Breakdown of effective phonon theory in one-dimensional chains with asymmetric interactions

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(Dated: today)

Abstract

Phonons are universal language for solid state theory. Effective phonon theory (self-consistent harmonic approximation) have been extensively used to access the weakly nonlinear effect in solid materials, which are standard content in textbook. In this manuscript, we test the effective phonon theory in one-dimensional chains with asymmetric interactions. It is found that simulation results agree well with theoretical predictions for symmetric cases, while significantly deviate from theoretical predictions for asymmetric cases. Our results imply the asymmetric interaction can provide stronger phonon-phonon interaction, which lead to break down of the effective phonon theory.
Nonlinearity play important roles in solid materials, which responds for thermodynamic and transport properties such as thermal expansion and thermal conductivity. Effective phonon theory (EPT) have been commonly used to assess the weakly nonlinear effect on phonons (normal modes in classical physics), whose basic ideal is to find a effective harmonic Hamiltonian to approximate the true nonlinear Hamiltonian (in early literature, also called self-consistent harmonic approximation) \([1]\). In the last decade, EPT have been extensively used to study low dimensional lattice models. These studies focus on one-dimensional (1D) momentum-conserved lattices and reported that the numerical results agree well with theoretical predictions even in strong nonlinearity limit \([2–6]\). It seemingly suggest EPT worked well for 1D lattice systems. However, Our investigation here shows things are not that simple. We find that simulation results agree well with theoretical predictions for 1D chains with symmetric nonlinear interactions, while obviously deviate from predictions for ones with asymmetric interactions.

A 1D momentum-conserved lattice are generally defined by the dimensionless Hamiltonian
\[
H = \sum_i \frac{p_i^2}{2} + V(x_i - x_{i-1})
\] (1)
where \(p_i\) and \(x_i\) are the \(i\)th particle momentum and displacement from the equilibrium position, respectively. \(V\) is the potential between two neighboring particles, which is given by
\[
V(x) = \frac{1}{2}x^2 + \frac{\alpha}{3}x^3 + \frac{\beta}{4}x^4
\] (2)
The lattice spacing is set to unity. This means the sound velocity \(c_s\) in the harmonic limit is equal to one in our models. The EPT calculate the effective particle force constants through self-consistently replacing the harmonic force constants by their thermal averages over all possible motions of particles. As a result, an effective harmonic potential approximate the nonlinear one (2) by
\[
\tilde{V}(x) = \frac{\eta^2}{2}x^2
\] (3)
where \(\eta\) is the renormalization factor. To do so, the phonon frequencies are renormalized to \(\tilde{\omega}_k = \eta\omega_k\) by the factor \(\eta\) as well, where \(k\) is mode number and \(\omega\) is the phonon frequency for (2) in harmonic limit. \(\eta\) is usually considered as \(k\)-independent, which is numerically confirmed in FPU-\(\beta\) models \([2, 5]\). Many theoretical methods were used to deal with model (2) to calculate renormalized factor \(\eta\), such as generalized virial theorem \([2, 3]\), Zwanzig-Mori
projection [4], weak turbulence theory [5] and self-consistent phonon theory [6]. It has been confirmed that these methods are equivalent [4–6]. In the present manuscript, we test two kinds of expressions for $\eta$ based on the theories mentioned above. One is given by [5]

$$\eta = \sqrt{\frac{<K>}{<U_h>}}$$

where $K$ and $U_h$ is the total kinetic and harmonic potential energy of model (2). Another slightly different expression was given by [3]

$$\eta = \sqrt{\frac{<\sum_{i=1}^{N} \delta_i^2> + \alpha <\sum_{i=1}^{N} \delta_i^4> + \beta <\sum_{i=1}^{N} \delta_i^4>}{<\sum_{i=1}^{N} \delta_i^2>}}$$

where $\delta_i \equiv x_i - x_{i-1}$. $<\cdots>$ in the above two expressions denotes averaging over the Gibbs measure.

We divide the potential (2) into two types according to its symmetry with respect to its zero point at $x = 0$. In the symmetric type, we fix $\alpha = 0$, which recovers the Fermi-Pasta-Ulam $\beta$ (FPU-$\beta$) models. In the asymmetric one, we fix $\beta = 1$ and varied $\alpha$ in the interval $0.2$ to ensure only one potential minimum at $x = 0$, which is the Fermi-Pasta-Ulam $\alpha \beta$ (FPU-\alpha\beta) models. Nonlinear parameter $\alpha$ also governs the degree of the interaction asymmetry.

By increasing $\alpha$ from zero where the potential is symmetric, one gets increasingly stronger asymmetry.

The effective sound velocity $\tilde{c}_s$ is an important outcome from EPT, which can be measured in a laboratory. Therefore, it is natural to consider $\tilde{c}_s$ as an observable to verify the effectiveness of EPT. Obviously, $\tilde{c}_s$ equals the renormalization factor $\eta$ in our dimensionless models. On the other hand, we can employ equilibrium fluctuation correlation method [7] (for an more detailed version, see [8]) to directly determine $\tilde{c}_s$ by simulations. The method has also been used to measure the effective sound velocity in FPU-\beta models and the results agree well with the theoretical predictions from Eqn. (5) [9]. We conduct numerical simulations at constant energy by integrating the equations of motion governed by (2) with periodic boundary conditions. We use random initial conditions by assigning velocities from a Gaussian distribution and zero relative displacements for each particle, respectively, with the two constraints that the total momentum is zero and the total energy is set to be a specified constant. The Runge-Kutta algorithm of 7-8th order is adopted with the time step 0.01 to ensure the conservation of the total system energy and momentum up to high accurate in the all run time. The system then evolves for a certain transient time in order to start the
measurements in well-defined equilibrium states. In order to confirm that the system has reached the thermal equilibrium state, we have checked that the value of energy localization to be $O(1)$ and the relative displacement and the velocity distributions of particles agrees well with the Gibbs statistics\[5\].

In Fig. 1, we compare the measured $\tilde{c}_s$ as a function of nonlinear parameters with the theoretical predictions from Eqs. (4) and (5) where $\langle \cdots \rangle$ is replaced by time average. It is clearly seen that the measured results agree well with the predictions of EPT for FPU-$\beta$ chains in the entire range of $\beta$ under study. In contrast, the systematic deviation from the predictions is clearly revealed as $\alpha$ increasing for FPU-$\alpha\beta$ chains. The theoretical results obviously underestimate the effective sound velocity of FPU-$\alpha\beta$ chains with larger asymmetry. These results imply that EPT does well for nonlinear chains with symmetric interactions, but break down for ones with asymmetric interactions.

For understanding the breakdown of EPT in 1D chains with asymmetric interactions, we shall perform a more microscopic measurement as follows. We directly extract the phonon frequency $\omega_m$ from the true dynamics governed by (2), then calculate the measured renormalization factor by $\eta_m = \frac{\omega_m}{\omega_h}$, where $\omega_h$ is the corresponding harmonic phonon frequency. To this aim, we shall analyze the power spectrum of velocity of a single particle randomly picked up from the chain at equilibrium. The same simulation process as mentioned above is used. A FFT algorithm is used to obtain the power spectrum with a time series of total time $10^5$ to ensure the high frequency resolution. The power spectrum is averaging over at least 20 trajectories to suppress the statistical fluctuations.

Figure. 2 shows the power spectrum of the single-particle velocity time series for FPU-$\beta$ model with $\beta=10$ and FPU-$\alpha\beta$ model with $\alpha=2$. In spite of strong nonlinearity and long system size ($N = 2048$ for both models), it is clearly seen that a few phonon peaks with the lowest frequencies is well distinguished from others whose peaks quickly decay into noise signals due to stronger the phonon-phonon interactions. It was commonly accepted that the long-wavelength phonons dominate the asymptotic behavior of 1D momentum-conserved lattices. This is the very reason that a long-wavelength approximations was extensively adopted in varied theories, such as the self-consistent mode-coupling theory\[10\] and hydrodynamics\[12,14\]. In addition, some important physical quantity, such as sound velocity, is defined in a long-wavelength limit. Therefore, it is fair to focus on the lowest frequency phonon peak. The separability of the lowest frequency phonon peak have been
FIG. 1: The effective sound velocity is plotted versus nonlinear parameters $\beta$ in FPU-$\beta$ chains (a) and $\alpha$ in FPU-$\alpha\beta$ chains (b) at equilibrium temperatures $T = 0.5$. The open triangles indicate the measured value by the equilibrium fluctuation correlation method for $N = 2048$ [7]. The red lines indicate the predictions from the Eqn. (4) and the blue lines indicate the predictions from the Eqn. (5), where $N = 128$.

checked for all parameters under investigation, and hence allow us to accurately measure its frequency and renormalization factor. Interestingly, our results intuitively display the image of “effective phonons” that was proposed on purely phenomenological basis in varied theories.

Figure. 2 also shows a notable difference between FPU-$\alpha\beta$ and FPU-$\beta$ models for linewidths of phonon peaks. The phonon peak for FPU-$\alpha\beta$ model is broader than the one for FPU-$\beta$ models by one order of magnitude under the current parameters. That means the asymmetric interactions provide stronger phonon-phonon interaction compared to the symmetric ones, which lead to shorter phonon lifetime. The results on phonon linewidths will be reported in our otherwise manuscript. Here, we focus on the effect of nonlinearity on phonon frequency.
FIG. 2: The phonon peaks in the low frequency regime for $N = 2048$ and $T = 0.5$. Blue solid line indicate the FPU-$\beta$ with $\beta = 10$; Red solid line indicate the FPU-$\alpha \beta$ with $\alpha = 2$ and $\beta = 1$. For comparison, the lowest harmonic frequency is also plotted by black solid line.

In Fig. 3, we plot the measured renormalization factor $\eta_m$ as the function of nonlinear parameters for two representative equilibrium temperatures 0.1 and 0.5, respectively. Meanwhile, we calculate the theoretical value of $\eta$ via the expressions (4) and (5), in which $<\cdots>$ was replaced by time average. For FPU-$\beta$ chains, the measured factor $\eta_m$ agree well with theoretical predictions in the entire parameter region being explored at both temperatures. In sharp contrast to that, the systematic deviation from the prediction is clearly seen again for FPU-$\alpha \beta$ chains at larger $\alpha$ at both temperatures. We also check that the $\eta_m$ is independent of systems size $N$ for both FPU-$\beta$ and FPU-$\alpha \beta$ models, as shown in Fig. 4. This result implies that the measured $\eta_m$ is independent of the wave numbers of phonons for the two models. Therefore, It is reasonable to measure the renormalization factor via the single phonon peak with the lowest frequency. The results further reveal that the EPT fail to renormalize the phonon frequency in chains with asymmetric interactions.

Naturally, a following question is if the measured renormalization factor can exactly
FIG. 3: The renormalization factor is plotted versus nonlinear parameters $\beta$ in FPU-$\beta$ chains and $\alpha$ in FPU-$\alpha\beta$ chains at equilibrium temperatures $T = 0.5$ and $T = 0.1$. The open circles indicate the measured value $\eta_m$. The red lines indicate the predictions from the Eqn. (4) and the blue lines indicate the predictions from the Eqn. (5).

predict the effective sound velocity for the chains under investigation. To check this, we compare the effective sound velocity obtained by $\eta$ with the measured one from the equilibrium fluctuation correlation method mentioned above. In Fig. 5, it is clearly seen that there is an excellent agreement between these two ways to obtain the effective sound velocity in both FPU-$\beta$ and FPU-$\alpha\beta$ models. These results confirm that one can obtain the correct renormalized frequency of phonon even in chains with larger interaction asymmetry where the EPT break down.

The effectiveness of EPT for FPU-$\beta$ chains even in a strongly nonlinear regime has also been confirmed by other authors [2, 3, 5], and be well understood under the frame of weak turbulence theory [4]. In these theoretical scenario, the FPU-$\beta$ dynamics with the strong nonlinear limit in thermal equilibrium can be effectively described by a system of weakly interacting renormalized normal modes. Such effective renormalization results mainly from
FIG. 4: The measured renormalization factor is plotted versus system size $N$ at equilibrium temperature $T = 0.5$ for FPU-$\beta$ chains with $\beta = 10$ (open circles) and FPU-$\alpha\beta$ chains with $\alpha = 2$ and $\beta = 1$ (open squares), where two horizontal lines are responding to their mean values, respectively.

the trivial resonant wave interactions, i.e., interactions with no momentum exchange. It is thus appropriate that for FPU-$\beta$ chains the mean-field approximation is employed as does EPT.

However, such a picture seemingly cannot extend to the chains with asymmetric interparticle interactions, as revealed by the results mentioned above. The deviation from the calculations in EPT in FPU-$\alpha\beta$ chains suggest that the asymmetric interactions may provide stronger nonlinearity than symmetric ones. Multich-phonon processes beyond the trivial resonant wave interactions should be considered, lead to breakdown of EPT. In fact, it was also found that asymmetric interactions results in stronger phonon-phonon interactions in the recent studies of energy equipartition [15] and heat conduction [16, 17] in FPU-$\alpha\beta$ chains. In the former case, shorter equipartition time was observed for FPU-$\alpha\beta$ chains comparing to the FPU-$\beta$ chains, and in the latter case, normal heat conduction was reported, against the abnormal heat conduction for FPU-$\beta$ chains.
FIG. 5: The measured sound velocity is plotted versus nonlinear parameters $\beta$ for FPU-$\beta$ chains (a) and FPU-$\alpha\beta$ chains (b) at the equilibrium temperature $T = 0.5$. The open circles indicate the values obtained by $\eta_m$ based on an analysis of the lowest frequency phonon peak for $N = 128$. The solid triangles indicate the values from measured values from the equilibrium fluctuation correlation method for $N = 2048$.

In summary, we check the EPT for both FPU-$\beta$ and FPU-$\alpha\beta$ models through an analysis of the lowest frequency phonon peak. It is found that the numerically measured renormalization factor and sound velocity agree well with the theoretical predictions for FPU-$\beta$ chains, whereas obviously deviate from predictions for FPU-$\alpha\beta$ chains. We stress that the asymmetric interactions play an important role responsible for breakdown of EPT, which provide stronger interactions among the phonons beyond the ones without momentum exchange occurred in the chains with symmetric interactions. We also confirm that the analysis based on the lowest frequency phonon peak can obtain the renormalized phonon frequency in momentum conserved chain with asymmetric interactions where EPT break down. It is a challenge to correct theories to effectively renormalize anharmonicity induced by asymmetric interactions.

Furthermore, the lowest frequency phonon peak analysis provide a test bed for the theories based on the long-wavelength approximations, such as the self-consistent mode coupling...
theory \[10\] and hydrodynamics \[12-14\]. The current work together with our recent reports on heat conduction \[16, 17\] have revealed the important roles of asymmetric interactions for phonon interactions in 1D momentum conserved nonlinear chains, which have been underestimated in conventional theories.

Acknowledgments

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