Unconventional Sound Propagation and Its Strong Coupling to Heat in Anharmonic Chains Under Pressure Fluctuations

Daxing Xiong

Department of Physics, Fuzhou University, Fuzhou 350108, Fujian, China

We propose a new numerical scheme to estimate sound mode correlations in general anharmonic chains. Contrary to the previous schemes, our method fully considers the role of pressure fluctuations. With this scheme the cross-correlations between heat and sound modes can also be measured, which thus helps test the decoupling hypothesis assumed in fluctuating hydrodynamic theory. Remarkably, we find that the traditional picture of sound propagation and the decoupling hypothesis can only be valid in a system of small pressure fluctuations. When the fluctuations are relatively large, the sound modes no longer show two ballistically moving peaks as usual and their coupling to heat mode can be dominated. Our results shed new light on how to improve the current nonlinear fluctuating hydrodynamic theory.

Most one-dimensional (1D) systems display anomalous transport. Among others, anomalous thermal transport is a paradigm that has attracted much interest in the past decades [1–5]. Generally, this anomalous behavior is resulted from the dimensional constraint inherent in 1D systems that causes the Fourier law, which describes \( J = -\kappa \nabla T \) with \( J \) the heat current, \( \nabla T \) the temperature gradient, and \( \kappa \) the thermal conductivity of a constant for a bulk material under a given temperature \( T \), invalid. This invalidity exhibits in \( \kappa \) being a power-law function of the system size \( L \), namely \( \kappa(L) \sim L^\alpha \), with \( 0 < \alpha < 1 \) showing superdiffusive transport. The origin of this superdiffusive behavior is usually traced back to the abnormal propagation of relevant conserved quantities fluctuations. These fluctuations control the system’s cooperative behavior, and their correlations propagation leads to the observed anomaly.

Fluctuating hydrodynamic theory [4] is quite useful in describing these fluctuations and correlations. For thermal transport in 1D systems, this theory assumes the fluctuations will induce three hydrodynamic (normal) modes—one heat mode and two sound modes, and such fluctuations propagation can be understood by a combination of these normal modes correlations. Under this framework, recently a nonlinear fluctuating hydrodynamic theory [5–7] has been proposed and great progress has been achieved: Narayan and Ramaswamy [5] first predicted \( \alpha = 1/3 \) by a renormalization group analysis; Van Beijeren [6] further supported that certain heat mode correlations for general anharmonic chains can be captured by the Kardar-Parisi-Zhang universality class [8] which exactly gives \( \alpha = 1/3 \); Spohn [7] reformulated the theory, advanced the predictions on more general grounds and suggested two generic universality classes of \( \alpha = 1/3 \) and \( 1/2 \).

In spite of these achievements, the current version of nonlinear fluctuating hydrodynamics (NFH) is not satisfactory and its exact predictions are still under debate. Some unsatisfactory points are: (i) In derivation of NFH, the diffusion and the noise terms present in the theory are not obtained from microscopic descriptions but instead added phenomenologically [9]; (ii) To predict the universality classes, a heuristic decoupling of modes is assumed, for which there has not yet been a firm analytic confirmation [10]; (iii) Even worse, the current NFH is based on the linearized hydrodynamics added constant pressure nonlinearity, while the pressure fluctuations are not taken into account [11].

Indeed, the relevant numerical test [12] based on the scheme suggested by NFH has verified the predictions in a good level, but also reported some deviations. This scheme focuses on the correlations of fluctuations of three conserved fields, i.e., the stretch, momentum, and energy, and further transforms them into normal modes correlations. But whenever one performs such transformation, the test will not be directly from dynamics as one does not know whether this transformation is always available. In addition, the test surely does not include the information of pressure fluctuations as the pressure is fixed at the starting point of simulations [12].

In this Letter we propose a new numerical scheme to estimate hydrodynamic modes correlations in general anharmonic chains. Our advance is to include the role of pressure fluctuations and to avoid any operators that cause the estimations away from the original dynamics. Using this scheme, we are able to reveal that the pressure fluctuations increase, the traditional picture of sound propagation and the decoupling hypothesis of hydrodynamic modes suggested in conventional NFH can be broken down in a quite unusual way. This first-hand information indicates the essential role of pressure fluctuations and would help develop a full NFH theory.

We consider a general momentum-conserving anharmonic chain with Hamiltonian:

\[
H = \sum_{m=1}^{L} \frac{p_m^2}{2} + V(r_{m+1} - r_m),
\]  

where \( p_m \) is the \( m \)th (totally \( L \) particles and all with unit mass) particle’s momentum, \( r_m \) is its displacement from equilibrium position, and \( V(\xi) \) is the interparticle
potential between two nearest-neighbor particles. To numerically estimate the hydrodynamic modes, we specialize the formalism in [4] to 1D case, whose hydrodynamic modes are defined by small values of the wave number $k$ and given as linear combinations of the Fourier components of the deviations from the equilibrium values of microscopic densities of particles:

$$\hat{n}(k, t) = \sum_{m=1}^{L} \exp(-ikr_m) - \delta_{k,0}\langle \hat{n} \rangle; \quad (2)$$

momentum:

$$\hat{p}(k, t) = \sum_{m=1}^{L} p_m(t) \exp(-ikr_m), \quad (3)$$

and energy:

$$\hat{e}(k, t) = \sum_{m=1}^{L} e_m(t) \exp(-ikr_m) - \delta_{k,0}\langle \hat{e} \rangle, \quad (4)$$

where $\delta$ represents the Kronecker delta function, $\langle \cdot \rangle$ denotes the ensemble average, $\langle \hat{n} \rangle$ and $\langle \hat{e} \rangle$ are the equilibrium values of the Fourier components $(k = 0)$ for densities of particle (1) and energy $[e_m(t) = \hat{p}_m^2/2 + V(r_{m+1} - r_m)/2 + V(r_m - r_{m-1})/2]$. In fact, such three quantities are regarded as the conserved fields of the system and this formalism assumes that all slow variables relevant to the long time behavior of hydrodynamics and related time correlations are the long-wavelength Fourier components of densities of these conserved fields plus their product $[6]$. Under this assumption, one obtains the heat mode:

$$\hat{a}_{\sigma_0}(k, t) = \left( \frac{1}{\langle \hat{n} \rangle k_B T^2 C_p} \right)^{1/2} \left[ \hat{e}(k, t) - \Delta \hat{n}(k, t) \right] \quad (5)$$

and the sound modes:

$$\hat{a}_{\sigma_{\pm}}(k, t) = \left( \frac{1}{\langle \hat{n} \rangle k_B T^2 C_p} \right)^{1/2} \left[ c_0^{-1} \hat{F}(k, t) + \sigma_{\pm} \hat{p}(k, t) \right], \quad (6)$$

with $c_0$ and $\sigma_{\pm} = \pm 1$ labelling the heat mode and two sound modes, respectively; $k_B$ the Boltzmann constant; $\hat{F}(k, t) = \sum_{m=1}^{L} F_m(t) \exp(-ikr_m) - \delta_{k,0}\langle \hat{F} \rangle$ the pressure fluctuation with $F_m(t) = -\partial V(r_{m+1} - r_m)/\partial r_m; C_p$ and $\hat{h} = (\langle \hat{e} \rangle + \langle \hat{F} \rangle)/\langle \hat{n} \rangle$ the specific heat at constant pressure $\langle \hat{F} \rangle$ and equilibrium enthalpy, per particle; $c_0$ the sound velocity. As can be seen, both definitions of $\hat{a}_{\sigma_0}$ and $\hat{a}_{\sigma_{\pm}}$ already involve the information of pressure. More importantly, the pressure fluctuations seem key for sound modes. Now since the Fourier transform is a linear transformation, in real space we have:

$$a_{\sigma_0}(m, t) = \left( \frac{1}{\langle \hat{n} \rangle k_B T^2 C_p} \right)^{1/2} \left[ \Delta e_m(t) - \Delta \hat{n}_m(t) \right] \quad (7)$$

and

$$a_{\sigma_{\pm}}(m, t) = \left( \frac{1}{\langle \hat{n} \rangle k_B T^2 C_p} \right)^{1/2} \left[ e_0^{-1} \Delta F_m(t) + \sigma_{\pm} \Delta p_m(t) \right], \quad (8)$$

where $\Delta \hat{A} = A_m(t) - \langle A \rangle$.

Note that both prefactors in Eqs. (9) and (10) are usually constant for given temperatures, in practice one only needs to concern with the variables

$$Q_m(t) = e_m(t) - hn_m(t), \quad (9)$$

and

$$S^+_m(t) = \sigma_0^{-1} F_m(t) + \sigma_{\pm} p_m(t). \quad (10)$$

Actually, $Q_m(t)$ is the density of heat evolved from a process in the system. This can be seen from $\partial Q_m(t)/\partial T = \kappa \nabla^2 T = 0$ [13], which is obtained by combining the continuous equations of energy and mass. Its correlation function $\rho_Q(m, t) = \langle \Delta Q_{m,t}(t) \Delta Q_{m,t}(0) \rangle$ has been confirmed to represent the heat mode correlation and studied in many publications [13, 14]. Hence, in the following we mainly focus on the sound modes and also their coupling to heat. We argue that $S^+_m(t)$ can be similarly regarded as the density relevant to sounds in the same process. Then, the sound mode correlations can be represented by

$$\rho_{S^\pm}(m, t) = \langle \Delta S^\pm_{m,t}(t) \Delta S^\pm_{m,t}(0) \rangle \langle \Delta S^\pm_{m,t}(0) \Delta S^\pm_{m,t}(0) \rangle^{-1}, \quad (11)$$

which facilitates our numerical estimation.

We first take a typical potential $V(\xi) = A\xi^3/3 + \xi^4/4$ ($A \geq 0$) [14, 15] for our applications. Such systems are called as the cubic-plus-quartic anharmonic chains. As $A$ varies, they represent most common properties of a general momentum-conserving anharmonic chain. A particular case ($A = 0$) is the purely quartic chain whose $V(\xi)$ (averaged pressure) is symmetric (zero). This system has been predicted/supposed to follow the universality class of $\alpha = 1/2$ [6, 7], although some numerical deviations were also reported [14]. A nonzero $A$ then adds potential’s asymmetry (system’s nonzero pressure) and makes them belong to another universality class of $\alpha = 1/3$. We expect that knowing the information of sound modes correlations will help understand such a transition.

Before proceed, let us first see the distribution and fluctuation of pressure under equilibrium ($T = 0.5$) for the systems. As depicted in Fig. [1] only for $A = 0$ or a relatively small $A \leq 1$, the pressure distribution $P(F)$ indicates a narrow peak [see Fig. [1a]], which causes the displacement distribution $P(\xi)$, i.e., the potential, mainly concentrated on one single well [see Fig. [1b]]. As $A$ increases, both $P(F)$ and $P(\xi)$ can appear in a wide range and seem to around two peaks. We stress that such unusual distributions should certainly affect
the correlations of hydrodynamics modes, but presently, their roles have not been included in the NFH theory [7]. Indeed, the estimation of the mean value \( \langle F \rangle \) and fluctuation \( \langle (F - \langle F \rangle)^2 \rangle \) of pressure further reveals that \( A_{cr} \approx 1 \) is a turning point [see Figs. 1c,d], below which the \( A \)-dependence of \( \langle F \rangle \) is linear (non-linear) and \( \langle (F - \langle F \rangle)^2 \rangle \) is small (large). Such a turning point has also been addressed by exploring the system’s dynamic structure factor [14]. Due to this turning property, one might infer that, the current NFH theory only considering the fixed pressure nonlinearity might be insufficient to describe the overall transport behavior.

Knowing \( A_{cr} \approx 1 \), we now start our estimation. According to Eqs. (10) and (11), the only left unknown parameter for the scheme is the sound velocity \( c_0 \). Generally, for a given \( V(\xi) \) one can resort to spohn’s formula [2]. But, as we aim at proposing a direct numerical test, we would like all the parameters are directly from dynamics. We thus choose to obtain \( c_0 \) from measuring the momentum correlation \( \rho_p(m,t) \equiv \langle \rho_{p_m}(t)\rho(0) \rangle \). This is an usual way to numerically measure \( c_0 \) [10], for which \( \rho_p(m,t) \) always displays two ballistic peaks moving with \( c_0 \) for all considered \( A \). Some typical \( c_0 \) are listed in Table I. We also note that spohn’s formula might be not so conveniently used for systems with multi-well potentials [17].

| \( A \) | 0 | 0.25 | 1 | 1.5 | 2 | 3 |
|---|---|---|---|---|---|---|
| \( c_0 \) | 1.022 | 1.019 | 1.004 | 0.985 | 0.918 | 0.612 |

TABLE I: The measured \( c_0 \) for different \( A \).

The next procedures of estimation are performed as follows: A long chain size of \( L = 7201 \) is chosen to ensure that an initial fluctuation located at the center can spread out at a time up to \( t = 2000 \); a coarse-grained description of space variable is adopted, for which the chain is divided into several bins of equal size 8; the Runge-Kutta algorithm of seventh to eighth order with a time step 0.05 is employed to evolve the system; a total ensemble of size about \( 8 \times 10^9 \) is used for the average.

Figure 2 depicts one branch of sound mode correlations \( \rho_{s^-}(m,t) \). We do not plot another branch \( \rho_{s^+}(m,t) \) as both ones bear the mirror symmetry. As shown, for \( A < 1 \) [see Figs. 2a,b], \( \rho_{s^-}(m,t) \) displays similar behaviors as predicted by NFH, i.e., on one side certain ballistically moving peaks and these peaks broaden as time increases. This implies that the current NFH might be almost valid in this range. However, unusual things take place for a large \( A \), where two other peaks from both the center and the opposite side emerge [see Figs. 2d]. These are not just small perturbations to the origin sound peak. In fact, a further increasing \( A \) can lead such additional peaks dominated [see Figs. 2e]. Finally, all the three peaks are overlapped for a quite large \( A \) [see Figs. 2f], indicating strong couplings. This detailed transition indicates that our present description for the sound mode correlation in NFH might not be available in this large \( A \) range and \( A_{cr} \approx 1 \) seems a borderline [see Figs. 2c].

With this borderline in mind, we next test the decoupling hypothesis that usually assumed in NFH. This is achieved by measuring the cross-correlation function

\[
C_{S^-Q}(m,t) = \langle \Delta S^-_i(0) \Delta Q_{1+m}(t) \rangle \quad (12)
\]

between heat and one branch of sound modes \( S^- \). This is already enough to obtain the full information of cross-correlations as we have confirmed that \( C_{QS^\pm}(m,t) = \langle \Delta Q_{i}(0) \Delta S_{1+m}^\pm(t) \rangle \equiv C_{S^\pm-Q}(m,t) = \langle \Delta S_i^\pm(0) \Delta Q_{1+m}(t) \rangle \) and there is a mirror symmetry between \( C_{QS^-}(m,t) \) and \( C_{QS^+}(m,t) \).

Figure 3 depicts \( C_{S^-Q}(m,t) \). As shown, compared to \( \rho_{s^-}(m,t) \), the results are more complicated and richer. For a relatively large \( A \), all the three locations of the peaks of \( \rho_{s^-}(m,t) \) exhibit cross-correlations [see Fig. 3d,e]. This is the case even for \( A_{cr} \approx 1 \) [see
Fig. 3: The cross-correlation $C_{S-Q}(m,t)$ between heat and one sound mode for three long times $t = 1000$ (dotted), $t = 1500$ (dashed), and $t = 2000$ (solid). The insets of (a,b) depict the peaks of $C_{S-Q}(m,t)$ decaying with $t$.

Fig. 4: The propagation of pressure fluctuations $\rho_F(m,t)$ for three long times $t = 1000$ (dotted), $t = 1500$ (dashed), and $t = 2000$ (solid). The inset in (c) is a zoom for the central peaks.

For a quite large $A$, the cross-correlation will be concentrated on the center [see Fig. 3(d)]. In this sense, the decoupling hypothesis of heat and sound modes is surely violated for $A \geq 1$, even though both heat and sound modes do have different moving velocities.

Turning back to small $A$, there are still distinctions between $A = 0$ and $A \neq 0$ [see Fig. 3(a,b)]: for a given $t$ $C_{S-Q}(m,t)$ of $A = 0$ looks like a single peak, but the peak is distorted for $A = 0.25$. Such distortion is different from the estimation using the NFH scheme [7], where no cross-correlation was detected [14]. But, it is indeed consistent with the same distortion shown in the heat mode correlation [14]. We would like to comment that this distortion would likely induce a new universality class of the scaling for thermal transport [14]. Another important point is that the peak of $A = 0$ ($A = 0.25$) decays as $t^{-0.97}$ ($t^{-0.68}$). Obviously, for $A = 0$ the exponent is close to $-1$, one thus infers that the decoupling hypothesis will be valid in this case. However, a longer tail of $A = 0.25$ indicates that even a small $A$ could induce long-time couplings, thus breaks the decoupling hypothesis.

So far we have shown that in a cubic-plus-quartic anharmonic chain the traditional pictures of sound mode propagation and the decoupling hypothesis can break down in an unusual way. To show that this is truly induced by the variation of pressure fluctuations, we finally suggest to study a correlation function of pressure

$$\rho_F(m,t) = \frac{\langle \Delta F_{t+m}(t) \Delta F_t(0) \rangle}{\langle \Delta F_t(0) \Delta F_t(0) \rangle}$$

(13)

to directly capture the role of pressure fluctuation in transport. Indeed, $\rho_F(m,t)$ indicates the most common properties of sound propagations (see Fig. 4). For $A < 1$, $\rho_F(m,t)$ follows similar manners as sound modes correlations. However, a quite unusual picture takes place for a large $A$: First, a center peak exhibits [see Fig. 4(d), but Fig. 4(c) seems to be a borderline], and it quickly becomes dominated [see Fig. 4(e)]. Nevertheless, this situation can not be persisted for ever, a larger $A$ will lower down the peak and make the three peaks overlapped. This is consistent with the strong couplings as shown in Fig. 3. All of these suggest that $\rho_F(m,t)$ can be used as an early indicator to explore the effects of pressure fluctuations on transport.

To summarize, we have proposed a new numerical scheme with a coarse-grained description of space variables to explore hydrodynamic modes correlations for general anharmonic chains. The novelty of this scheme lies not only in a full consideration of the role of pressure fluctuations, which has been neglected in the current NFH [7,11], but also in that it is a purely dynamic method, i.e., all the relevant quantities are directly obtained from dynamic simulations. Using this scheme, we have shown that for a typical anharmonic chain of cubic-plus-quartic interparticle interactions, the sound modes propagation and their coupling properties to heat can follow a quite distinct way as the current NFH predicted. Indeed, the sound modes look strongly dependent on the strength of pressure fluctuations and there is a border-line $A_{c\tau} \approx 1$, above which the traditional picture of NFH breaks down. The decoupling hypothesis between hydrodynamic modes under this consideration should be taken more care. In fact, our results indicate that the current NFH seems to only work fine in anharmonic chains with symmetric (even) potentials under both zero averaged pressure and small pressure fluctuations. Thus, further advance of NFH should certainly take pressure fluctuations into account.

Over all, this new scheme is quite general. It could be easily extended to other anharmonic chains with a
FIG. 5: \( \rho_p(m,t) \) for three times \( t = 300 \) (dotted), \( t = 600 \) (dashed), and \( t = 900 \) (solid). The insets in (b-d) are a zoom for the result of \( t = 900 \).

different potential [13], or having additional degrees of freedom [19]. It could also shed new light on some special systems [20,25] whose thermal conduction has been conjectured to follow Fourier’s law. As to this latter case, one can quickly examine the propagation of pressure fluctuations \( \rho_p(m,t) \) for a rotor chain with Hamiltonian [1] and \( V(\xi) = 1 - \cos(\xi) \) [20,21]. Such a system has a striking feature that its heat conduction undergoes a crossover from abnormal to normal behaviors as the system’s temperature increases. In the language of NFH, the normal behavior at a high temperature is attributed to the destruction of the conservation of stretch [22,23]. However, in Fig. 5 we clearly demonstrate that \( \rho_p(m,t) \) seems key to this temperature-dependent crossover. This provides a new perspective to understand the origin of the validity of Fourier’s law in a rotor chain [26].

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* Electronic address: phyxiongdx@fzu.edu.cn

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without decaying as the system size increases.