Predicting and identifying finite-size effects in current spectra of one-dimensional oscillator chains

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The existence of a finite-size effect in one-dimensional oscillator systems causing the energy current power spectrum to saturate to a constant value at low frequencies is discussed. It is shown that a mode-coupling theory presented in earlier papers can be used to predict the frequency of onset of this finite-size effect. This can be used by researchers to plan simulations with large enough numbers of particles to avoid the presence of this finite-size effect.

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I. INTRODUCTION

Transport in one-dimensional (1D) systems has been intensely studied for decades [1,2]. One topic of interest has been the asymptotic exponent with which the heat current power spectrum diverges at low frequencies. That is, the heat current power spectrum, $\tilde{C}_\kappa(\omega)$, is thought to diverge as some $\omega^{-\alpha}$ with α becoming constant at some sufficiently low frequency. Various theoretical proposals have been put forward to explain the variety of results seen [2–7]. However, current laboratory experiments are unable to measure current power spectra to the precision needed to test these theories. Thus, for the time being, we are forced to rely on simulations to test theories on the mechanisms of heat conduction in 1D systems. To date the results of these simulations has often been quite contradictory [1,2].

Critically in these studies it is necessary to try to determine the low-frequency asymptotic transport behavior in 1D systems. So, it is the limit as the system length $L \to \infty$ and $\omega \to 0$ that is of most interest. Thus, where simulations are being used in an attempt to approach this limit it becomes crucial to be able to discern whether results of the simulation display finite-size effects. In many papers reporting simulation results of this sort the authors tentatively identify finite-size effects in the low-frequency parts of the simulation data (e.g., Ref. [8]). In some papers authors carry out simulations for several chain lengths in order to identify whether observed low-frequency behavior is a finite-size effect (e.g., Ref. [9]). In other cases arguments have been carried on within the literature about whether an observed low-frequency behavior is the desired asymptotic behavior or just a finite-size effect (see Ref. [10] and follow-up comments in Refs. [11,12]).

The identification of finite-size effects is crucial to the discussion of what constitute asymptotic behavior in necessarily finite systems, which are simulated. Despite this, relatively little has been written explicitly on the nature of the finite-size effects seen in transport in 1D chains. To the extent that finite-size effects appear in the literature, it is pointed to in the low-frequency behavior of simulation results being used to examine something else. An exception to this is a recent paper [13] that paid much-needed attention to this topic. In that paper the authors examine the effect of periodic recurrence in the state correlation function $R(t) = \langle \mathbf{r}(0)\mathbf{r}(t)\rangle$, where $\mathbf{r}(t)$ is simply the phase space state vector of the system at time t. $R(t)$ is observed to exhibit a recurrence with period L/v_s, where L is the system length and v_s is the thermodynamic speed of sound in the system. They show that in a diatomic hard-point gas model the recurrences in $R(t)$ give rise to a periodic oscillation in the energy current correlation function. On the other hand, in the FPU-β system, while the recurrence in $R(t)$ is present it does not give rise to any oscillations in the current correlation function.

In the present paper we intend to demonstrate the source of another finite-size effect. It is quite well known that in the heat current power spectra of 1D chains a saturation is often seen at the lowest frequencies. Running simulations at several system lengths generally reveals this to be a finite-size effect [9]. This is a particularly troubling finite-size effect since it could easily lead to misidentification of the asymptotic exponent α. The saturation is presumably due to the absence of modes below a cutoff frequency, which could contribute to transport at those frequencies. However, as we will demonstrate in this paper, it is possible to use mode-coupling theory to predict the frequency at which this finite-size saturation will occur for any given chain length. This is extremely useful since it allows simulations to be planned in which the investigator can be confident that this finite-size saturation will not occur.

II. THEORY

The finite-size effect that will be discussed in the present paper turns out to be predicted by mode-coupling theory. Furthermore, the frequency at which it manifests can be predicted from mode-coupling theory. We will, thus, briefly review a few key aspects of mode-coupling theory focusing on the specific version of the theory that we will use to predict onset of the effect that is of current interest. Many varieties of mode-coupling theory can be constructed. A good early review is found in Ref. [14]. A particularly influential construction of mode-coupling theory can be found in Ref. [15]. Mode-coupling theories of various types have been used by various researchers to try to explain what the limiting value of the exponent, α, should be and these have resulted in a variety of often contradictory predictions. Early examples are well summarized in Refs. [1,2]. A good example of the approach, and its difficulties, is presented in Refs. [8,16], where a very conventional mode-coupling theory approach is employed to predict that modes damp on time scales that scale as $k^{-5/6}$ rather than the k^{-2} behavior of classical hydrodynamics. This is then used to predict $\alpha = 2/5$, except that in Ref. [8] a midfrequency regime with $\tilde{C}_\kappa(\omega) \approx \omega^{-1/2}$ is predicted in some

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cases. However, this approach was criticized as internally inconsistent in Ref. [17], where it is pointed out that $\omega \sim k$ was incorrectly used in obtaining the damping time scales. In that paper it is argued using renormalization group theory that $\alpha \sim 1/3$. A somewhat different mode-coupling approach, using an Ansatz for the time scaling of damping, was employed more recently in Ref. [18], where it was found that $\alpha = 2/5$ in purely longitudinal systems (what is usually meant by 1D heat transport) but that $\alpha = 1/3$ in systems with transverse motions (which some authors call "quasi-1D"). However, this was criticized in Ref. [6], where still another mode-coupling approach (separation of phase and amplitude dynamics) yields a prediction of $\alpha = 1/3$. In that same paper, however, the numerical results show different behavior for the FPU-β system, which the authors speculate is indicative that it belongs to a different universality class.

The foregoing paragraph simply shows that there is currently considerable controversy over the form of the mode-coupling theory that should be used, or, indeed, whether mode-coupling theory can even reliably predict α. It is also clear that the simulation results in the literature have been limited in their ability to distinguish conclusively between various proposed values of α. For the present paper we are not concerned with the value of α. Nor are we directly concerned with the distinctions among the various mode-coupling theories referenced above. We will instead use a simpler (even crude) form of mode-coupling theory, which was previously introduced in Refs. [7,19]. This theory is somewhat less ambitious than the ones presented in Refs. [6,8,16,18] in that it requires input of high-frequency behavior of the various current power spectra. However, given this input—which could come from theory, experiment, or simulation—it predicts the low-frequency behavior of the power spectra with no adjustable parameters. Further, it is able not only to predict the power α but actually predicts the absolute size of the heat current power spectrum. This theory is fully presented in Refs. [7,19], so all that will be presented here is a condensed description of the theory focusing on those aspects that are particularly relevant to prediction of the finite-size effect that is the topic of this paper.

We start from the assumption that energy is carried in the system by sound modes and that the contribution due to each sound mode is simply $c\delta\epsilon(k',t)$, where c is the thermodynamic speed of sound and $\delta\epsilon(k',t)$ is the k'th mode of the spatial Fourier transform of the deviation from equilibrium of the energy density at time t. Each mode of the energy-density deviation is assumed to damp exponentially as

$$\delta\epsilon(k',t) = \delta\epsilon(k',0)e^{-\Gamma k'^2|t|}, \tag{1}$$

where Γ is a sound damping coefficient. However, unlike in classical hydrodynamics, Γ is assumed to be a microscopic variable with dependence on k' so that each mode has its own sound-damping coefficient, $\Gamma_{k'}$. In the harmonic limit we expect that $\langle[\delta\epsilon(k',t)]^2\rangle = 1/\beta^2$, where $\beta = 1/k_B T$. Thus, we can obtain the energy-current power spectrum by Fourier-transforming these mode contributions with respect to time and then summing over all modes. This gives

$$\tilde{C}_\kappa(\omega) = \frac{2c^2}{L\beta^2}\sum_{k'}\frac{\Gamma_{k'}k'^2}{\omega^2 + (\Gamma_{k'}k'^2)^2}, \tag{2}$$

where L is the system length, and the sum is over the whole reciprocal lattice restricted to the number of particles, N, in the system.

We now *speculate* that the microscopic sound-damping coefficient can be obtained by direct analogy with the macroscopic sound damping coefficient via

$$\Gamma_{k'} = \Gamma_{\omega'/c} \equiv \Gamma(\omega') = \frac{\gamma - 1}{\rho c_P}\kappa(\omega') + \frac{1}{\rho}\zeta(\omega'), \tag{3}$$

where c_P is the constant pressure specific heat capacity, ρ is the mass density, $\gamma \equiv c_P/c_V$ is the ratio of specific heat capacities, and $\kappa(\omega')$ and $\zeta(\omega')$ are the microscopic heat capacity and microscopic bulk viscosity, respectively, as defined from the appropriate Kubo relations

$$\kappa(\omega) = \frac{\beta^2 k_B}{2}\tilde{C}_\kappa(\omega), \tag{4}$$

$$\zeta(\omega) = \frac{\beta}{2}\tilde{C}_\zeta(\omega). \tag{5}$$

At first sight this looks nonsensical since $\tilde{C}_\kappa(\omega)$ depends on itself through the dependence of $\Gamma_{k'}$ on $\kappa(\omega')$. However, the sum in Eq. (2) can be shown to be dominated by terms corresponding to modes with $\Gamma_{k'}k'^2 \simeq \omega$. This relieves the circularity so that $\tilde{C}_\kappa(\omega)$ at any ω is determined by the much-higher-frequency parts of $\kappa(\omega)$ and $\zeta(\omega)$. This is an example of a "mode cascade."

The terms in the reciprocal lattice sum are Lorentzians. The way certain terms dominate below the frequency cutoffs described above is simply that this is the frequency scale of the turnover of the Lorentzian curve. Thus, for any term due to k' where $\Gamma_{k'}k'^2 \ll \omega$, the term gives a "flat" contribution, essentially independent of ω. If the minimum wave vector in the reciprocal lattice is $k'_{\min}$, then at all frequencies lower than $\Gamma_{k'_{\min}}{k'_{\min}}^2$ the predicted energy current power spectrum is flat.

Thus, assuming we have a target minimum frequency, $\omega_{\min}$, the above provides a prescription for finding the minimum number of particles that must be simulated in order to avoid seeing finite-size effects. The main difficulty is that we do not, *a priori*, know $\Gamma_{k'_{\min}}$. In some systems (such as the pure quartic chain studied in Ref. [7]) it is possible to get at least a rough analytical prediction of this quantity, which could be fed into the mode-mode coupling theory. In most systems this is not possible. However, in these systems short simulations can be carried out to obtain $\Gamma_{k'}$ at high frequencies. These short simulations are usually orders of magnitude less numerically intensive than the simulations that will actually probe the behavior down to $\omega_{\min}$. Having completed these short simulations the current power spectra can be fed into the mode-mode coupling theory to generate a prediction of the lower-frequency behavior of the heat-current power spectrum.

A key point is that the sum in the theory can be carried out for any system size. That is, it is not restricted to being carried out using the system size of the simulation runs that is being used to feed the high-frequency behaviors into the theory. Thus, because of the mode cascade, we can obtain predictions of low-frequency behavior, including finite-size saturation, by feeding relatively short-run data into the theory, as long as the sum in the theory is carried out using the reciprocal lattice of a

larger system. From this point on we will distinguish between N, which is the number particles actually used in a simulation, from n, which will be taken as the system size used for a reciprocal lattice sum within the mode-coupling theory.

III. NUMERICAL RESULTS

We work with a cubic-plus-quartic chain (an FPU-$\alpha\beta$ chain with the harmonic coefficient set to zero). For all runs in this paper we use the parameters $\alpha = 2$, $B = 1$, $P = 0$, $T = 1$, which were well studied in Ref. [19].

Figure 1 shows how a short set of simulation runs can be used as input to the mode-mode coupling theory to predict how many particles are needed in the chain to ensure that no finite-size effects are seen at the lowest frequencies of a longer set of runs. A set of runs with number of particles, $N = 2^{10}$, and final time, $t_f = 2^{18}$, were used to generate theoretical predictions out to frequencies below 2^{-22} for several target values of n. These show that to see no finite-size effects at these frequencies, a minimum of 2^{14} particles are needed. A set of runs with $N = 2^{14}$, $t_f = 2^{22}$ follow the $N = 2^{14}$ prediction quite well at low frequencies where the theory is valid. A theoretical curve generated from the $N = 2^{14}$ simulations demonstrates that the theoretical prediction is not appreciably influenced by the value of N used in the simulation data that is used as input to the theory.

Figure 2 shows simulation runs for two values of N and corresponding theoretical predictions. The finite-size effects predicted in the $N = 2^{10}$ curve are clear in the data from the simulation that used $N = 2^{10}$. This clearly demonstrates that the finite-size saturation predicted by the mode-mode coupling is observed in the simulations.

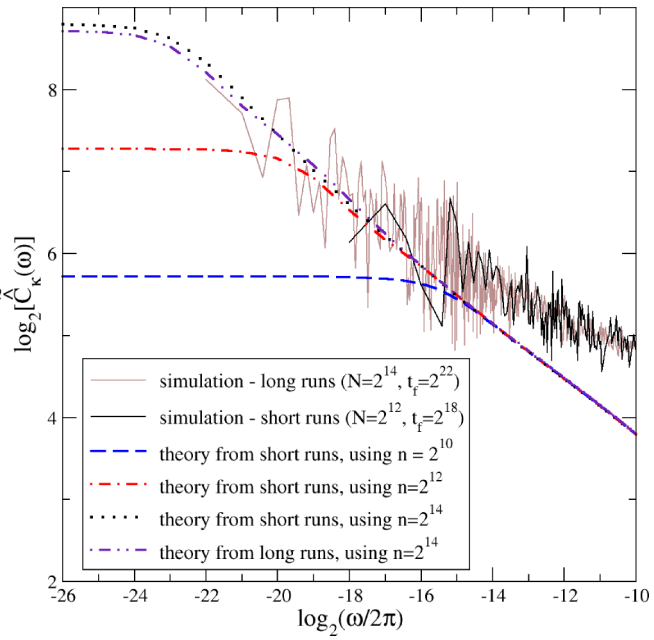

FIG. 1. (Color online) Energy current power spectrum for a set of short runs ($N = 2^{12}$,$t_f = 2^{18}$) and long runs ($N = 2^{12}$,$t_f = 2^{18}$). Also shown are theoretical curves generated by the mode-mode coupling theory from Ref. [7]. These were generated from the short-run data using $n = 2^{10}$, 2^{12}, and 2^{14}. For comparison, the theoretical curve generated from the long runs is also shown.

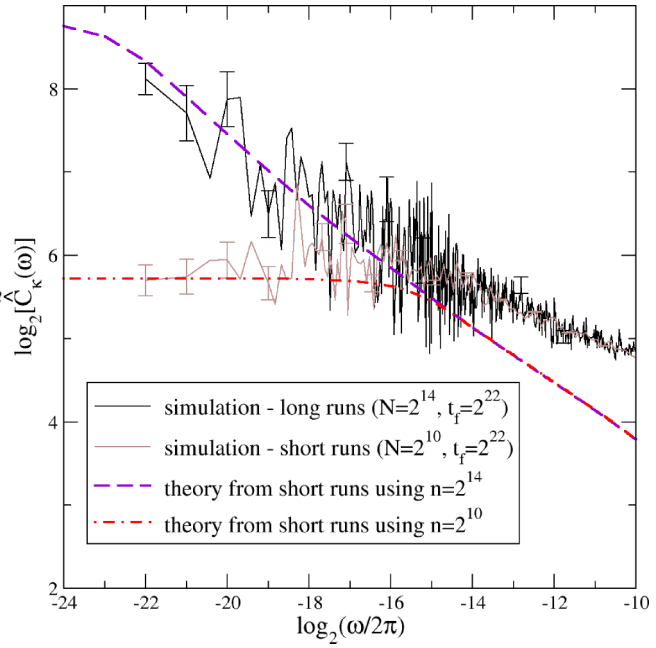

FIG. 2. (Color online) Energy-current power spectrum for a set of long runs ($N = 2^{14}$,$t_f = 2^{22}$) and a set of shorter runs ($N = 2^{10}$,$t_f = 2^{22}$). Also shown are theoretical curves generated from the shorter runs using $n = 2^{10}$ and 2^{12}.

IV. DISCUSSION AND CONCLUSIONS

Our aim in the present paper is very practical. We aim to provide a prescription that any researcher can apply when they wish to simulate a 1D system to determine how large their system needs to be to probe the behavior of the thermal conductivity down to a target frequency. We have shown that this prescription works well for a restricted version of the FPU-$\alpha\beta$ system. It can be expected to work for any system for which the mode-mode coupling theory introduced in Ref. [7] applies. It is not currently known what the range of applicability of this theory is. However, on the strength of its success with FPU systems it is probably applicable to any 1D chain with polynomial interparticle potentials and no onsite potentials. We also have evidence, which will be presented in a forthcoming paper, that the theory applies to at least some systems with hard-core and step-function potentials. It is known not to apply to the momentum-conserving-ding-a-ling system [20], which has a mix of hard-core and harmonic potentials.

Beyond providing a practical tool, this paper also further demonstrates the ability of the mode-mode coupling theory of Ref. [7] to predict a number of features of transport in 1D chains. It is now known, for FPU-like systems, that provided high-frequency data for the current power spectra this theory can

(i) predict the low-frequency heat current power spectrum, where if its asymptotic behavior is assumed to be $\langle |j_\kappa(\omega)|^2 \rangle \sim C\omega^{-\alpha}$, then the theory predicts both C and α with no adjustable parameters [7];

(ii) predict that the heat-current power spectrum and momentum-current power spectrum go with the same power of ω at low frequencies if the ratio of specific heat capacities $\gamma \equiv c_P/c_V \neq 1$ [7,19];

(iii) explain that the criterion for determining which universality class ($\alpha = 1/2$ or $\alpha < 1/2$) a system belongs to is determined by whether or not $\gamma = 1$ [21];

(iv) predict the frequency of onset of finite-size saturation.

It remains to explore what other systems this theory applies to. Additionally, it is still unclear exactly what the asymptotic behavior of the heat-current power spectrum in the $\gamma \neq 1$ universality class. Some authors propose that it is $1/3$ [2], while others propose that it is $2/5$ [3–5]. The mode-mode coupling theory of Ref. [7] predicts a somewhat more complicated asymptotic behavior, but this can only be seen at frequencies that remain inaccessibly low in all known systems.

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