

Universality classes for thermal transport in one-dimensional oscillator systems

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Two universality classes for thermal transport in one-dimensional oscillator systems are proposed. In class A the asymptotic behavior of the frequency dependent thermal conductivity is $\kappa(\omega) \sim \omega^{-1/2}$, whereas the bulk viscosity is finite. In class B the asymptotic behavior of the thermal conductivity is $\kappa \sim \omega^{-\alpha}$, where $\alpha < 0.4$, and the frequency dependent bulk viscosity has the same asymptotic behavior as the thermal conductivity. It is further proposed that the criterion for membership in class A is that the ratio of specific heat capacities $\gamma \equiv c_P/c_V = 1$. A one-dimensional cubic-plus-quartic coupled oscillator is examined at conditions for which $\gamma = 1$ but $P \neq 0$. It is found that the system belongs to class A, in agreement with the proposed criterion. Additionally, it is proposed that examination of whether a system has a well-defined bulk Prandtl number is a more reliable way of determining whether a system is in class A or class B.

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I. INTRODUCTION

Despite decades of research, anomalous thermal transport in one-dimensional classical systems continues to present many puzzles. While a few one-dimensional systems are thought to have finite thermal conductivities [1–3], most one-dimensional systems exhibit anomalous thermal conduction [4,5]. This is seen either by noting that the thermal conductivity depends on the system length or, equivalently, that the heat current power spectrum diverges at low frequencies according to some power law, $|j_\epsilon(\omega)|^2 \sim \omega^{-\alpha}$, where $0 < \alpha < 1$. The criteria for a system to have a finite thermal conductivity are not currently known. The presence of on-site potentials appears to be one important criterion [1,6,7]. However, some systems without on-site potentials [3,8] seem to have finite thermal conductivities.

One area of recent progress in the study of systems with no on-site potentials is the recognition that there may be at least two universality classes of systems with anomalous thermal conductivity. These have different values of the exponent, α . The details of these universality classes are still somewhat unclear. That is, what values are taken on by α in these classes? What determines to which class a given system belongs? The current consensus seems to be that described in [5]. However, a similar but significantly different proposal is contained in [9,10]. These two proposals agree that there are (at least) two universality classes. In one, which for brevity we will call class A, both proposals agree that $\alpha = 1/2$. In the other, which we will call class B, there is still much disagreement about the value of α , but it seems clear that $\alpha < 0.4$. It should be noted that there remains some disagreement about the value of α in class A, with some authors finding evidence that $\alpha = 2/5$ [11–13]. Overall, given the lack of consistent results across systems, it is possible that there are more than two universality classes.

In [5] and elsewhere it is argued that $\alpha = 1/3$ in class B. On the other hand, [9] paints a somewhat more complicated picture in which α goes through an infinite number of transitions at different frequencies, going asymptotically to a limiting value

$\alpha^* = (3 - \sqrt{5})/2$ which is only observed at inaccessibly low frequencies.

For the present paper we will work under the assumption that there are only two universality classes: class A with $\alpha = 1/2$ and class B with $\alpha = 1/3$ or a similar value; the exact value of α in class B is unimportant to the discussion in this paper except insofar as $\alpha \leq 0.4$. We will not entertain the possibility that $\alpha = 2/5$ in class A. In part this is because, as we will show in this paper, the behavior of the system under study is much more consistent with $\alpha = 1/2$.

Evidence has been provided [14,15], that the criteria for membership in class A are:

- (1) The interparticle potential is even when expanded about its minimum.
- (2) The system pressure is zero.

Various other authors present evidence for this, or at least that even interparticle potentials are special.

On the other hand, in [9] theoretical arguments were put forth that the criterion for membership in class A is that the system's specific heat ratio is $\gamma \equiv c_P/c_V = 1$. The argument in [9] suggests that this should be the criterion for membership in class A, regardless of the form of the interparticle potential. The two proposals are strongly overlapping since any system with an even potential at zero pressure will have $\gamma = 1$. The evidence presented in [15] and [9] is consistent with both proposals since all examples that have been examined with $\gamma = 1$ have also had even potentials and $P = 0$. However, the case of $\gamma = 1$ has not been examined for systems with non-even interparticle potential and non-zero pressure. Thus, a simple test of the two proposals would be to examine a system which has $\gamma = 1$ but a non-even potential and non-zero pressure. This is the primary goal of the present paper. As a secondary goal, we will propose a way of identifying membership in class B which is more reliable than trying to determine the value of α .

II. MODE COUPLING THEORY

The argument for $\gamma = 1$ resulting in $\alpha = 1/2$ is contained within a simple mode coupling theory which was presented in [9] and [10]. Because the theory is quite fully presented in those papers we will here present only a brief summary of the

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main features, focusing on the argument regarding the special nature of $\gamma = 1$.

In a classic paper [16], a sophisticated development of mode coupling was used to show that, in general, the long-time tails of all of the current correlation functions in a fluid should have leading terms which go as $t^{-d/2}$, where d is the dimensionality of the system. In one dimension, where shear viscosity is undefined, the relevant expressions from [16] reduce to

$$C_\zeta(t) \simeq \left[\frac{M_{+-}}{(\Gamma_s)^{1/2}} + \frac{M_{HH}}{(2D_T)^{1/2}} \right] \left(\frac{1}{4\pi t} \right)^{1/2}, \quad (1)$$

$$C_\kappa(t) \simeq \left[\frac{K_{+-}}{(\Gamma_s)^{1/2}} \right] \left(\frac{1}{4\pi t} \right)^{1/2}, \quad (2)$$

where $C_\zeta(t)$ and $C_\kappa(t)$ are the momentum current correlation function and heat current correlation functions, respectively, m is the mass per particle, ρ is the mass density, c_P is the constant pressure specific heat capacity, c_V is the constant volume specific heat capacity, $\gamma \equiv c_P/c_V$ is the ratio of specific heats, $D_T = m\kappa/\rho c_P$ is the thermal diffusivity, $\Gamma_s = (\gamma - 1)D_T + D_\ell$ is the sound damping coefficient, κ is the thermal conductivity, $D_\ell = (4\eta/3 + \zeta)/\rho$ is the longitudinal diffusivity, η is the shear viscosity (which vanishes in 1D) and ζ is the bulk viscosity. Via Green-Kubo integrals, $C_\zeta(t)$ and $C_\kappa(t)$ are related to the system's bulk viscosity and thermal conductivity, respectively. The symbols, M_{+-} , M_{HH} , and K_{+-} are defined in [16] as

$$M_{+-} = \frac{1}{\beta^2} \left[1 - \frac{\gamma - 1}{\alpha_P T} + \frac{\rho}{c} \left(\frac{\partial c}{\partial \rho} \right) \right], \quad (3)$$

$$M_{HH} = \frac{1}{2\beta^2} (\gamma - 1)^2 \left[1 - \frac{1}{\alpha_P c_P} \left(\frac{\partial c_P}{\partial T} \right)_P + \frac{1}{\alpha_P} \left(\frac{\partial \alpha_P}{\partial T} \right)_P \right], \quad (4)$$

$$K_{+-} = \frac{c^2}{\beta^2}. \quad (5)$$

For a system with $\gamma = 1$ it was shown in [9] that the prefactor in square brackets $[\dots]$ in the momentum current correlation function is zero. Thus, the possibility exists that the bulk viscosity of a one-dimensional system with $\gamma = 1$ is well defined, whereas it is anomalous in other one-dimensional systems in much the same way that the thermal conductivity is.

A very simple mode coupling theory can be obtained from the assumption that the sound damping coefficient, Γ_s is a frequency dependent phenomenological parameter of the system of the form

$$\Gamma_s(\omega') = \frac{\gamma - 1}{\rho c_P} \kappa(\omega') + \frac{1}{\rho} \zeta(\omega'), \quad (6)$$

where $\kappa(\omega')$ and ζ' are the frequency dependent thermal conductivity and bulk viscosity as defined through Green-Kubo integrals. Further, the $k \rightarrow 0$ limit of the energy current power spectrum, $\tilde{C}_\epsilon(\omega)$, is shown to be obtainable from this

frequency dependent damping coefficient via

$$\tilde{C}_\epsilon(\omega) = \frac{2c^2}{L\beta^2} \sum_{k'} \frac{\Gamma_s(ck')k'^2}{\omega^2 + [\Gamma_s(ck')k'^2]^2}, \quad (7)$$

where k' is the wave vector and the sum is taken over the whole reciprocal lattice.

At first sight this theory seems pathological since $\tilde{C}_\epsilon(\omega)$ depends on $\Gamma_s(\omega')$, but $\Gamma_s(\omega')$ in turn depends on $\tilde{C}_\epsilon(\omega)$ via the Green-Kubo integral for the thermal conductivity. The theory is saved from this circularity by the fact that Eq. (7) is dominated by terms due to modes with $\Gamma_s(ck')k'^2 \simeq \omega$. As a result, a ‘‘mode cascade’’ results in which the thermal conductivity at any (sufficiently low) frequency is entirely determined by the thermal conductivity and bulk viscosity at much higher frequency.

Two main cases now become evident. If $\gamma = 1$ then the $\kappa(\omega')$ term in Eq. (6) is zero and the thermal conductivity is entirely determined by the bulk viscosity. Since, for $\gamma = 1$, the bulk viscosity appears to be finite a simple argument [9] leads to the prediction that $\kappa(\omega) \sim \omega^{-1/2}$. This is class A.

On the other hand, if $\gamma \neq 1$ a more complicated situation arises. At any frequency, ω , the thermal conductivity, $\kappa(\omega)$, is determined by the behavior of $\kappa(\omega')$ and $\zeta(\omega')$ at much higher frequencies, ω' . Meanwhile, due to Eq. (1), the bulk viscosity, $\zeta(\omega)$ is determined in a similar way, via both Γ_s and D_T by the higher frequency behaviors of κ and ζ . As is suggested by the ‘‘toy model’’ in the Appendix of [9], this could lead to a situation in which both the energy and momentum power spectra exhibit an infinity of segments with differing exponent α , separated by ‘‘kinks’’ at which the value of α changes, but always converging to a universal value $\alpha^* = (3 - \sqrt{5})/2 \simeq 0.382$. One characteristic of this picture is that, while both κ and ζ are anomalous, they would have the same power-law behavior at all sufficiently low frequencies. Thus, the bulk Prandtl number, Pr_ζ , should be well defined. This distinctive behavior is observed for the cubic-plus quartic system in [10]. We, therefore, suggest that the existence of a well defined bulk Prandtl number at low frequencies is a good signal that a system is a member of class B. Given the well known difficulties in accurately determining the value of α for a system, this may be a much more reliable way of determining whether a system belongs to class B.

III. SYSTEM OF INTEREST

One of the best studied one-dimensional oscillator chains is the FPU- $\alpha\beta$ system, which has been studied via simulations since a number of pioneering papers in the 1960s [17,18]. A variant on this system is the cubic-plus-quartic system which was examined in [10]. This is simply the FPU- $\alpha\beta$ system with the harmonic coefficient set to zero. It was argued in [10] that the harmonic term is unimportant in the context of the mechanisms responsible for heat transport in oscillator chains. Further, the cubic-plus-quartic system can be re-expanded about its minimum to recover a harmonic coefficient, albeit one which is not independent of the cubic and quartic coefficients. Thus, the cubic-plus-quartic system can be seen as a restricted set within the parameter space of the FPU- $\alpha\beta$ system, but this restricted set spans behavior from

harmonic to highly anharmonic. Because it is slightly faster to numerically integrate than the full FPU- $\alpha\beta$ system it is an ideal test system for our present purposes.

The system is defined by the Hamiltonian

$$H(p, q) = \sum_{i=0}^N \frac{p_i^2}{2m} + \frac{A}{3}(q_i - q_{i-1} - a)^3 + \frac{B}{4}(q_i - q_{i-1} - a)^4, \quad (8)$$

where p_i and q_i are the canonical momentum and position of the i th particle, N is the number of particles in the system, m is the particle mass, A and B are the cubic and quartic coefficients of the interparticle potential, respectively, and a is an arbitrary interparticle spacing at which the zero (not the equilibrium) of the potential occurs. In most discussions the cubic and quartic coefficients are called α and β , but we choose to call them A and B to avoid confusion with the limiting exponent of the heat current power spectrum and the inverse temperature, $\beta = 1/k_B T$, where k_B is Boltzmann's constant and T is the temperature.

The thermodynamics of this system are presented in detail in [10]. We will just summarize some key features of current interest. Of particular interest in the present paper is the specific heat ratio, $\gamma \equiv c_P/c_V$. We will wish to find conditions under which the cubic-plus-quartic system has $\gamma = 1$. It is worthwhile noting the standard thermodynamic identity

$$\gamma - 1 = \frac{\ell \alpha_P^2 \gamma T}{\chi_T c_P}, \quad (9)$$

where $\ell \equiv L/N$ is the system length per particle, α_P is the thermal expansion coefficient at constant pressure and χ_T is the isothermal compressibility. So whenever $\alpha_P = 0$ we should expect that $\gamma = 1$; it may be more intuitively clear how to find conditions under which a system without even symmetry in its potential might have $\alpha_P = 0$ than it is to think directly about when $\gamma = 1$.

This gives us a heuristic argument which narrows our search for conditions under which $\gamma = 1$. Consider that at $P = 0$ as the temperature of the system is increased the population of particles on the ‘‘shoulder’’ of the potential increases. Thus, the system expands if $A > 0$. But at low temperatures we could also populate the shoulder by changing the pressure. Again, if $A > 0$ then we must put the system under tension ($P < 0$) to do this. On the other hand, the constant pressure, constant temperature distribution function is $\exp[-\beta(H - PL)]$. As the temperature is increased the energy increases and the PL in the exponent becomes insignificant. So the infinite temperature limit of the particle distribution function is independent of the pressure. This can be seen explicitly by examining the expectation value of the interparticle distance. So, it should be possible to find pressures far enough from zero that the system contracts as the temperature increases. Thus, for any finite temperature there must be some intermediate pressure at which the system neither expands nor contracts—that is $\alpha_P = 0$.

Let us make the above, heuristic, argument more precise. Following [10] we define

$$\bar{X}_n(T, P) \equiv \frac{\int_{-\infty}^{\infty} X^n \exp\{-\beta[V(X) + PX]\}}{\int_{-\infty}^{\infty} dX \exp\{-\beta[V(X) + PX]\}} = \langle X^n \rangle, \quad (10)$$

then it is easy to show [10] that the equilibrium distance between particles is

$$\ell = a + \bar{X}_1, \quad (11)$$

the thermal expansion coefficient is

$$\alpha_P = \frac{1}{\ell} \frac{1}{k_B T^2} \left[\frac{A}{3}(\bar{X}_4 - \bar{X}_3 \bar{X}_1) + \frac{B}{4}(\bar{X}_5 - \bar{X}_4 \bar{X}_1) + P(\bar{X}_2 - \bar{X}_1^2) \right], \quad (12)$$

the isothermal compressibility is

$$\chi_T = \frac{\beta}{\ell} (\bar{X}_2 - \bar{X}_1^2), \quad (13)$$

and the constant pressure specific heat capacity per particle is

$$c_P = k_B \beta^2 \left[\frac{1}{2\beta^2} + \frac{A^2}{9}(\bar{X}_6 - \bar{X}_3^2) + \frac{B^2}{16}(\bar{X}_8 - \bar{X}_4^2) + P^2(\bar{X}_2 - \bar{X}_1^2) + \frac{AB}{6}(\bar{X}_7 - \bar{X}_4 \bar{X}_3) + \frac{2AP}{3}(\bar{X}_4 - \bar{X}_3 \bar{X}_1) + \frac{BP}{2}(\bar{X}_5 - \bar{X}_4 \bar{X}_1) \right]. \quad (14)$$

With these, thermodynamic identities allow us to obtain all other equilibrium thermodynamic quantities—of greatest interest are γ and the thermodynamic speed of sound, c . These can be expressed in terms of the above using standard thermodynamic identities. The expressions themselves are too large to usefully write in a publication.

This gives us the tools that we need to search parameter space for conditions under which the cubic-plus-quartic system has $\gamma = 1$. By the heuristic argument presented above we would expect that for any $A > 0$ and finite temperature we should be able to find $\gamma = 1$ at some $P < 0$ (system under tension). Alternatively, we could choose $A < 0$ and find $\gamma = 1$ at some $P > 0$. A plot showing an example of this parameter space search is shown in Fig. 1.

IV. RESULTS

We have carried out a set of simulations of the cubic-plus-quartic system to test the system for membership in class A or class B under several sets of parameters. If $A = 0$ (pure quartic system) and $P = 0$, then it is already known [9] that the system belongs to class A. Similarly, under all of the conditions examined [10] ($A > 0$, $P = 0$) the system displays a well-defined bulk Prandtl number and energy current power-law exponent $\alpha \leq 0.4$, and so it is in class B. For the present paper we have examined two new conditions under which $\gamma = 1$: $A = -2.0$ with $P = 0.5926$, and $A = 1.89$ with $P = -0.5$. We have done simulations under these sets of parameters and also for some sets of conditions ‘‘nearby’’ in parameter space but with $\gamma \neq 1$.

We simulate using the same fourth-order symplectic integrator that was used in [10]. In all cases, the system is

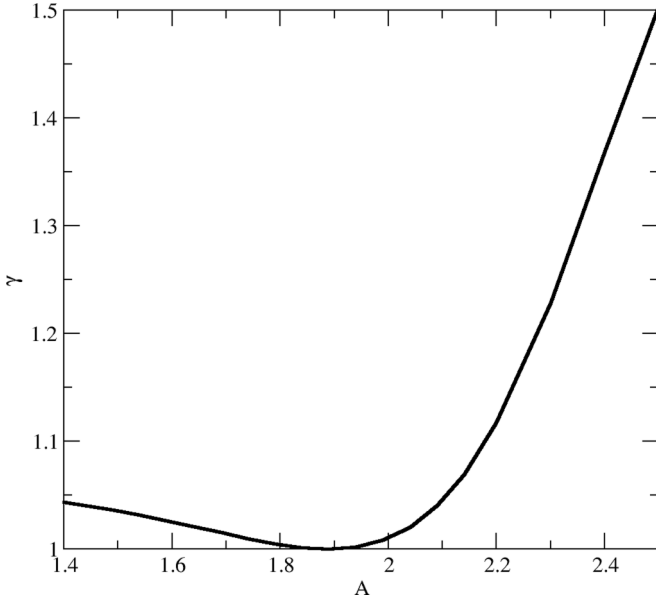


FIG. 1. Variation of γ with A for the cubic-plus-quartic system with $B = 1$, $T = 1$, $P = -0.5$. More detailed plots show that $\gamma = 1$ at $A \simeq 1.89$.

initialized into an equilibrium state by randomly generating particle positions and momenta from the Boltzmann statistics of the constant temperature, constant pressure ensemble. We check the system energy and system momentum of all runs to ensure that floating-point and truncation errors have not caused them to drift by too much. Symplectic integrators are especially advantageous in this regard since they do not result in secular variations of the energy and momentum. We have also checked that our initialization routine produces the expected means and standard deviations of the system energy and length as predicted by equilibrium statistical mechanics. Finally, we also use sum rules described in [19] for the average squared stress, $\langle \tau^2 \rangle$, and average squared energy current, $\langle j_\epsilon^2 \rangle$, to check that the statistics of the currents is representative of those for a true (infinite) ensemble. This step is important since the squared currents follow highly non-Gaussian distributions with long tails. Thus, it is very easy for a finite set of simulation runs to inadequately sample or oversample the tails of these distributions. Results of this checking are shown in Table I.

As expected, at both of the sets of parameter with $\gamma = 1$ the bulk viscosity is finite but the thermal conductivity diverges at low ω , so the bulk Prandtl number is undefined. Figures 2 and 3 include lines at slopes of $-1/2$ and are consistent with

TABLE I. Thermodynamic checking for simulation runs with $\gamma = 1$.

| Quantity | $A = 1.89, P = -0.5$ | | $A = -2.0, P = 0.5926$ | |
|--------------------------------|----------------------|--------------------|------------------------|-------------------|
| | Theory | Simulation | Theory | Simulation |
| $\langle \ell \rangle$ | -0.630 | -0.631 ± 0.001 | 0.6667 | 0.668 ± 0.001 |
| $\langle E \rangle$ | 0.2931 | 0.293 ± 0.002 | 0.1964 | 0.196 ± 0.001 |
| $\langle j_\epsilon^2 \rangle$ | 1.2365 | 1.236 ± 0.005 | 1.333 | 1.26 ± 0.07 |
| $\langle \tau^2 \rangle$ | 2.4729 | 2.472 ± 0.006 | 2.6670 | 2.667 ± 0.004 |

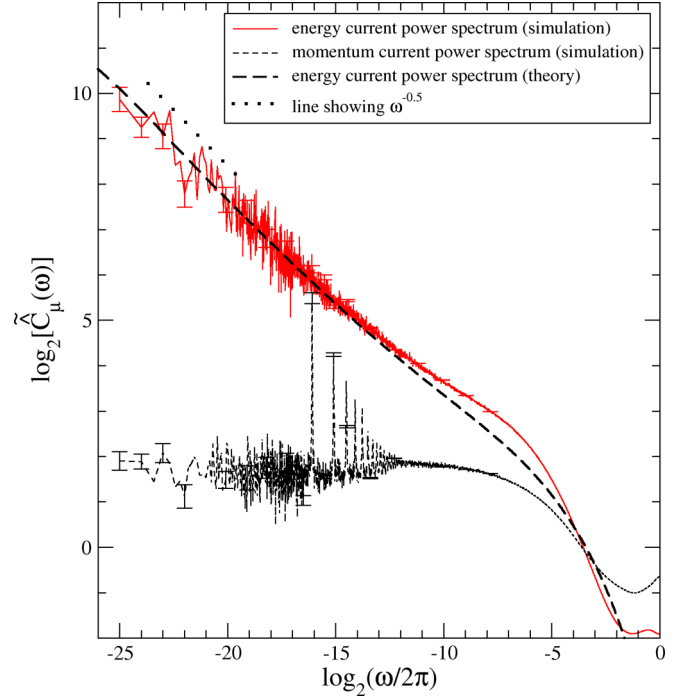


FIG. 2. (Color online) Current power spectra of the cubic+quartic system with $N = 2^{15}$, final time $= 2^{25}$, $\alpha = 1.89$, and $P = -0.5$. The thin red line is the simulated energy current power spectrum, the thin black dashed line is the simulated momentum current power spectrum, the heavy dashed black line is the energy current power spectrum from theory, and the heavy dotted line indicates the slope of pure $\omega^{-1/2}$ behavior. Selected error bars show one standard error among simulation results.

$\kappa \sim \omega^{-1/2}$. More will be said about this below. Thus, even though $P \neq 0$ and the system's interparticle potential does not have even symmetry, the system is a member of class A under these conditions.

Similar runs using parameters for which $\gamma \neq 1$ were carried out. The parameters chosen were $A = -2.7$, $P = 0.5926$, and $A = 2.0$, $P = -0.5$. These runs have the characteristic behavior that the energy and momentum current power spectra follow the same power law at low frequencies. Thus, a well defined bulk Prandtl number exists for these conditions. Further, the low frequency limit of α is significantly less than $1/2$. Thus, the system is a member of class B with these parameter sets.

In view of the continued disagreement over whether α is $1/2$ or $2/5$ for systems belonging to class A, it is worth examining the runs shown in Figs. 2 and 3 in more detail. Taking linear regressions of the results at frequencies below 2^{-16} we obtain the slopes shown in Table II. These are far more consistent

TABLE II. Slopes of portions of plots in Figs. 2 and 3 for frequencies less than 2^{-16} .

| A | P | Slope |
|------|--------|------------------|
| 1.89 | -0.5 | -0.47 ± 0.02 |
| -2.0 | 0.5926 | -0.49 ± 0.02 |

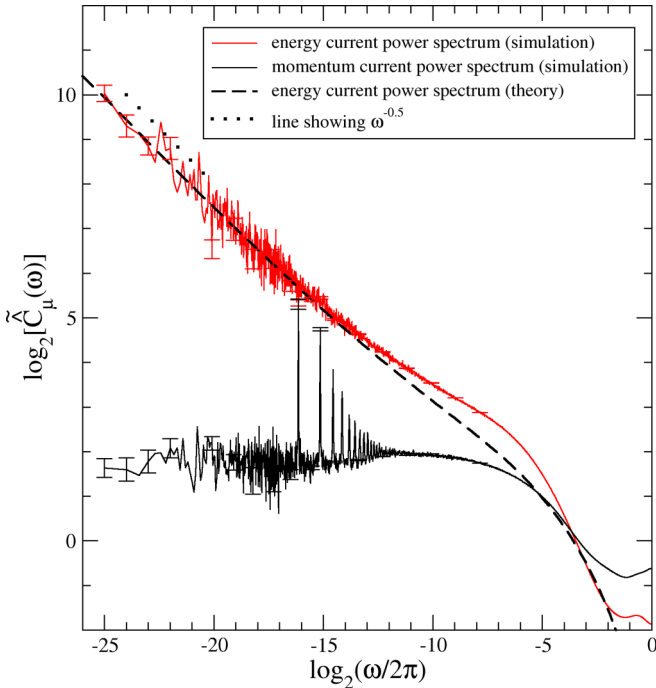


FIG. 3. (Color online) Current power spectra of the cubic+quartic system with $N = 2^{15}$, final time = 2^{25} , $\alpha = -2.0$, and $P = 0.5926$. The thin red line is the simulated energy current power spectrum, the thin black line is the simulated momentum current power spectrum, the heavy dashed black line is the energy current power spectrum from theory, and the heavy dotted line indicates the slope of pure $\omega^{-1/2}$ behavior. Selected error bars show one standard error among simulation results.

with $\alpha = 1/2$ than they are with $\alpha = 2/5$. Specifically, the 95% confidence intervals for the slopes exclude $\alpha = 2/5$.

V. DISCUSSION AND CONCLUSIONS

The key result is that, for the cubic-plus-quartic system, the criterion for membership in class A is that $\gamma = 1$. Secondly, we can say with some confidence that for this system, when it is in class A the asymptotic exponent is $\alpha = 1/2$, not $\alpha = 2/5$.

To what extent can this result be generalized to other one-dimensional systems? While more study will be needed to determine this, the nature of the mode-coupling theory which predicted this criterion allows us to speculate. It is not yet known what systems the simple mode coupling theory is valid for, but the only fundamental assumptions underlying the theory [9] are:

- (1) The system is in local thermodynamic equilibrium, at least over sufficiently long length scales.
- (2) The microscopic sound damping coefficient can be at least approximated by Eq. (6).

Given that this seems to be true for FPU chains, it seems likely that it is true for any other coupled oscillator systems with power-law potentials and with some nonlinearity to couple the harmonic modes. A preliminary study of a system with discrete, impulsive collisions shows that transport in that system is also governed by this theory. This will be presented in a future paper. On the other hand, the “momentum conserving ding-a-ling” system [3] appears not to be described by this mode coupling theory. It is not clear why. Does the system fail to maintain local thermodynamic equilibrium? Does the unusual nature of the system produce completely different sound damping behavior? Answering these questions could provide broader insights.

The additional condition for systems to divide neatly into the class A and class B proposed in this paper is that, for systems with $\gamma = 1$, the bulk viscosity is finite. The theory does not predict this. All it predicts is that any $t^{1/2}$ term in the momentum current correlation function is identically zero if $\gamma = 1$. One can think of the theory, with its mode cascade, as a normalization group flow. If it is “seeded” with an initial, relatively high-frequency $\omega^{-1/2}$ behavior, as originally predicted by [16] then this leads to a cascade through $\omega^{-1/3}$, $\omega^{-2/5}$ and so on converging towards the universal $\omega^{-\alpha^*}$ as described in [9,10]. If $\gamma = 1$ and it is “seeded” with a constant bulk viscosity then it results in $\omega^{-1/2}$ behavior. However, nothing in the theory tells us, a priori, what to seed the theory with. Thus, much additional work remains to be done. Other universality classes are not ruled out. For example, a system with $\gamma = 1$ but a non-constant bulk viscosity would produce very different behavior. The cascade through $\omega^{-1/2}$, $\omega^{-1/3}$, $\omega^{-2/5}$, ... would explain the persistent lack of consistency of results in numerical studies of heat conduction in one-dimensional systems. Indeed, the seed of the cascade is presumably some “mid-frequency” behavior which may not be $\omega^{-1/2}$. This will result in a different cascade, still going asymptotically towards $\alpha = \alpha^*$, but passing through values of α which are nearly, but not quite $1/3$, $2/5$, ... This would explain the preponderance of reported values of α that are between $1/3$ and $2/5$.

Finally, there is evidence [14] that conventional hydrodynamics breaks down in these systems so that peak widths scale as $\omega^{3/2}$ rather than as ω^2 . The mode coupling theory used in the present study assumes the ω^2 scaling of conventional hydrodynamics. It would be interesting to recast the theory using the $\omega^{3/2}$ scaling proposed in [14] in order to see whether this provides better prediction of the transport.

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