Thermal conductivity of one-dimensional lattices with self-consistent heat baths: a heuristic derivation

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We derive the thermal conductivities of one-dimensional harmonic and anharmonic lattices with self-consistent heat baths (BRV lattice) from the Single-Mode Relaxation Time (SMRT) approximation. For harmonic lattice, we obtain the same result as previous works. However, our approach is heuristic and reveals phonon picture explicitly within the heat transport process. The results for harmonic and anharmonic lattices are compared with numerical calculations from Green-Kubo formula. The consistency between derivation and simulation strongly supports that effective (renormalized) phonons are energy carriers in anharmonic lattices although there exist some other excitations such as solitons and breathers.

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Heat conduction exhibits diversified behaviors for one-dimensional lattices in terms of heat current $j$ as the function of lattice length $N$, $\alpha$. Harmonic lattice possesses ballistic heat transport in which the heat current is independent of the lattice length, $j \sim N^0$. Anharmonic lattices without external potential such as FPU-like lattices have anomalous heat conduction $3$ in the sense $j \sim N^{-\alpha}$, where $0 < \alpha < 1$. Anharmonic lattices with external potential such as Frenkel-Kontorova (FK) and $\phi^4$ lattices show normal Fourier’s heat conduction $3, 6$ since $j \sim N^{-1}$. After intensive numerical simulations over the last decade, it has been commonly accepted that anharmonicity and external potential are sufficient to induce Fourier’s heat conduction law. In fact, Bolsterli, Rich and Visscher (BRV) have obtained in 1970 the Fourier’s heat conduction by attaching external heat baths to every atom of a harmonic chain $3$. In this so-called BRV lattice, the interaction between heat baths and harmonic chain resembles the external anharmonic forces.

The BRV lattice plays a fundamental role in understanding the Fourier’s law in one-dimensional lattices as exemplified by recent studies $8, 9$. In Ref. $9$, Bonetto, Lebowitz and Lukkarinen revisit the thermal transport of BRV lattice with a mathematically rigorous treatment. In addition, they also obtain the same result from the derivation of Green-Kubo formula. In Ref. $9$, they deal with the quantum BRV lattice and obtain the exact result in the classical (high-temperature) limit. However, the phonon picture during thermal transport is not reflected explicitly in their approaches. Harmonic lattice only allows phonons as the collective motion. There is no doubt that phonons should be the energy carriers for harmonic lattice. However for anharmonic lattices, there are some other collective motions such as solitons $10$ and breathers $11$ existing as the consequence of anharmonicity. They are proposed as the energy carriers responsible for some novel transport phenomena, e.g. thermal rectifying in asymmetric nanotubes $12$, anomalous heat conduction in FPU-$\beta$ lattice $13$ and so on $14, 15$. An investigation for anharmonic BRV lattices where external heat baths are attached to every atom of an anharmonic chain is desirable and this may shed some light on the role of energy carriers for anharmonic lattice.

In this work, we study the thermal conductivities of BRV lattices from a different approach named as the Single-Mode Relaxation Time (SMRT) approximation from Boltzmann equation $16, 17$. Both harmonic and anharmonic BRV lattices have been considered. The results from SMRT approximation are also compared with numerical simulations from Green-Kubo method. The harmonic BRV lattice is described as a one-dimensional harmonic chain of $N$ atoms attached by independent Langevin heat baths. The Hamiltonian of this harmonic chain reads

$$H = \sum_{i=1}^{N} \left( \frac{1}{2} p_i^2 + \frac{1}{2} \omega^2 (q_{i+1} - q_i)^2 + \frac{1}{2} \gamma^2 q_i^2 \right) \quad (1)$$

where $q_i$ is the $i$’th atom’s displacement from its equilibrium position. $\omega^2$ and $\gamma^2$ represent the strength of inter-atom and external potential respectively. For a chain with lattice constant $a$ and atom mass $m$, we adopt the dimensionless units by setting $a = m = 1$. A periodic boundary condition $q_{N+1} = q_1$ is used. The heat bath attached to every atom is modeled by stochastic Langevin heat bath. The coupling strength is determined by the friction coefficient $\lambda$ in Langevin dynamics. Thus the equation of motion of the harmonic BRV lattice is expressed as

$$\ddot{q}_i = \frac{\partial H}{\partial q_i} + \xi_i - \lambda \dot{q}_i \quad (2)$$

where $\xi_i$ is the Gaussian white noise with $\langle \xi_i(t) \rangle = 0$ and $\langle \xi_i(t) \xi_j(0) \rangle = 2 \lambda k_B T \delta(t)$. 
According to the SMRT approximation\[16, 17\], the thermal conductivity for one-dimensional system has a compact expression

$$\kappa = \frac{c}{\pi} \int_0^\pi v^2(k)\tau(k)dk \quad (3)$$

where $c$ is the specific heat, $k$ the phonon wavevector, $v(k)$ the group velocity, and $\tau(k)$ the phonon relaxation time of mode $k$. We focus on the classical transport processes where specific heat $c = k_B$ for harmonic lattice with Hamiltonian Eq. \[11\].

To obtain the group velocity $v(k)$, we need to find the phonon dispersion relation. From Eq. \[11\], one readily obtains the following dispersion relation $\omega_k = \sqrt{4\sin^2 k/2 + \nu^2}$ for $k \in [0, \pi]$ with $\nu^2 = \gamma^2/\omega^2$. Thus the phonon group velocity is obtained

$$v(k) = \frac{\partial \omega_k}{\partial k} = \omega \frac{\sin k}{\sqrt{4\sin^2 k/2 + \nu^2}} \quad (4)$$

If the system has no external potential, i.e. $\gamma = 0$, the phonon group velocity is $v(k) = \omega \cos k/2$. The existence of external potential shifts the phonon band off the zero point and reduces the phonon group velocity, as can be seen from Eq. \[4\].

To analyze the phonon relaxation time $\tau(k)$, we consider the velocity auto-correlation function $\langle \dot{q}_k(t)\dot{q}_k(0) \rangle$ for mode $k$. Here $q_k$ is the counterpart of $q_i$ in mode space after some canonical transformation $q_k = \sum_{i=1}^N S_kq_i$. $S$ is the transformation matrix. We use symbol $k$ to represent wavevector and mode index simultaneously since it will not cause confusion. After canonical transformation, the Hamiltonian can be decomposed into separated harmonic oscillators specified by a frequency $\omega_k$. Performing the transformation on both sides of Eq. \[2\], we obtain the separated equation of motion in mode space: $\ddot{q}_k(t) = -\omega_k^2q_k + \xi_k(t) - \lambda k\dot{q}_k$. After transformation, $\xi_k$ still obeys the statistical properties of Gaussian white noise. Especially, the statistical properties of the fluctuations will not depend on the choice of the potential form. The above Langevin equation can be solved\[18\] by setting the first term on the right hand side to zero: $\dot{q}_k(t) = q_k(0)e^{-\lambda t} + \int_0^t dt' e^{-\lambda(t-t')}\xi_k(t')$. Substituting the solution of $\dot{q}_k(t)$ into the velocity auto-correlation function, we have

$$\langle \dot{q}_k(t)\dot{q}_k(0) \rangle = \langle \dot{q}_k^2(0) \rangle e^{-\lambda t} \quad (5)$$

The ensemble average of the terms containing $\xi_k(t)$ vanish due to the statistical property of Gaussian white noise. The velocity auto-correlation function decays exponentially with a characteristic time of $1/\lambda$. Therefore we come to the conclusion that the phonons acquire a frequency-independent relaxation time $\tau(k) = 1/\lambda$ due to the coupling with the external Langevin heat bath.

FIG. 1: (Color online) Thermal conductivity $\kappa$ vs $\nu$. Solid curve is from Eq. \[6\], and bullets are numerical results from Green-Kubo method. The parameters are $\omega = 1, \lambda = 0.25, T = 1$ for a lattice with $N = 100$. The Boltzmann constant $k_B$ is set to unity.

As a result, the thermal conductivity can be obtained from Eq. \[6\]

$$\kappa = \frac{k_B}{\pi} \int_0^\pi \left( \frac{\omega \sin k}{\sqrt{4\sin^2 k/2 + \nu^2}} \right)^2 \frac{1}{\lambda} \frac{d\nu}{d\lambda} \quad (6)$$

Thus we have obtained the same exact result as in previous works\[8\] from a heuristic derivation. The phonon picture for the thermal transport is explicitly revealed in our derivation.

As we have mentioned in the introduction, it has been proved that the Green-Kubo formula renders the same result\[8\]. Here we calculate the thermal conductivities of harmonic BRV lattice by Green-Kubo formula numerically. The advantage of numerical Green-Kubo method lies in the fact that it can be easily extended to anharmonic BRV lattice where no existing theoretical analysis has ever been applied. The thermal conductivity is calculated from\[8\]

$$\kappa = \frac{1}{k_B T^2 N} \int_0^\infty (J(t)J(0))dt \quad (7)$$

where $J(t) = \sum_{i=1}^N j_i$ and $j_i = \dot{q}_i \frac{V(q_i, q_{i+1})}{\delta V}$ is the heat current within the chain. $V(q_i, q_{i+1})$ represents the inter-atom potential. The length and temperature independence of $\kappa$ has been verified by Green-Kubo simulations (not shown here). In Fig[4] we plot the thermal conductivity as a function of $\nu$ at $\omega = 1, \lambda = 0.25, T = 1$.
for a length \( N = 100 \). The numerical result for a 100-atoms chain has already approached the continuous-limit result. There is no surprise since the mean-free-path \( l(k) \) of phonons \( l(k) = v(k)\tau(k) \sim \omega/\lambda \sim 4 \) is much shorter than the chain length \( N = 100 \).

Next we shall consider the anharmonic BRV lattice. As we have seen above, the existence of external potential only affects the group velocity. For simplicity, we only consider the anharmonic BRV lattice without external potential term. First we consider the anharmonic case containing FPU-\( \beta \) chain. The Hamiltonian of FPU-\( \beta \) chain is

\[
H = \sum_{i=1}^{N} \left[ \frac{1}{2} p_i^2 + \frac{1}{2} (q_{i+1} - q_i)^2 + \frac{1}{4} (q_{i+1} - q_i)^4 \right] \tag{8}
\]

Due to the anharmonic interaction, the canonical transformation of Eq. (2) yields coupled equations of motion in mode space. In this case, we need to evoke the effective phonon theory\([10]\), which considers the phonon-phonon interaction as a kind of mean field. The anharmonic Hamiltonian can be viewed as weakly coupled effective phonons with a renormalized frequency \( \omega_k \). Thus by ignoring the weakly coupled interactions within effective phonons, we obtain the approximate equations of motion in mode space: \( \dot{q}_k = -\omega_k^2 q_k + \xi_k - \lambda q_k \). The statistical properties of the fluctuations don’t depend on the choice of the potential form. With similar analysis, the relaxation time for effective phonons is still the frequency-independent \( 1/\lambda \). The major anharmonic effect comes from the group velocity of effective phonons. According to the effective phonon theory, the effective phonon frequency \( \dot{\omega}_k \) in FPU-\( \beta \) chain is proportional to the phonon frequency \( \omega_k = 2 \sin k/2 \) with a temperature(anharmonicity)-dependent prefactor, i.e. \( \dot{\omega}_k = \sqrt{\alpha} \omega_k \). The temperature-dependent coefficient \( \alpha \) has the following analytic expression

\[
\alpha = 1 + \int_{0}^{\infty} \phi^4 \int_{0}^{\infty} e^{-\beta(\phi^2/2 + \phi^4/4)} d\phi \int_{0}^{\infty} \phi^2 e^{-\beta(\phi^2/2 + \phi^4/4)} d\phi \]

\( \beta \equiv 1/k_B T \). From this, we obtain the group velocity of effective phonons: \( v(k) = \partial \omega_k / \partial k = \sqrt{\alpha} \cos k/2 \).

The anharmonic interaction will also make the specific heat a function of temperature. This effect cannot be neglected when temperature is not very low. For a chain with \( N \) atoms, the specific heat is determined by

\[
c \equiv \langle H \rangle / NT.
\]

As a result of energy equipartition theory, the contribution to specific heat from kinetic energy is half of the Boltzmann constant \( k_B / 2 \). The contribution from potential energy can be derived by using the equality \( Nk_B T = \sum_{i=1}^{N} \langle q_i^2 \rangle / m_i \). Substituting the Hamiltonian, Eq. (8), into the above equality and using the definition of specific heat, one can obtain the specific heat for FPU-\( \beta \)

\[
c = k_B \left[ 1 - \frac{\int_{0}^{\infty} \phi^4 e^{-\beta(\phi^2/2 + \phi^4/4)} d\phi}{\int_{0}^{\infty} e^{-\beta(\phi^2/2 + \phi^4/4)} d\phi} \right] \tag{9}
\]

The low and high temperature limit value of \( c \) are \( k_B \) and \( k_B / 4 \), respectively. The temperature-dependent \( c \) is plotted in Fig. 2. The monotonically decreasing specific heat as the function of temperature looks counter-intuitive as we all know that the specific heat of real material is a monotonically increasing function of temperature. We have to emphasize two things clearly here. First we only deal with classical specific heat. For harmonic chain, the classical specific heat is a temperature-independent constant \( k_B \). Second, we have introduced the anharmonic interaction. The anharmonic interaction actually reduces the specific heat. Thus the ”counter-intuitively” decreasing specific heat with temperature is a classically anharmonicity-induced result.

The thermal conductivity of FPU-\( \beta \) BRV lattice can be derived from Eq. (3) as

\[
\kappa = \frac{c}{\pi} \int_{0}^{\pi} \left( \sqrt{\alpha} \cos k/2 \right)^2 \frac{1}{\lambda} dk = \frac{ca}{2\lambda} \tag{10}
\]

Thus, \( \kappa \) depends on temperature via the product of \( c \) and \( \alpha \). To verify this prediction, we perform the Green-Kubo calculations of \( \kappa \). The results are plotted in Fig. 3. Solid curve is our prediction of Eq. (10) and red solid circles are the numerical values of \( \kappa \). Our prediction agrees very well with the Green-Kubo calculations for a very wide temperature range of about four orders of magnitudes.

It must be emphasized that our prediction is derived only by assuming effective phonons as the energy carriers and ignoring the weak interactions between them.

The consistency between theoretical analysis and numerical simulations clearly demonstrate that it is effective phonons, a kind of renormalized phonons due to anhar-
The final expression of $\kappa$ obtained is from Eq. (10) for FPU-\(\beta\) and symmetric FPU-\(\alpha\) BRV lattices, respectively. Solid circles and hollow circles are the numerical Green-Kubo results for FPU-\(\beta\) and symmetric FPU-\(\alpha\) BRV lattices, respectively. The horizontal line marks the value of $\kappa$ for harmonic BRV lattice. The simulations are performed at $\lambda = 0.25$ for a lattice with $N = 100$. Boltzmann constant $k_B$ has been set to unity.

Besides FPU-\(\beta\) BRV lattice, we also consider another simple anharmonic BRV lattice containing a symmetric FPU-\(\alpha\) chain

$$H = \sum_{i=1}^{N} \left[ \frac{1}{2} p_i^2 + \frac{1}{2} (q_{i+1} - q_i)^2 + \frac{1}{3} |q_{i+1} - q_i|^3 \right]$$

(11)

The expression of specific heat $c$ and coefficient $\alpha$ are obtained

$$c = k_B \left[ 1 - \frac{\int_{0}^{\infty} \phi^3 e^{-\beta(\phi^2 + \phi^4)} d\phi}{\int_{0}^{\infty} e^{-\beta(\phi^2 + \phi^4)} d\phi} \right]$$

$$\alpha = 1 + \frac{\int_{0}^{\infty} \phi^3 e^{-\beta(\phi^2 + \phi^4)} d\phi}{\int_{0}^{\infty} \phi^2 e^{-\beta(\phi^2 + \phi^4)} d\phi}$$

(12)

As we have discussed for FPU-\(\beta\) BRV lattice, the symmetric FPU-\(\alpha\) BRV lattice also has a frequency-independent phonon relaxation time, i.e. $\tau(k) = 1/\lambda$. The final expression of $\kappa$ is also the same as Eq. (10). Here we should keep in mind that the specific heat $c$ and $\alpha$ are now coming from Eq. (12). This prediction is plotted in Fig. 3 as the dotted curve. The numerical results (hollow circles in Fig. 3) are in good agreement with this prediction.

In summary, we have derived analytically the thermal conductivities of harmonic and anharmonic BRV lattices from the SMRT approximation. The derivation is heuristic and the phonon (effective phonon) picture is explicit during derivation. For harmonic BRV lattice, we obtain the same exact result as in previous works. For anharmonic BRV lattices, we obtain the approximate results and compare them with numerical simulations from the Green-Kubo formula. The consistency between our theoretical results and numerical simulations demonstrates that the effective (renormalized) phonons should be the fundamental energy carriers of anharmonic lattices. The contributions from solitons and breathers, if any, are negligible at least for FPU-like lattices.

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