangle_c = \left\langle \frac{p_n^2}{2m} \right\rangle + W_\gamma + V_\rho. \tag{14}$$

Note that $\langle p_n^2/m \rangle = k_B T$, where T is the kinetic temperature of the system in the canonical ensemble. In the thermodynamic limit $N \to \infty$, the microcanonical ensemble is generally equivalent to the canonical ensemble if the energy of the microcanonical system equals the internal energy of its corresponding canonical system, i.e., $\varepsilon = \langle \varepsilon \rangle_c$. Under such a hypothesis, the temperature of microcanonical systems can be written as

$$k_B T = 2(\varepsilon - W_\gamma - V_\rho). \tag{15}$$

Equation (15) gives a general relation between the temperature and the energy density of a dynamical system, from the perspective of the microcanonical ensemble.

One can immediately assure Eq. (15) for the harmonic system, for which $W(\delta q_n) = k\delta q_n^2/2$ and $V(q_n) = f_0 q_n^2/2$. Here k is the coupling strength and f_0 the strength of the harmonic on-site potential. According to Eq. (11),

$$W_\gamma = \frac{k}{2}\gamma^2, \quad V_\rho = \frac{f_0}{2}\rho^2. \tag{16}$$

It is then straightforward to obtain the temperature of the harmonic system as

$$k_B T = \varepsilon, \tag{17}$$

which is consistent with the equipartition theorem.

III. RESULTS FOR TWO MODELS

In this section, we apply our approach to the temperature of two one-dimensional nonlinear lattices, i.e., the FPU-β lattice and the ϕ^4 lattice. The approach is then validated in two ways. First, according to Rugh's method [11,12], Ψ can be written by Eq. (4) [18]. In order to obtain the temperature (denoted by T_R) of the systems in terms of Eqs. (2) and (4), we employ the *SABA*$_2C$ symplectic algorithm [32], which is of a ten-order symplectic integrator, to integrate the equations of motion derived from the Hamiltonian Eq. (5). In our simulations, the integration time step is $\Delta t = 0.01$ and the energy drift can be less than 10^{-6} for simulations of 10^8 time steps.

Second, we compare the SCPT results with those by a "thermalization method," since temperature is well defined when the system is in contact with a heat bath. As a first step, the systems are fully thermalized by linking each site to a Langevin heat bath [33,34] at temperature T_b. After thermalization, heat baths are removed and the energy density ε of the isolated Hamiltonian systems Eq. (5) can be obtained. Here, the energy density is averaged over 10^4 realizations, in order to reduce the fluctuations due to the finite-size effects. Then the temperature $T(\varepsilon)$ in terms of Eq. (15) is compared with the temperature of heat baths T_b.

In our numerical simulations, the Boltzmann's constant k_B and the mass m are set as units, i.e., $k_B = 1$ and $m = 1$. But for the sake of clarification, we keep k_B and m in all the following formulas.

A. FPU-β lattice

The FPU-β lattice, originally proposed to study the problem of energy equipartition [35], has on-site potential $V(x) = 0$ and interaction potential

$$W(\delta x_n) = \frac{k}{2}\delta q_n^2 + \frac{\beta}{4}\delta q_n^4. \tag{18}$$

In terms of Eq. (11), one can easily obtain the average interaction potential

$$W_\gamma = \frac{k}{2}\gamma^2 + \frac{3}{4}\beta\gamma^4. \tag{19}$$

Noting that sinusoidal terms in the summation of Eq. (13) are canceled, one can explicitly get the two-point correlation function

$$\gamma^2 = \frac{-k + \sqrt{k^2 + 12\beta k_B T}}{6\beta} \tag{20}$$

and the effective force constant

$$f_c = k + 3\beta\gamma^2. \tag{21}$$

Therefore, in terms of Eq. (15), the temperature of the FPU-β system can be explicitly given by

$$k_B T = \frac{36\beta\varepsilon + 2k^2 - 2k\sqrt{k^2 + 9\beta\varepsilon}}{27\beta}. \tag{22}$$

Note that, for harmonic limit $\beta \to 0$ in Eq. (22), one finds $k_B T = \varepsilon$, which is consistent with Eq. (17). For the limit $\beta \to \infty$, one finds $k_B T = \frac{4}{3}\varepsilon$.

We compare the results obtained by numerical simulations in terms of Rugh's method with that by SCPT. Figure 1(a) depicts temperature versus the nonlinear strength β with fixed energy density $\varepsilon = 1$, showing that differences between T and T_R are slight. The temperature T as the function of the energy density ε, with fixed nonlinear strength $\beta = 1$, is shown in Fig. 1(b). One can see an excellent agreement between Rugh's method and SCPT.

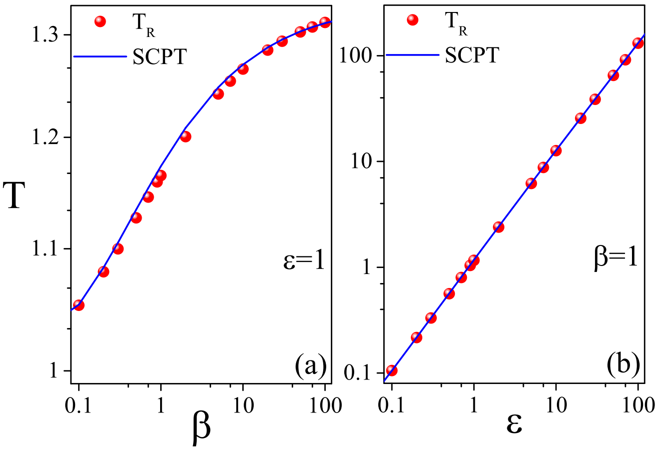

FIG. 1. Comparing the temperature obtained by SCPT with that by Rugh's dynamical approach (as denoted by T_R) for the FPU-β model. (a) Temperature as a function of the nonlinear strength β with fixed energy density $\varepsilon = 1$ and (b) temperature as a function of the energy density ε with fixed nonlinear strength $\beta = 1$. Here $k = 1$ and $N = 1024$.

Next, Langevin heat baths at temperature T_b are connected to each site for a long time to guarantee the systems are fully thermalized at T_b. We obtain the energy density for the Hamiltonian Eq. (5); then we calculate the temperature T according to Eq. (22). For comparison with the thermalization method, one can see in Fig. 2(a) that the temperature T calculated by SCPT slightly fluctuates around the reference line

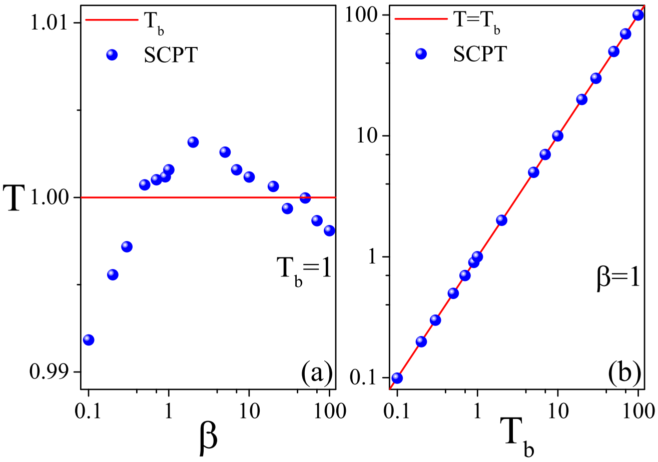

FIG. 2. Comparing temperature obtained by SCPT with the temperature of heat bath used to thermalize the FPU-β system (see text for details). (a) Temperature versus the nonlinear strength β when the temperature of heat bath $T_b = 1$. The solid line corresponds to the reference value $T_b = 1$. (b) Temperature versus T_b with fixed $\beta = 1$. The solid line represents the reference line $T = T_b$. One can see a good agreement between T and T_b. Here $k = 1$ and $N = 1024$.

$T_b = 1$. The change of T with T_b is depicted in Fig. 2(b), in which one finds that temperature obtained by SCPT coincides with the solid line $T = T_b$. These results indicate the validity of our approach.

B. ϕ^4 lattice

The ϕ^4 lattice is a typical model in which total momentum is not conserved. Its Hamiltonian consists of not only a harmonic interaction potential

$$W(\delta q_n) = \frac{k}{2}\delta q_n^2, \tag{23}$$

but also of a quartic on-site potential

$$V(q_n) = \frac{\lambda}{4}q_n^4. \tag{24}$$

In terms of Eq. (11), W_γ and V_ρ are given by

$$\begin{aligned} W_\gamma &= \frac{k}{2}\gamma^2, \\ V_\rho &= \frac{3}{4}\lambda\rho^4. \end{aligned} \tag{25}$$

The summation of Eq. (12) can be replaced by an integral as the system size is large, which yields

$$\rho^2 = \frac{k_B T}{\sqrt{3\lambda\rho^2(3\lambda\rho^2 + 4k)}}. \tag{26}$$

Then the effective force constant f in Eq. (7) is given by

$$f = 3\lambda\rho^2 = \frac{3\lambda k_B T}{\sqrt{f(f + 4k)}}. \tag{27}$$

Solving Eq. (13) as well as Eq. (10), we can get the relation between γ and f,

$$\gamma^2 = \frac{k_B T}{k} - \frac{f^2}{3\lambda k}. \tag{28}$$

Finally, according to Eq. (15), the temperature of the ϕ^4 system is given by

$$k_B T = \varepsilon + \frac{f^2}{12\lambda}. \tag{29}$$

Considering Eqs. (27) and (29), one gets the following equation:

$$16(k_B T - \varepsilon)^2 - k_B^2 T^2 + 16k\sqrt{\frac{4}{3\lambda}}(k_B T - \varepsilon)^{\frac{3}{2}} = 0. \tag{30}$$

The temperature of the ϕ^4 system can be equivalently obtained by solving Eq. (30). Like for the FPU-β model, one gets $k_B T = \varepsilon$ in the harmonic limit $\lambda \to 0$ and $k_B T = \frac{4}{3}\varepsilon$ in the strong nonlinearity limit $\lambda \to \infty$.

Similar to the FPU-β model, we first compare our results with those by Rugh's method. It is seen from Fig. 3(a) that the deviation between T and T_R is small for fixed $\varepsilon = 1$. Figure 3(b) shows T as a function of the energy density ε, with fixed nonlinear strength $\lambda = 1$. An excellent consistency between T and T_R can be observed.

As for comparison with the thermalization method for the ϕ^4 model, one can see in Fig. 4(a) that T obtained by SCPT is slightly larger than the thermostat temperature, which is fixed at $T_b = 1$. In Fig. 4(b), we illustrate the temperature T as a function of T_b. The nice consistency between T and T_b is observed, which supports the validity of our theory for the ϕ^4 model.

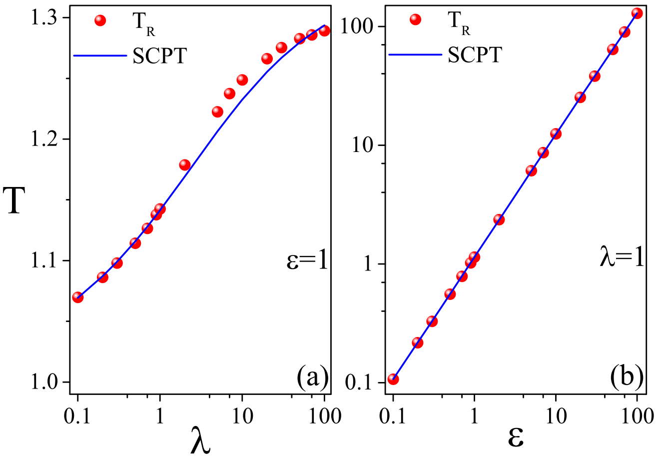

FIG. 3. Comparing the temperature obtained by SCPT with that by Rugh's dynamical approach for the ϕ^4 model. (a) Temperature as a function of the nonlinear strength λ with fixed energy density $\varepsilon = 1$ and (b) temperature as a function of the energy density ε with fixed nonlinear strength $\lambda = 1$. Here $k = 1$ and $N = 1024$.

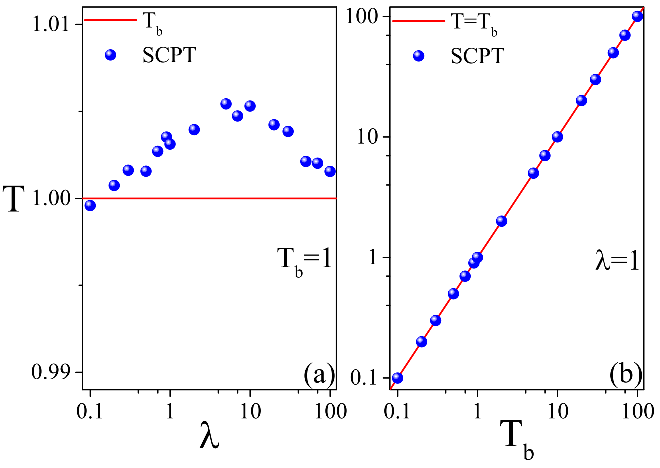

FIG. 4. Comparing the temperature obtained by SCPT with the temperature of heat bath used to thermalize the ϕ^4 system (see text for details). (a) Temperature versus the nonlinear strength λ as the temperature of heat bath $T_b = 1$. The solid line corresponds to the reference value $T_b = 1$. (b) Temperature versus T_b with fixed $\lambda = 1$. The solid line represents the reference line $T = T_b$. One can see a good agreement between T and T_b. Here $k = 1$ and $N = 1024$.

IV. SUMMARY AND DISCUSSIONS

In summary, we presented an analytical approach to measure temperature in nonlinear dynamical systems in the microcanonical ensemble and we gave a general relation between temperature and energy density for nonlinear interacting lattice systems. As an exemplification, we applied our approach to two typical nonlinear lattices: the FPU-β lattice and the ϕ^4

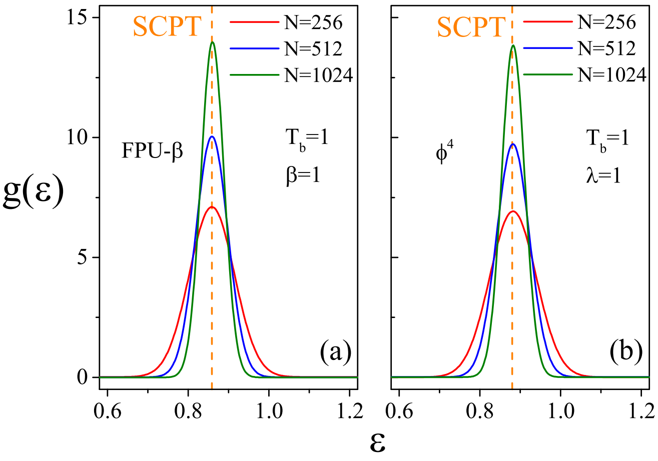

FIG. 5. Energy density distribution g(ε) for (a) the FPU-β lattice and (b) the ϕ^4 lattice. The red, blue, and green solid lines correspond to the number of particles $N = 256$, 512, and 1024, respectively. The orange dashed lines represent the average energy density obtained by SCPT. Here nonlinearity strengths are given by $\beta = 1$ and λ=1. And the thermostat temperatures are $T_b = 1$ for both cases. The distributions are obtained in terms of average over 10^4 realizations.

lattice. Furthermore, the dynamical approach to temperature and the thermalization method were used in order to validate our approach. Our results show that the approach is consistent with the two methods for both models, indicating its validity. In comparison with Rugh's numerical method, our approach is especially effective for systems of large size. Note that our method can be in principle generalized to high-dimensional systems of nonlocal interactions (e.g., next-nearest neighbor interactions).

SCPT actually lies in the canonical ensemble, while the systems we considered are in the microcanonical ensemble. The energy is a constant (restricted to a very narrow range) for a system in the microcanonical ensemble, while it fluctuates between zero and infinity for the system in the canonical ensemble. How can we ensure the temperature derived from a canonical ensemble can measure a system in the microcanonical ensemble? To explain the problem, we first examined the energy distribution of the systems. After full thermalization, we obtained the probability density function of the energy density over 10^4 statistical samples. In Fig. 5, we depicted the distribution of energy density for the two models, i.e., the FPU-β model [Fig. 5(a)] and the ϕ_4 model [Fig. 5(b)]. As one can see, for both models, the probability density is a normal distribution and the average $\langle\varepsilon\rangle$ (the most probable value corresponding to the peak) agrees with that calculated by SCPT [Eq. (15)] denoted by the dashed line. Moreover, as the number of particles increases, the distribution becomes sharper and sharper. It is thus reasonable to conjecture that the distribution approaches a δ function when $N \to \infty$, which corresponds to the microcanonical ensemble with $\varepsilon = \langle\varepsilon\rangle$. In fact, it has been indicated that the ratio of the canonical temperature and the microcanonical temperature is $(N-2)/N$, which approaches 1 when $N \to \infty$ [12]. Secondly, we examined the finite size effects of our calculations, as shown in Fig. 6. Rugh's method coincides with our approach with small deviations, which is practically satisfactory when $N > 1000$ for the FPU-β [Fig. 6(a)] and the ϕ_4 model [Fig. 6(b)]. For the thermalization method,

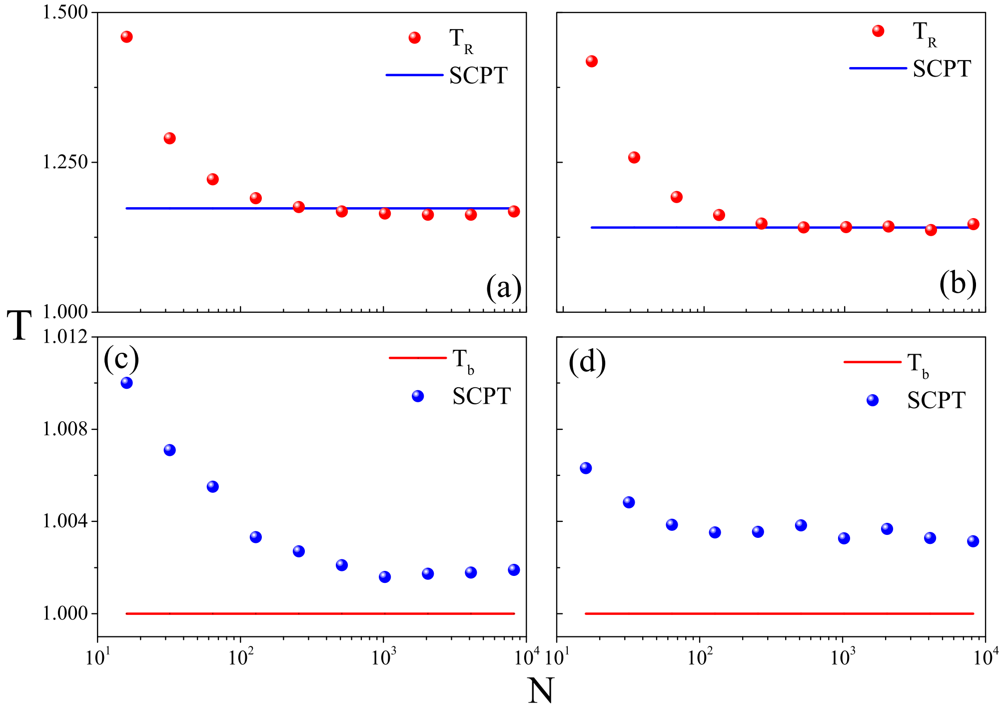

FIG. 6. Temperature T as a function of the system size N. First, our approach is compared with Rugh's method for (a) the FPU-β model and (b) the ϕ^4 model, respectively. Second, our approach is compared with the thermalization method (see text for details) for (c) the FPU-β model and (d) the ϕ^4 model, respectively. In our calculations, the parameters are given by $\beta = 1$, $\lambda = 1$, and $\varepsilon = 1$.

one can see the fluctuations of SCPT calculations [Figs. 6(c) and 6(d)] since the average energy density obtained after thermalization has finite size dependence. Yet, the relative difference between T and T_b is less than 0.5% as $N > 100$. The discrepancy mainly comes from invalidity of the assumption of ensemble equivalence at small system size. We thus propose our approach as an analytically viable approach to the calculation of temperature in interacting systems of many particles.

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