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Effective phonons in anharmonic lattices: Anomalous *vs.* normal heat conduction

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Abstract. – We study heat conduction in one-dimensional (1D) anharmonic lattices analytically and numerically by using an effective phonon theory. It is found that every effective phonon mode oscillates quasi-periodically. By weighting the power spectrum of the total heat flux in the Debye formula, we obtain a unified formalism that can explain anomalous heat conduction in momentum conserved lattices without on-site potential and normal heat conduction in lattices with on-site potential. Our results agree very well with numerical ones for existing models such as the Fermi-Pasta-Ulam model, the Frenkel-Kontorova model and the ϕ^4 model etc.

Recent years has witnessed increasing studies on heat conduction in one-dimensional (1D) anharmonic (nonlinear) lattices [1]. On the one hand, people would like to know whether or not Fourier's law of heat conduction for bulk material is still valid in 1D systems. This is a fundamental question in non-equilibrium statistical mechanics. In fact, it is not trivial at all as a rigorous proof is still not possible. On the other hand, the fast development of nano technology makes it possible to fabricate 1D or quasi 1D systems such as nanowire and/or nanotube etc and to measure its transport properties. To understand heat conduction properties in such systems is of great interest in heat control and management at nanoscale. Numerically, an anomalous heat conduction — heat conductivity diverges with system size— has been observed in momentum conserved systems without on-site potential such as the Fermi-Pasta-Ulam (FPU) lattice [2], and a normal heat conduction has been found in the systems with on-site potential like the Frenkel-Kontorova model [3] and the ϕ^4 model [4, 5].

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Unfortunately, up to now a general theory to predict the heat conduction behavior in a 1D system is still lacking.

In this letter, we investigate analytically and numerically the physical mechanism leading to the anomalous and the normal heat conduction in 1D anharmonic (nonlinear) lattices from an *effective phonon theory*. The theory is based on the ergodic hypothesis (equipartition theorem). As will be seen, our analytical result can explain the anomalous and normal heat conduction observed numerically in different models.

We consider a 1D anharmonic (nonlinear) lattice with the Hamiltonian

$$H = \sum_{i=1}^{N} \left[\frac{1}{2} m_i \dot{x}_i^2 + V(\delta x_{i,i+1}) + U(x_i) \right] \tag{1}$$

with periodic boundary condition $x_1 = x_{N+1}$. Here we chose mass $m_i = 1$ for all lattices. $\dot{x}_i = \mathrm{d}x_i/\mathrm{d}t$. $\delta x_{i,i+1} = x_i - x_{i+1}$. Without loss of generality, we write the inter-particle potential $V(\delta x_{i,i+1})$ and the on-site potential $U(x_i)$ as

$$V(\delta x_{i,i+1}) = \sum_{s=2}^{\infty} g_s \frac{(\delta x_{i,i+1})^s}{s}, \;\; U(x_i) = \sum_{s=2}^{\infty} \sigma_s \frac{x_i^s}{s}, \tag{2}$$

respectively. The canonical transformation which diagonalizes the harmonic Hamiltonian is $\boldsymbol{X} = \boldsymbol{BQ}$, where $X_i = (x_i \,\mathrm{or}\, \dot{x}_i)$, $Q_k = (q_k \,\mathrm{or}\, p_k)$, and B_{ik} are [6]

$$B_{ik} = \begin{cases} \sqrt{\frac{2}{N}} G_k \cos \frac{2i\pi(k-1)}{N}, & k = 1, ..., \left[\frac{N}{2}\right] + 1, \\ \sqrt{\frac{2}{N}} G_k \sin \frac{2i\pi(N-k+1)}{N}, & k = \left[\frac{N}{2}\right] + 2, ..., N, \end{cases}$$

where $\left[\frac{N}{2}\right]$ is the integer part of $\frac{N}{2}$, and $G_k = 1/\sqrt{2}$ for $k = 1$ and $k = N/2 + 1$ if N is even, otherwise $G_k = 1$. The spectrum of the harmonic lattice is $\omega_k = 2 \sin (k-1)\pi/N$.

Under the *ergodic hypothesis*, the system obeys the generalized equipartition theorem [7] $k_B T = \left\langle q_k \frac{\partial H}{\partial q_k} \right\rangle$, here $\langle \cdot \rangle$ denotes the canonical ensemble average. The force in k space has two parts

$$-F_k = \frac{\partial H}{\partial q_k} = \sum_{i=1}^{N} \sum_{s=2}^{\infty} \left(\omega_k g_s (\delta x_{i,i+1})^{s-1} \gamma_{ik} + \sigma_s x_i^{s-1} B_{ik} \right),$$

where the new matrix γ_{ik} is defined as in ref. [6], $\gamma_{ik} = 0$ for $k = 1$ and $\gamma_{ik} = (1/\omega_k)(B_{ik} - B_{i+1k})$ otherwise. γ_{ik} satisfy $\sum_{i=1}^{N} \delta x_{i,i+1} \gamma_{ik} = \omega_k q_k$, $\sum_{k=2}^{N} \gamma_{ik} \omega_k q_k = \delta x_{i,i+1}$. The generalized equipartition theorem becomes

$$\begin{aligned} k_B T &= \sum_{i=1}^{N} \sum_{s=2}^{\infty} \left(\omega_k g_s \langle (\delta x_{i,i+1})^{s-1} q_k \rangle \gamma_{ik} + \sigma_s \langle x_i^{s-1} q_k \rangle B_{ik} \right), \\ &\approx \sum_{s=2}^{\infty} \left[g_s \frac{\langle \sum_{i=1}^{N} (\delta x_{i,i+1})^s \rangle}{\langle \sum_{i=1}^{N} (\delta x_{i,i+1})^2 \rangle} \omega_k^2 + \sigma_s \frac{\langle \sum_{i=1}^{N} x_i^s \rangle}{\langle \sum_{i=1}^{N} x_i^2 \rangle} \right] \langle q_k^2 \rangle, \\ &\equiv \alpha(\omega_k^2 + \gamma) \langle q_k^2 \rangle, \end{aligned} \tag{3}$$

where

$$\alpha = \frac{\sum_{s=2}^{\infty} g_s \langle \sum_{i=1}^{N} (\delta x_{i,i+1})^s \rangle}{\langle \sum_{i=1}^{N} (\delta x_{i,i+1})^2 \rangle},$$

and

$$\gamma = \frac{1}{\alpha}\frac{\sum_{s=2}^{\infty}\sigma_s\langle\sum_{i=1}^{N}x_i^s\rangle}{\langle\sum_{i=1}^{N}x_i^2\rangle}.$$

In analogy with a harmonic lattice where $k_BT = \omega_k^2\langle q_k^2\rangle$, we define effective phonons in 1D anharmonic lattices. The frequencies of the effective phonon are

$$\hat{\omega}_k^2 = \alpha(\omega_k^2 + \gamma), \tag{4}$$

here k is wave vector with replacement $k \to 2\pi(k-1)/N$ and $\omega_k = 2\sin\frac{k}{2}$. The corresponding velocities are

$$v_k = \frac{\partial\hat{\omega}_k}{\partial k} = \frac{\sqrt{\alpha}\ \omega_k}{\sqrt{\omega_k^2+\gamma}}\cos\frac{k}{2}. \tag{5}$$

It has been found [6, 8] numerically that the approximation in eq. (3) is feasible for anharmonic lattices without on-site potential such as the FPU-β model ($U(x) = 0$, $V(x) = x^2/2 + \beta x^4/4$, we take $\beta = 1$ in this paper) and the H_4 model ($U(x) = 0$, $V(x) = x^4/4$); α is found to be independent of mode k and lattice length.

In order to check if eq. (3) is suitable for the anharmonic chains with on-site potential, we study numerically γ for the ϕ^4 model ($U(x) = x^2/2, V(x) = x^4/4$) and the quartic ϕ^4 model ($U(x) = x^4/4, V(x) = x^4/4$). We find that γ is independent of k and the chain length provided the chain is long enough. For example, $\gamma \simeq 1.065$ for the ϕ^4 model with chain length $N \geq 64$ at temperature $T = 1$. In fig. 1, we show $\langle p_k^2\rangle/(\hat{\omega}_k^2\langle q_k^2\rangle)$ and dispersion relation $\hat{\omega}_k$ for quartic ϕ^4 (upper panel) and ϕ^4 (lower panel) models. $\langle p_k^2\rangle/(\hat{\omega}_k^2\langle q_k^2\rangle)$ is very close to one for all k in both models. We also find that γ increases with temperature as $\gamma \sim T^{0.61\pm0.01}$ (see, fig. 2). Therefore, we can conclude that the approximation is good for both anharmonic chains with and without on-site potential under ergodic hypothesis.

It should be pointed out that the approximation in eq. (3) is a kind of mean-field approximation. It is based on our numerical observation as a rigorous proof is not possible,. The phonon-phonon interaction is implicitly contained in the two coefficients α and γ.

The heat conductivity can be derived from the Debye formula

$$\kappa = \sum_k c_k v_k^2 \tau_k,$$

where c_k, v_k, and τ_k are specific heat, phonon velocity and phonon relaxation time of mode k, respectively. Generally, the contribution from phonons of different frequencies should in principle be weighted but this is not reflected in the Debye formula. Since the heat conductivity is a transport coefficient of heat energy which manifest itself by heat flux, this weight factor must be the power spectrum of the total heat flux. Thus we rewrite the Debye formula for 1D anharmonic lattices as,

$$\kappa = \sum_k P_k c_k v_k^2 \tau_k,\ 0 < k \leq 2\pi,$$

in which P_k is the normalized power spectrum of the total heat flux. Moreover, the Debye formula does not give an explicit expression of the phonon relaxation time τ_k. From our numerical calculations, we find that each mode oscillates quasi-periodically for both lattices with and without on-site potential (see fig. 3). It is therefore reasonable to assume that the phonon relaxation time is proportional to the quasi-period of each mode, *i.e.*, $\tau_k = \lambda\frac{2\pi}{\hat{\omega}_k}$, where the prefactor λ is only temperature dependent and will be discussed in another paper.

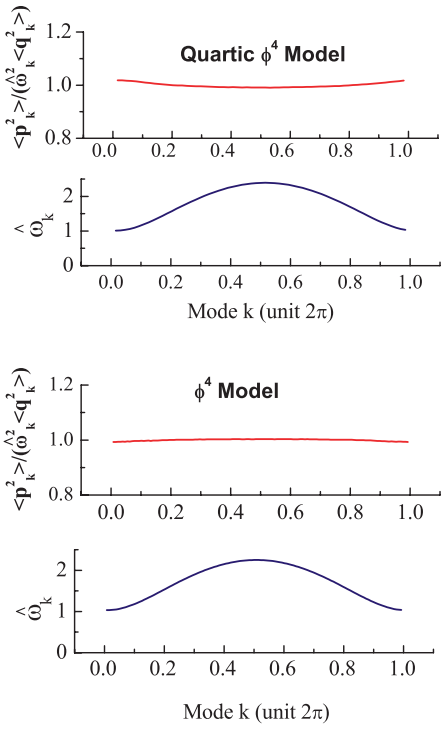

Fig. 1

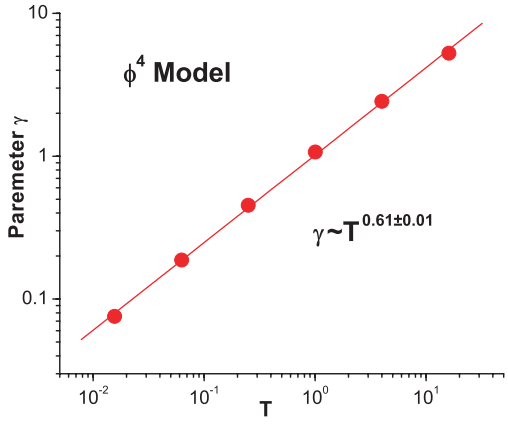

Fig. 2

Fig. 1 – The energy ratio, $\langle p_k^2\rangle/\hat{\omega}_k^2\langle q_k^2\rangle$, and dispersion relation $\hat{\omega}_k$ *vs.* k for the ϕ^4 model (lower panel) and the quartic ϕ^4 model (upper panel). $N = 128$ for the ϕ^4 model, and $N = 64$ for the quartic ϕ^4 model. Temperature is set to $T = 1$.

Fig. 2 – Parameter γ *vs.* temperature T for the ϕ^4 model.

To deal with the size dependence of the heat conductivity, it is more convenient to consider the mean-free-path rather than the relaxation time. The mean-free-path of the effective phonons is defined by

$$l_k = v_k\tau_k = 2\pi\lambda\frac{\omega_k}{\omega_k^2+\gamma}\cos\frac{k}{2}. \tag{6}$$

For systems without on-site potential where $\gamma = 0$, l_k reduces to

$$l_k = \frac{2\pi\lambda}{\omega_k}\cos\frac{k}{2}.$$

In the long-wavelength limit, $k \to 0$, the mean-free-path $l_k \propto 1/k$, becomes divergent. However, for systems with on-site potential where $\gamma > 0$, the mean-free-path of any effective phonon is finite. This difference results in different heat conduction behaviors in systems without on-site potential and systems with on-site potential.

The modified Debye formula of thermal conductivity can be expressed in a continuous form in the thermodynamical limit:

$$\kappa = \frac{N}{2\pi}\int_0^{2\pi} P(k)c_k v_k l_k \mathrm{d}k = c\lambda\sqrt{\alpha}\int_0^{2\pi} P(k)\frac{\omega_k^2}{(\omega_k^2+\gamma)^{3/2}}\cos^2\frac{k}{2}\mathrm{d}k, \tag{7}$$

where $c = \sum_k c_k$. By definition, $P(k)\mathrm{d}k = P(\omega)\mathrm{d}\omega$, and $P(\omega)$ is the Fourier transform of the auto-correlation function of the total heat flux $J(t)$.

Equation (7) is the main analytical result of this letter. Whether the heat conduction in a 1D system is normal or anomalous depends on whether the integral of eq. (7) is finite or infinite. For systems with on-site potential such as the FK model and the ϕ^4 model where $\gamma > 0$, all integrands except the normalized power spectrum $P(k)$ are finite. Since $P(k)$ should be normalized over the phonon spectrum $\int_0^{2\pi} P(k)\mathrm{d}k = 1$, the integral of eq. (7) for systems with on-site potential is always finite. Thus even without knowing exact knowledge of $P(k)$, we can predict that heat conduction of systems with on-site potential obeys Fourier's Law. However for systems without on-site potential, $\gamma = 0$ which implicitly means the momentum conservation. The integral of eq. (7) reduces to $\int_0^{2\pi} P(k)\frac{\cos^2\frac{k}{2}}{\omega_k}\mathrm{d}k$. In the long-wavelength limit, $\omega_k \approx k$, the integral has a singularity at $k \to 0$. This singularity originates from the infinite mean-free-path of the effective phonon of the long-wavelength limit and is proportional to $1/k$. Since the effective phonon of the long-wavelength is the most dominant part for heat transfer, the systems without on-site potential will exhibit an anomalous heat conduction. In the following we shall apply the above theory to two typical classes of Hamiltonian systems, the FPU model, a representative model without on-site potential, and the ϕ^4 model, a representative one with on-site potential. As shall be seen soon our theory gives predictions in good agreement with numerical simulations.

Systems without on-site potential. – In the Hamiltonian (1), $U(x) = 0$ means momentum conservation, and $\gamma = 0$ in eq. (3). Here we focus on the FPU-β model. The details of renormalized frequencies of effective phonons will be discussed as well as the effective phonon speed and the heat conductivity with respect to lattice length.

In the FPU-β model, $V(x) = x^2/2 + x^4/4$ and $U(x) = 0$. α is determined only by temperature [6, 9]. In this model, α has a simple analytic expression

$$\alpha = 1 + \frac{\left\langle \sum_{i=1}^{N} \left(\delta x_{i,i+1}\right)^4 \right\rangle}{\left\langle \sum_{i=1}^{N} \left(\delta x_{i,i+1}\right)^2 \right\rangle} = 1 + \frac{\int_{-\infty}^{\infty} \phi^4 e^{-V(\phi)/T}\mathrm{d}\phi}{\int_{-\infty}^{\infty} \phi^2 e^{-V(\phi)/T}\mathrm{d}\phi} \tag{8}$$

this equation is equivalent to the eq. (11) of ref. [9].

If the effective phonons of long wavelength are dominant in heat transfer, which is true for a system of large size, the speed of the energy transport can be approximated by the speed of the effective phonon with the longest wavelength

$$v = \sqrt{\alpha}\cos\frac{\pi}{N}. \tag{9}$$

In fig. 4 we draw the above analytical v *vs.* temperature for two different system sizes and compare them with the numerical ones from Aoki and Kuznezov [10]. The agreement between our analytical results (9) and the numerical ones is very good in a very wide range of temperature (five orders of magnitudes.)

In the thermodynamic limit $N \to \infty$, the size dependence of heat conductivity only depends on the integral

$$\kappa \propto \int_0^{2\pi} P(k)\frac{\cos^2\frac{k}{2}}{\omega_k}\mathrm{d}k. \tag{10}$$

If the effective phonons of long wavelength dominate the heat transfer, and $P(k) \propto k^{-\delta}$ ($\delta > 0$) asymptotically in the long-wavelength limit, then, the heat conductivity is a system-size–dependent quantity, $\kappa \propto k^{-\delta} \propto N^{\delta}$. The numerical calculation of the power spectrum of the

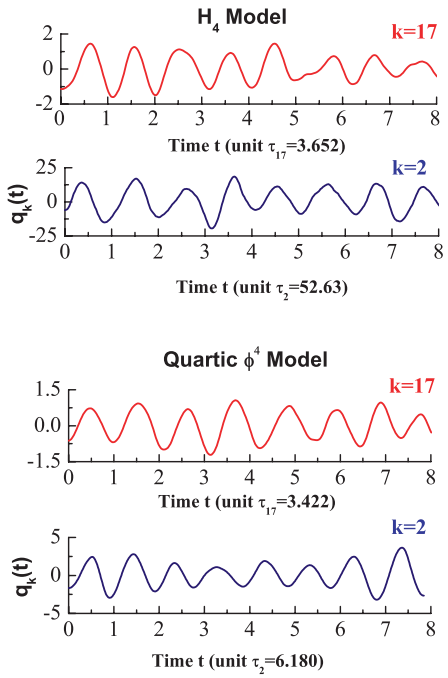

Fig. 3

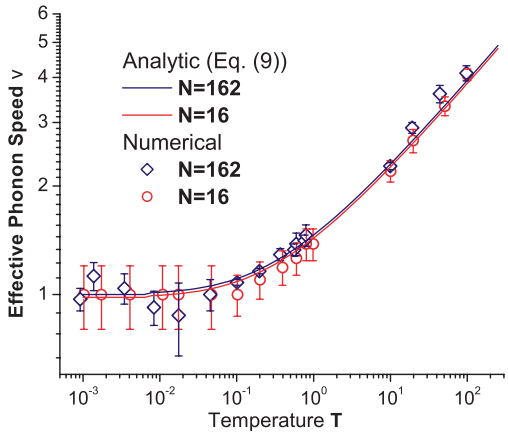

Fig. 4

Fig. 3 – Time behaviors of $q_k(t)$ of the H_4 model and the quartic ϕ^4 model. $N = 64$ and $T = 1$ for both models. $\tau_k = 2\pi/\hat{\omega}_k$.

Fig. 4 – The effective phonon speed in the FPU-β model *vs.* temperature. The numerical results come from the lower panel of fig. 3 in ref. [10]

total heat flux in the FPU-β model has shown that $\delta \approx 0.37 \sim 0.4$ [2]. This divergent behavior of thermal conductivity has been observed in the FPU model by different groups [2, 4, 10].

Systems with on-site potential. – Things turn out to be different for systems with on-site potential. Having an on-site potential means that $\gamma > 0$ and the momentum conservation is broken. A phonon band gap appears around zero frequency. Under the ergodic assumption, heat conduction in such systems obeys Fourier's law. For the sake of simplicity, we only discuss the ϕ^4 model.

The ϕ^4 model has a quadratic inter particle potential, $V(x) = x^2/2$ and a quartic external potential $U(x) = x^4/4$. Therefore, we have $\alpha = 1$ and $\gamma = \langle\sum_{i=1}^{N} x_i^4\rangle/\langle\sum_{i=1}^{N} x_i^2\rangle$. The ensemble average has no simple analytic expression. At temperature $T = 1$, the numerical value $\gamma \approx 1.065$ is found to be independent of length at least for $N \geq 64$. The dispersion relation, $\hat{\omega}_k = \sqrt{4\sin^2\frac{k}{2} + 1.065}$, is shown in fig. 1.

The mean-free-path l_k depends on temperature via the parameters γ and λ, $l_k = v_k\tau_k = 2\lambda\pi\sin k/(4\sin^2\frac{k}{2} + \gamma)$. In the low-temperature limit, the ϕ^4 model reduces to the harmonic model where λ is infinity. Therefore, λ should decrease with temperature. From fig. 2, we can see that γ increases monotonically with temperature. As a result, the mean-free-path decreases as temperature is increased, since the heat conductivity is independent of N when N is larger than the mean-free-path. The higher the temperature, the smaller the size effect for the ϕ^4 model as observed by Aoki and Kuznezov [10].

In summary, from an effective phonon theory, we have derived an analytic formula for heat conductivity in 1D nonlinear lattices, eq. (7). We find that the phonon-phonon interaction due to the anharmonicity (nonlinearity) can be written as an effective harmonic one in terms of the ensemble average, so we can attribute the heat transfer to the effective phonons which can be treated in the same way as phonons in the harmonic lattice. The difference between system without on-site potential and system with on-site potential lies in their renormalized frequencies. For systems without on-site potential, there exists a zero-frequency mode with infinite mean-free-path which is the physical mechanism for the anomalous heat conduction. For systems with on-site potential, a phonon band gap near zero frequency appears leading to the normal heat conduction, *i.e.* heat conduction obeys Fourier's Law.

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