Variational approach to renormalized phonon in momentum-nonconserving nonlinear lattices

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received 16 March 2016; accepted in final form 24 May 2016
published online 13 June 2016

PACS 05.45.-a – Nonlinear dynamics and chaos
PACS 63.20.-e – Phonons in crystal lattices
PACS 45.10.Db – Variational and optimization methods

Abstract – In this letter, we extend a previously proposed variational approach to systematically investigate general momentum-nonconserving nonlinear lattices. Two intrinsic identities characterizing optimal reference systems are firstly revealed, which enables us to derive explicit expressions for optimal variational parameters. The resulting optimal harmonic reference systems provide information for the band gap as well as the dispersion of renormalized phonons in momentum-nonconserving nonlinear lattices. As a demonstration, we consider the one-dimensional $\phi^4$ lattice. We show that the phonon band gap endows a simple power-law temperature dependence in the weak stochasticity regime where predicted dispersion is reliable by comparing with numerical results. In addition, an exact relation between ensemble averages of the $\phi^4$ lattice in the whole temperature range is found, regardless of the existence of the strong stochasticity threshold.

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Introduction. – The understanding of the microscopic foundation of Fourier’s law is a long-standing problem in statistical physics. One of the promising ways along this direction is the study of heat conduction in low-dimensional nonlinear lattices [1–3]. Among the investigations, an interesting perspective is to find a nonlinear lattice which displays normal heat conduction, namely, where Fourier’s law holds. After numerous numerical simulations [4–9], a consensus that one-dimensional (1D) nonlinear lattices with on-site potentials can establish normal heat conduction has been reached. Unraveling the microscopic mechanism of heat transfer across such momentum-nonconserving (MNC) lattices thus may provide crucial insights to the foundation of Fourier’s law.

Phenomenologically [10], the heat conductivity $\kappa$ can be approximately obtained via the Peierls formula, i.e., $\kappa = \sum_k C_k v_k l_k$, where $k$ is the phonon wave number, $C_k$ the specific heat of the phonon mode, $v_k$ its phonon group velocity and $l_k$ the corresponding mean free path (MFP). Following this spirit, a theoretical proposal for phonon heat transport based on renormalized phonon has been carried out [11,12]. Nevertheless, flaws in its phonon description [13] may produce wrong phonon information, which limits its ability and generality. Trying to understand the process of heat conduction from the phonon point of view, theoretical investigations on the phonon properties seems to be a necessary step. Thus a unified phonon theory which is capable of dealing with various nonlinear lattices is of primary interest and importance at the present stage. However, the attempts concerning phonon properties in MNC lattices are fewer [11,12,14], compared with studies carried out on momentum-conserving (MC) counterparts exhibiting anomalous heat conduction [15–23]. More efforts should be devoted to the former.

In a previous study [23], we have demonstrated the advantages of a variational approach in describing renormalized phonons in MC nonlinear lattices with either symmetric or asymmetric nearest-neighbor potentials compared with existing quasi-harmonic theories. Moreover, besides our method, we found that the nonlinear fluctuating hydrodynamics (NFH) [24] can also provide good estimation for the sound velocity of MC nonlinear lattices. Since the concept of sound velocity is invalid in MNC nonlinear lattices, we deduce that the NFH cannot be able to give information on the renormalized phonons, although it can still describe correlation functions of these
systems [25]. Therefore, an interesting question arises whether the variational approach can be exploited for this class of models.

The purpose of this work is thus twofold: i) By putting the proposed variational approach onto a more general ground, we show that MNC nonlinear lattices can be tackled within the framework of the variational approach, which makes our theory a candidate for a unified phonon theory, and ii) we determine temperature-dependent phonon properties of MNC nonlinear lattices using this method and confirm the validity of the so-obtained results with the aid of molecular dynamics (MD) simulations as well as a tuning fork method [26]. As a demonstration, we consider one of archetype 1D nonlinear lattices in classical statistical mechanics, namely, 1D $\phi^4$ lattice. We conclude that the approach opens a new perspective to understand renormalized phonons in various nonlinear lattices.

The paper is organized as follows. In the second section, we present the general aspects of the extended variational approach. Two intrinsic relations satisfied by the optimal variational parameters are also obtained. In the third section, we focus on a comprehensive study of a specific nonlinear lattice. We found a power-law temperature dependence of the phonon band gap valid in the weak stochasticity regime as well as a rigorous relation between ensemble averages of the nonlinear lattice. Finally, we briefly summarize our main findings in the last section.

The methodologies. – We consider 1D nonlinear lattices described by the general Hamiltonian [27]

$$
H = \sum_{n=1}^{N} \left[ \frac{p_n^2}{2} + V(q_n - q_{n-1}) + U(q_n) \right],
$$

where $N$ is the particle number, $p_n$ denotes the momentum of $n$-th particle, $q_n = x_n - na$ denotes the displacement of $n$-th particle from its equilibrium position $na$ with $x_n$ the absolute position and $a$ the equilibrium distance for the interaction bond (for systems with zero pressure, it coincides with the lattice spacing), and $V$ represents the interparticle potential, $U$ is the on-site potential. We use periodic boundary conditions such that $q_0 = q_N$. For brevity and without loss of generality, we take $m = 1$ and $\alpha = 1$ as the unit of mass and length, respectively.

For simplicity, we introduce $\delta_n \equiv q_n - q_{n-1}$. The system evolves according to the equations of motion (EOMs)

$$
\dot{q}_n = p_n,
\dot{p}_n = V'(\delta_{n+1}) - V'(\delta_n) - U'(q_n),
$$

where the dot and the prime denote the time and spatial derivative, respectively. Notice that lattices with asymmetric interparticle potentials ($V(\delta) \neq V(-\delta)$) will induce nonvanishing internal pressure, here we only consider lattices with symmetric ones. The extension to systems involving asymmetric potentials is straightforward [23]. Accordingly, nonlinear potentials with the following general forms are of special interest:

$$
V(\delta_n) = \sum_{s=1}^{\infty} \frac{f_{2s}}{2s} \delta_n^{2s},
U(q_n) = \sum_{k=1}^{\infty} \frac{g_{2k}}{2k} q_n^{2k},
$$

Coefficients are chosen in such a way that potentials exhibit a single-well character.

In order to utilize a variational approach, the basic routine is to introduce a reference system with a trial Hamiltonian $H_0$ and prepare the nonlinear system and the reference system at the same temperature, then determines optimal reference systems from variational principles [28], the resulting optimal variational parameters inevitably take temperature dependence.

For systems with zero pressure, the Helmholtz free energy $F$ determines its thermodynamic properties. Since nonlinear lattices in thermal equilibrium behave like weakly interacting renormalized phonons [18,20,26], the free energy of the nonlinear lattices can be divided into two parts, one is the contribution of the free renormalized phonon gas described by a harmonic Hamiltonian, the other comes from the phonon-phonon interaction. However, the interaction is complicated, approximations should be taken. Intuitively, we adopt the well-known first-order cumulant inequalities of the free energy [29]

$$
F \leq F_0 + \langle H - H_0 \rangle_{\rho_0}, \quad (6)
$$

and

$$
F \geq F_0 + \langle H - H_0 \rangle_{\rho}, \quad (7)
$$

as the variational principles, where $F_0$ is the Helmholtz free energy of the reference system, $\rho_0 \equiv e^{-\beta_0(H_0 - F_0)}$ and $\rho \equiv e^{-\beta(H - F)}$ stand for the canonical measure of the reference system and the nonlinear lattice, respectively, $\beta_T \equiv 1/T$ is the inverse temperature (we set $k_B = 1$).

The trial Hamiltonian $H_0$ contains a set of adjustable parameters $\{\chi_i\}$, an optimal reference system can be obtained by varying those parameters such that bounds of the variational principle go to a relative minimum or maximum. Generally, without specific forms of $H$ and $H_0$, the condition for the bounds (cf., eqs. (6) and (7)) to be stationary with respect to one of the parameters $\chi_i$ is equivalent to

$$
\left\langle \frac{\partial H_0}{\partial \chi_i} \right\rangle_{\rho_0} = 0,
$$

and

$$
\left\langle \frac{\partial H_0}{\partial \chi_i} \right\rangle_{\rho} = \left\langle \frac{\partial H_0}{\partial \chi_i} \right\rangle_{\rho_0},$$

for eqs. (6) and (7), respectively, where $\langle A; B \rangle$ stands for the connected expectation value (cumulant):
The main concern of the present work is to obtain the phonon information in the nonlinear point lattice from a theoretical point of view. Phonon bears a solid basis only in harmonic systems, therefore, a harmonic reference system is chosen in the theory. Anharmonic references such as the Toda systems are out of the present scope. For homogeneous nonlinear lattices with the chosen nearest-neighbor interactions as well as on-site potentials (cf., eqs. (4) and (5)), it is sufficient to consider the following trial harmonic Hamiltonian [31]:

\[ H_0 = \sum_{n=1}^{N} \left[ \frac{k_n^2}{2} + \frac{\Omega^2}{2} \delta_n^2 + \frac{\gamma}{2} \delta_n^2 \right], \quad (10) \]

in which \( \Omega^2 \), and \( \gamma \) are variational parameters with \( \Omega^2 \) being the effective elastic constant, and \( \gamma \) the strength of the on-site potential. For later convenience, we refer to the optimal harmonic system with the property eq. (8) or eq. (9) to the upper bound harmonic (UH) or lower bound harmonic (LH) system, respectively. The corresponding dispersion relation of the harmonic system reads

\[ \omega_n^2 = 4\Omega^2 \sin^2 \frac{ka}{2} + \gamma \quad (11) \]

where \( k \) is the wave number and \( a \) the lattice spacing. As can be seen, \( \gamma \) also quantifies the phonon band gap. This dispersion relation with optimal parameters can be regarded as estimations of the actual dispersion in nonlinear lattices.

In order to obtain simple expressions for the optimal parameters, we should utilize the virial identity [32]

\[ \langle \nabla \cdot f \rangle_\rho = \beta_T \langle f \cdot \nabla H \rangle_\rho \quad (12) \]

for any polynomial \( f \) which depends only on coordinates. If we take a special choice \( f = \vec{q} \) with \( \vec{q} = (q_1, q_2, \cdots, q_N) \) a vector consists of all the coordinates of the system with \( N \) particles, we arrive at the generalized equipartition theorem (GET) [33]

\[ \langle q_n \partial H / \partial q_n \rangle_\rho = \beta_T^{-1} \quad (13) \]

For the UH system, by choosing \( f = \vec{q}(H-H_0) \) in eq. (12) and noting the GET as well as eq. (8), we find \( \langle \vec{q} \cdot \nabla H \rangle_\rho = \langle \vec{q} \cdot \nabla H_0 \rangle_\rho \) after some algebras. With the concrete forms of \( H \) and \( H_0 \), it leads to the following self-consistent equations:

\[ \Omega_U^2 = \sum_{n=1}^{N} f_{2n} \langle \delta_n^{2n} \rangle_\rho / \langle \delta_n^2 \rangle_\rho \quad (14) \]

\[ \gamma_U = \sum_{n=1}^{N} g_{2n} \langle \delta_n^{2n} \rangle_\rho / \langle \delta_n^2 \rangle_\rho \quad (15) \]

with \( \Omega_U^2 \) and \( \gamma_U \), estimations of the phonon dispersion (eq. (11)) as well as phonon band gap via the UH system are thus determined.

While for the LH system, we apply the GET to both \( H \) and \( H_0 \) and use properties \( \langle \delta_n^2 \rangle_\rho = \langle \delta_n^{2n} \rangle_\rho = \langle \dot{q}_n^2 \rangle_\rho \) (cf., eq. (9)), similar forms can be obtained as follows:

\[ \Omega_L^2 = \sum_{n=1}^{N} f_{2n} \langle \dot{q}_n^{2n} \rangle_\rho / \langle \dot{q}_n^2 \rangle_\rho \quad (16) \]

\[ \gamma_L = \sum_{n=1}^{N} g_{2n} \langle \dot{q}_n^{2n} \rangle_\rho / \langle \dot{q}_n^2 \rangle_\rho \quad (17) \]

However, unlike \( \Omega_U^2 \) and \( \gamma_U \), these two parameters are totally determined by ensemble averages of the nonlinear lattice. With \( \Omega_L^2 \) and \( \gamma_L \), we can find another estimation of the phonon band gap and the phonon dispersion. It is worthwhile to mention that the above results can be applied to MC lattices, actually, \( \Omega_U^2 \) and \( \Omega_L^2 \) reduce to the known results for the FPU-\( \beta \) lattice [23].

The \( \phi^4 \) lattice. – To verify the predictions of the variational approach, we consider the 1D \( \phi^4 \) lattice described by the following potentials [7–9]

\[ V(\delta) = \frac{K}{2} \delta^2, \quad U(q) = \frac{\lambda}{4} q^4, \quad (18) \]

which corresponds to a special case of eqs. (4) and (5) with \( f_2 = K \) and \( q_4 = \lambda \), respectively, and all other terms vanish. It is evident that only the on-site potential exhibits a nonlinearity. Although the study below is limited to the \( \phi^4 \) lattice, we should emphasise that the present theory (specifically, eqs. (14)–(17)) can be easily extended to other MNC lattices as well, provided that their potentials satisfy the forms as defined by eqs. (4) and (5). Our future work will address this aspect in more details.

Being one of the archetype 1D nonlinear lattices in classical statistical mechanics, the \( \phi^4 \) lattice has two advantages, on the one hand, the existence of renormalized phonons in this model has been confirmed by the use of the tuning fork method very recently [26], thus we can compare theoretical predictions with numerical results, on the other hand, the dynamics of this model has been studied extensively, especially the existence of a strong stochasticity threshold (SST). The SST is identified as a critical energy density \( \varepsilon_c \) where the scaling behavior of the maximum Lyapunov exponent changes significantly [34,35]. For the \( \phi^4 \) lattice, it was demonstrated that \( \varepsilon_c = 0.5 \) which corresponds to a temperature \( T = 0.6 \). We will show that the temperature dependence of the phonon band gap manifests distinct behaviors as temperature increases. The SST also determines the validity regime of the optimal harmonic reference systems. In the following, we will give a detailed study of the \( \phi^4 \) lattice by using our variational approach together with numerical simulations. For simplicity and without loss of generality, we only present details
with $K = 1$ and $\lambda = 1$, results with other parameter sets share similarities.

**Predictions of the variational approach.** Before going into details, we observe that $\Omega_2^2$ share similarities. The numerator of eq. (15) consists of only one term $\langle q_n^4 \rangle_{\rho_0}$. For a quadratic Hamiltonian, it is straightforward to show that $\langle q_n^4 \rangle_{\rho_0} = 3 \langle q_n^2 \rangle_{\rho_0}^2$ [31], then the self-consistent equation (eq. (15)) reduces to

$$\gamma_U = 3 \langle q_n^2 \rangle_{\rho_0}. \tag{19}$$

Note that $\langle q_n^2 \rangle_{\rho_0}$ can be directly computed from the Helmholtz free energy $F_0$ via

$$\sum_n \langle q_n^2 \rangle_{\rho_0} = 2 \frac{\partial}{\partial T} F_0. \tag{20}$$

For the harmonic system, $F_0$ can be expressed as $-\beta^{-1} \sum k \ln \frac{2\pi}{\beta \omega_k}$ with $\omega_k^2 = 4 \sin^2 \frac{k\pi}{4} + \gamma$, the above equation thus leads to

$$\gamma_U = \frac{3}{N \beta T} \sum_k \frac{1}{\omega_k^2}. \tag{21}$$

In the large $N$ limit, the summation can be replaced by an integral, after some arrangements, the self-consistent equation (eq. (21)) turns into a quartic equation

$$\gamma_U^4 + 4 \gamma_U^3 = \frac{9}{\beta \beta T^2}. \tag{22}$$

The temperature dependence of $\gamma_U$ is explicit. In the low-temperature regime ($\gamma_U \ll 4$) we infer that $\gamma_U \propto T^{2/3}$.

Predictions from the LH system are quite straightforward. Equation (17) implies that $\gamma_L$ has the following form:

$$\gamma_L = \frac{\langle q_n^4 \rangle_{\rho}}{\langle q_n^2 \rangle_{\rho}}. \tag{23}$$

which coincides with the prediction of the effective phonon theory (EPT) [19]. The temperature dependence of $\gamma_L$ comes from temperature-dependent ensemble averages of the nonlinear lattice. Unlike $\gamma_U$, the value of $\gamma_L$ relies on MD simulations, we cannot obtain it self-consistently. In the low-temperature limit, $\gamma_L$ has the following power-law temperature dependence [12]:

$$\gamma_L \simeq 1.23 T^{2/3}. \tag{24}$$

The validity regime of this low-temperature behavior will be identified by using MD simulations together with the SST in the following.

![Fig. 1](Color online) Temperature dependence of $\gamma$ for 1D $\phi^4$ lattice. The solid green line denotes the dependence of $\gamma_U$ (eq. (22)). The dashed red line stands for the behavior of $\gamma_L$ in the low-temperature limit (eq. (24)). The blue circles are values of $\gamma_U$ at temperature $T$ using MD results for $\langle q_n^4 \rangle_{\rho}$ and $\langle q_n^2 \rangle_{\rho}$ at the same temperature. The black dashed line indicates the temperature corresponds to the strong stochasticity threshold.

**Numerical simulations.** In this part, we utilize MD simulations to verify the above predictions. A symplectic integrator SABA$_2$ with a corrector SABA$_2$C [36] is adopted to integrate the EOMs of the $\phi^4$ lattice with a time step $\hbar = 0.02$. We take an initial condition such that the displacement of every particle is set to be zero and their velocities are randomly chosen from a Gaussian distribution at temperature $T$, after the initialization, a transient time of order $10^7$ is used to equilibrate the system with $N = 1024$.

The temperature dependence of $\gamma$ are shown in fig. 1. We determine $\gamma_U$ by numerically solving eq. (22) and getting its positive real solution. As for $\gamma_L$, we insert MD results for $\langle q_n^4 \rangle_{\rho}$ and $\langle q_n^2 \rangle_{\rho}$ obtained at temperature $T$ into eq. (23) to obtain its value at that temperature. The low-temperature behavior of $\gamma_L$ (eq. (24)) is depicted in the figure as a dashed-dotted line. It’s clearly seen that such a low-temperature behavior deviates from simulation results of $\gamma_L$ when $T \leq 0.6$. Note that $T = 0.6$ is just the SST found in the $\phi^4$ lattice [34,35]. Therefore the so-obtained low-temperature behavior of $\gamma_L$ is valid only in the weak stochasticity regime, once the system enters a strong chaotic regime, the simple power-law temperature dependence is not enough to capture the fast dynamics in the phase space.

Using the predicted $\gamma_U$ and $\gamma_L$ (cf., eqs. (22) and (23)), we can check the validity of the dispersion eq. (11) of optimal harmonic reference systems. We choose the tuning fork method introduced in [26] to obtain MD results for the actual dispersion of the 1D $\phi^4$ lattice. The comparisons between theoretical predictions and MD results are shown in fig. 2. The figure shows results for three different temperatures. One of the temperatures ($T = 0.1$) is well below the SST, implying that harmonic references should be good approximations. From fig. 2(a), we can see that this is indeed the case. The predictions of the LH system

40002-p4
and the UH system both show a perfect agreement with MD results, since the values of γ_L and γ_U differ slightly at T = 0.1 as depicted in fig. 1. As the temperature increases to 0.8 which is comparable to the SST, discrepancies between theoretical predictions and MD results appear near k = 0 and k = π as displayed in fig. 2(b). But in the middle range of k, the two harmonic systems still can offer good estimations for the dispersion. The inset shows that the LH system is better than the UH system. When the temperature is well above the SST, the system is in a strong chaotic regime. Thus in fig. 2(c), we find for T = 5 that our theoretical approximation eq. (11) cannot capture the actual dispersion of renormalized phonon in the lattice. Noting the largest MFP in this case is almost 2 as shown in the inset, it means that the phonon-phonon interaction is very strong in this regime. Such that the first-order cumulant approximation adopting in the variational principle is no longer capable of dealing with lattices in the high-temperature regime, higher-order corrections to the free energy should be taken into account.

Exact relations for ensemble averages. More surprisingly, although the variational approach takes an approximate way to get information of nonlinear lattices, we find that it can produce some rigorous results for the nonlinear lattice. Noting the identity of the LH system \( \langle \delta_{n}^{2} \rangle_{\rho} = \langle \delta_{n}^{2} \rangle_{\rho} \) and using eq. (20), we find γ_L also satisfies the following equation:

\[
\gamma_{L}^{2} + 4\gamma_{L} = \frac{1}{\beta_{T}^{2}} (\rho_{n}^{2})_{\rho}.
\]

By combining eq. (23), an identity of the 1D \( \phi^{4} \) lattice is revealed:

\[
\langle q_{n}^{4} \rangle_{\rho}^{2} + 4\langle q_{n}^{2} \rangle_{\rho} (\rho_{n}^{2})_{\rho} = T^{2}.
\]

Obviously, it is distinct from the simple relation in quadratic Hamiltonians, namely, \( \langle q_{n}^{2} \rangle_{\rho} = 3\langle q_{n}^{2} \rangle_{\rho}^{2} \). Moreover, it is worthwhile to mention that this relation is valid in the whole temperature range even though \( \langle q_{n}^{2} \rangle_{\rho} \) and \( \langle q_{n}^{2} \rangle_{\rho} \) have different temperature dependence in the weak and strong stochasticity regime separated by the SST.

If we combine eq. (26) with the GET (eq. (13)) for the \( \phi^{4} \) lattice with \( K = 1, \lambda = 1 \)

\[
(2q_{n}^{2} - 2q_{n}q_{n-1})_{\rho} + \langle q_{n}^{4} \rangle_{\rho} = T,
\]

we will further get relations hold between various ensemble averages, for instance,

\[
\langle q_{n}^{4} \rangle_{\rho} = T(q_{n}q_{n-1})_{\rho} + \langle q_{n}^{2} \rangle_{\rho}^{2},
\]

\[
\langle q_{n}^{4} \rangle_{\rho}(q_{n}q_{n-1})_{\rho} = (\rho_{n} - q_{n}q_{n-1})^{2}.\]

Therefore, in this model, it is apparent that the ensemble averages of on-site quantities, e.g., \( q_{n}^{2} \), can be fully determined by the ensemble averages of non-on-site terms such as \( q_{n}q_{n-1} \).

Summary. – In summary, we have extended a previously proposed variational approach to study phonon properties of general nonlinear lattices with on-site potentials, which makes our theory a possible candidate for a unified phonon theory. Intrinsic relations characterizing optimal reference system, namely, the LH system and the UH system, are revealed, from which we can obtain explicit forms for optimal variational parameters. Estimates for the phonon bad gap as well as the phonon dispersion are also obtained.

As a specific case, we present a thorough study of the 1D \( \phi^{4} \) lattice by utilizing the variational approach. In the low-temperature regime, a power-law temperature dependence
for $\gamma_L$ qualifying the phonon band gap is found by using a complementary method, namely, the transfer integral operator method. In comparison with results obtained via MD simulations, we find that such low-temperature behavior is valid only in the weak stochasticity regime where the temperature is below the SST.

We further compare the theoretical predictions of the phonon dispersion with MD results for the actual phonon dispersion of the 1D $\phi^4$ lattice. At a low temperature below the SST, the agreement between theoretical and numerical results is good. At an intermediate temperature which is comparable to the SST, a discrepancy begins to appear between theoretical and numerical results. We find that the LH system works better than the UH system. When the system enters a high-temperature regime, the predictions fail, it seems that higher-order corrections to the free energy must be taken into account.

Moreover, we find that the variational approach produces rigorous results for the nonlinear lattice, such as an exact relation between the ensemble averages of $q_n^2$ and $q_n^4$, that is valid ranging from low-temperature to high-temperature regime regardless of the existence of SST. This finding together with the generalized equipartition theorem will lead to interesting relations holding between ensemble averages of the 1D $\phi^4$ lattice.

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The authors thank W. Sti, S. Liu and N. Li for highly useful discussions. Support from the National Basic Research Program of China with Grant No. 2012CB921401 is gratefully acknowledged. The work is also supported by the National Nature Science Foundation of China.

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