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Energy super-diffusion in 1d deterministic nonlinear lattices with broken standard momentum

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Abstract. The property of total momentum conservation is a key issue in determining the energy diffusion behavior for 1d nonlinear lattices. The super-diffusion of energy has been found for 1d momentum conserving nonlinear lattices with the only exception of 1d coupled rotator model. However, for all the other 1d momentum non-conserving nonlinear lattices studied so far, the energy diffusion is normal. Here we investigate the energy diffusion in a 1d nonlinear lattice model with inverse couplings. For the standard definition of momentum, this 1d inverse coupling model does not preserve the total momentum while it exhibits energy super-diffusion behavior. In particular, with a parity transformation, this 1d inverse coupling model can be mapped into the well-known 1d FPU-β model although they have different phonon dispersion relations. In contrary to the 1d FPU-β model where the long-wave length phonons are responsible for the super-diffusion behavior, the short-wave length phonons contribute to the super-diffusion of energy in the 1d inverse coupling model.

1 Introduction

Since the first ever discovery of anomalous heat conduction for 1d nonlinear Fermi-Pasta-Ulam β (FPU-β) lattice [1], revealing the physical mechanism behind this anomalous heat conduction behavior has attracted great attention [2–5]. Among many properties of 1d FPU-β lattice model, the conservation of total momentum has been thought to be the key issue which eventually gives rise to the anomalous heat conduction [6,7]. The numerical simulations confirm that the anomalous heat conduction can be found for the 1d nonlinear lattice if the total momentum is conserved [1,8], except for the special 1d coupled rotator model [9,10]. On the other hand, the normal heat conduction can be obtained for 1d nonlinear lattice with on-site potential where the conservation of total momentum is broken [11–13]. Recent numerical results seem suggesting that asymmetry in momentum conserving lattices can induce normal heat conduction [14–16], but later works demonstrate that this might be a finite size effect and anomalous heat conduction will be approached for asymmetric momentum conserving lattices in the thermodynamical limit [17,18]. Although momentum conserved 1d nonlinear lattice models can exhibit anomalous or normal heat conduction behavior if we take the 1d coupled rotator lattice into consideration, the 1d nonlinear lattices with broken momentum conservation all show normal heat conduction behavior without any exception.

As the lattice system has no particle transport, heat conduction can be directly related to energy diffusion. It has been proved that the behavior of heat conduction has a one-to-one correspondence with the property of energy diffusion in 1D symmetric nonlinear lattice systems [19,20]. The size-dependence of thermal conductivity κ can be generally described as a power-law function of system length L as $\kappa \propto L^{\alpha}$ [2–5]. The exponent $\alpha = 0$ represents the normal heat conduction and $\alpha = 1$ describes the ballistic heat conduction. For $0 < \alpha < 1$, the system exhibits the anomalous heat conduction behavior. On the other hand, the energy diffusion can be characterized by the Mean Square Displacement (MSD) $\left\langle \Delta x^2(t)\right\rangle_E$ of energy fluctuation. The time-dependence of energy diffusion $\left\langle \Delta x^2(t)\right\rangle_E$ can be generally described as $\left\langle \Delta x^2(t)\right\rangle_E \propto t^{\beta}$ [21]. The normal and ballistic energy diffusions correspond to $\beta = 1$ and $\beta = 2$, respectively. For $1 < \beta < 2$, the system exhibits anomalous super-diffusion behavior.

The connection theory claims that $\alpha = \beta - 1$ directly relating heat conduction with energy diffusion [19]. According to the connection theory, normal (anomalous) heat conduction corresponds to normal (anomalous)

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energy diffusion. This theoretical relation has been verified by numerical simulations in 1D symmetric nonlinear lattices including the FPU-β lattice with anomalous heat conduction [21], and the FK, ϕ^4 and coupled rotator model with normal heat conduction [21,22]. In particular, this relation enables us to numerically study the heat conduction problem via the energy diffusion method, which can be performed more efficiently and accurately by considering micro-canonical simulation without heat baths included.

Recently, it has been found that a 1d chain model of charged particle with magnetic field shows energy super-diffusion behavior while the standard total momentum is not conserved due to the broken time-reversal symmetry [23,24]. The conservation of standard momentum is replaced by the new conservation of a pseudomomentum induced by the magnetic field. However, the equation of motions of the charged particles are composed of the deterministic dynamics from the model Hamiltonian and the *artificially* introduced conservative noises. The obtained super-diffusive behavior is not the direct result of the model Hamiltonian itself. Up to now, there is no 1D Hamiltonian system with broken momentum conservation where super-diffusion of energy can be obtained through its own deterministic dynamics.

In this paper, we investigate the transport property of the new proposed 1d inverse coupling model [25]. With the standard definition of momentum, the total momentum is broken for this 1d inverse coupling model. However, the super-diffusion of energy will be obtained for this momentum non-conserved 1d inverse coupling model. With a canonical transformation, this 1d inverse coupling model with broken momentum conservation can be mapped into the well-known FPU-β model with momentum conservation. Unlike the 1d FPU-β model where the long-wave length phonons contribute for the super-diffusion of energy, the phonon dispersion relation obtained for this 1d inverse coupling model reveals that the short-wave length phonons are responsible for the energy super-diffusion behavior. The model and main results will be presented and discussed in Section 2 and the summary will be concluded in Section 3.

2 Model and numerical results

According to reference [25], the 1d inverse coupling lattice toy model is proposed from a spring-disk chain model. In Figure 1, the schematic picture of the 1d inverse coupling model is plotted where each atom labeled "i" can oscillate from its equilibrium position. It can be seen that the increase of x_i will tend to reduce the value of x_{i-1} of its neighborhood. As a result, the dimensionless Hamiltonian of the 1d nonlinear inverse coupling model can be expressed as:

$$H=\sum_i\left[\frac{p_i^2}{2}+\frac{1}{2}(x_i+x_{i-1})^2+\frac{1}{4}(x_i+x_{i-1})^4\right]=\sum_i H_i, \quad (1)$$

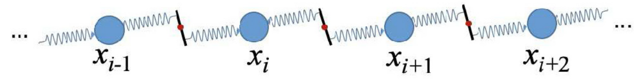

Fig. 1. The schematic picture of the proposed 1D inverse-coupling model. x_i is the displacement from its equilibrium position for ith site. The increase of x_i will tend to reduce the value of x_{i-1} of its neighborhood acting as inverse coupling.

where p_i is the momentum of the ith atom. For simplicity, the periodic boundary condition $x_0 = x_N$ is applied if total N sites are considered.

In order to understand the property of the 1d nonlinear inverse coupling model, we first analyze the linear inverse coupling model with Hamiltonian:

$$H=\sum_i\left[\frac{p_i^2}{2}+\frac{1}{2}(x_i+x_{i-1})^2\right]. \quad (2)$$

It is straightforward to derive that the time derivative of the total momentum $\sum_i p_i$ follows as

$$\frac{d\sum_i p_i}{dt}=-\sum_i(x_{i-1}+2x_i+x_{i+1})\neq 0. \quad (3)$$

With the standard definition of momentum, the total momentum for the 1d inverse coupling model is not conserved. This broken of total momentum is simply due to the lack of translational symmetry.

To obtain the phonon dispersion relation, the equation of motion of the linear inverse coupling model can be obtained as $d^2x_i/dt^2 = -(x_{i-1} + 2x_i + x_{i+1})$, which can be solved by considering the travelling wave solution as $x_i(t) \propto e^{-j(\omega t-ki)}$ with j the imaginary unit, k the wave vector and ω the frequency. The phonon dispersion relation can be derived as

$$\omega_k = 2\cos\frac{k}{2}, \quad -\pi < k \leq \pi. \quad (4)$$

As a result, the 1d linear inverse coupling model has the phonon modes with the cosine dependence of wave vector k. This is totally different with the conventional phonon dispersion relation $\omega_k = 2\sin(k/2), -\pi < k \leq \pi$ in linear Harmonic lattice where the phonon modes have the sinusoidal dependence.

The new dispersion relation for 1d linear inverse coupling model is plotted as a dashed line in Figure 2. It can be seen that $\omega_{k=0} = 2$ at long-wave length limit is not a zero frequency phonon mode. However, the linear inverse coupling model does have zero frequency phonon mode with $\omega_{k=\pi} = 0$, which is shifted to the Brillouin zone boundary. This π shift can be understood as the phase factor $e^{j\pi} = -1$ contributed by the inverse couplings. Therefore, the breaking of translational symmetry makes the momentum not conserved any more, while the zero frequency phonon mode is maintained as a result of lacking on-site potential.

It is known that for 1d Harmonic lattice, the long-wave length phonons with $k \to 0$ have the fastest phonon

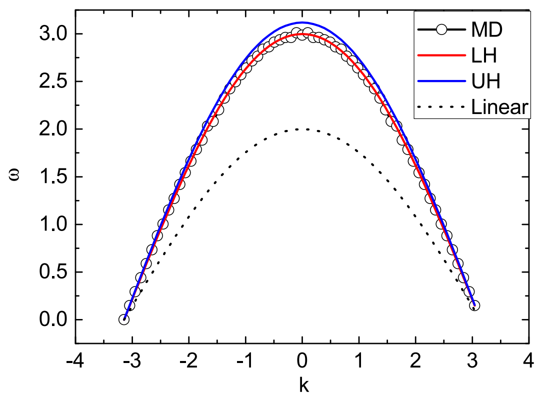

Fig. 2. The phonon dispersion relation for inverse-coupling model. The dashed line is the analytic result for linear inverse-coupling model as $\omega_k = 2\cos(k/2)$. The red (LH) and blue (UH) solid lines are the renormalized phonon predictions for lower limit of equation (7) and upper limit of equation (8), respectively. The circles are the numerical results of ω_k^R from Molecular Dynamics (MD) simulations with parameter of energy density $e = 1$ corresponding to a temperature $T \approx 1.16$. The numerical ω_k^R lies between the predictions of lower limit and upper limit and close to lower limit prediction with this energy density.

transport speed or sound velocity as $c_s = d\omega_k/dk = \cos(k/2) = 1$ in the limit of $k = 0$. While for the 1d linear inverse coupling model:

$$c_s = \left|\frac{d\omega_k}{dk}_{|k\to\pi}\right| = \left|\frac{d(2\cos\frac{k}{2})}{dk}_{|k\to\pi}\right| = \left|-\sin\frac{k}{2}_{|k\to\pi}\right| = 1, \tag{5}$$

the short-wave length phonons with $k \to \pi$ have the fastest phonon transport speed.

For the 1d nonlinear inverse coupling model described by equation (1), a renormalized phonon dispersion relation ω_k^R can be derived with the renormalization phonon theory as that done for FPU-β model [26–34]. The resulted dispersion relation ω_k^R for 1d nonlinear inverse coupling model is still cosine dependent and can be expressed as:

$$\omega_k^R = \sqrt{\alpha}\omega_k = 2\sqrt{\alpha}\cos\frac{k}{2}, \tag{6}$$

where the renormalization coefficient α is mode-independent function of the temperature T due to the nonlinear interaction. According to the variational renormalization phonon theory [33], the coefficient α has a lower and upper limit expressions as α_L and α_U respectively. In particular, the coefficient α can be obtained as [26–34]:

$$\alpha_L = 1 + \frac{\int_0^\infty x^4 e^{-(x^2/2+x^4/4)/T}}{\int_0^\infty x^2 e^{-(x^2/2+x^4/4)/T}}, \tag{7}$$

$$\alpha_U = \frac{1}{2}\left(1 + \sqrt{1+12T}\right). \tag{8}$$

The coefficient α is only temperature dependent or equivalently nonlinearity dependent. The difference between two predictions of lower limit α_L and upper limit α_U is very small. As a result, the sound velocity c_s for 1d nonlinear inverse coupling model is also temperature dependent as $c_s = \sqrt{\alpha}$. But here, the phonons with the sound velocity are the short-wave length phonons with $k \to \pi$.

In order to verify the dispersion relation of equation (6) in the 1d nonlinear inverse coupling model, we apply the resonance phonon approach method to numerically calculate the renormalized phonons ω_k^R [35,36]. In Figure 2, the numerical results of renormalized phonon frequencies ω_k^R are plotted for the inverse coupling model. The microscopic numerical simulations are performed with energy density $e = 1$ corresponding to temperature $T = 1.16$. The theoretical lower limit α_L and upper limit α_U are also plotted as red and blue lines respectively for comparisons. It can be seen that the numerical results at this temperature are between the two predictions of α_L and α_U and close to the lower limit α_L. Therefore, the dispersion relations in linear and nonlinear inverse coupling models share the same property that the long-wave length limit phonon mode at $k = 0$ does not have zero frequency. This is the result of the breaking of translational symmetry and momentum conservation. On the other hand, the zero frequency phonon mode still exists at the Brillouin zone boundary at $k = \pm\pi$ since there is no on-site potential to lift the zero frequency mode.

Before we study the energy diffusion for the 1d inverse coupling model without momentum conservation, we compare it with the well known 1d FPU-β model with momentum conservation. The FPU-β model has the following dimensionless Hamiltonian as

$$H = \sum_i \left[\frac{p_i^2}{2} + \frac{1}{2}(x_i - x_{i-1})^2 + \frac{1}{4}(x_i - x_{i-1})^4\right]. \tag{9}$$

In contrary to the inverse coupling model, here the increase of the displacement q_i tends to increase the value q_{i-1} of its neighborhood. Although the 1d inverse coupling model and the 1d FPU-β model have different physical properties such as the conservation of total momentum and the phonon dispersion relation, they can be connected by a parity transformation as:

$$x_i \to (-1)^i x_i. \tag{10}$$

As a result, the 1d inverse coupling model has no translational symmetry as the Lagrangian of inverse coupling model is not invariant under the transformation $x_i \to x_i + s$ with s some constant. However, the Lagrangian for 1d inverse coupling model is invariant under this transformation

$$h^s : x_i \to x_i + (-1)^i s. \tag{11}$$

According to Noether's theorem, one can define the following parity-momentum quantity I_p:

$$I_p = \sum_{i=1} \frac{\partial L}{\partial \dot{x_i}}\frac{dh^s}{ds} = \sum_{i=1}(-1)^i p_i \tag{12}$$

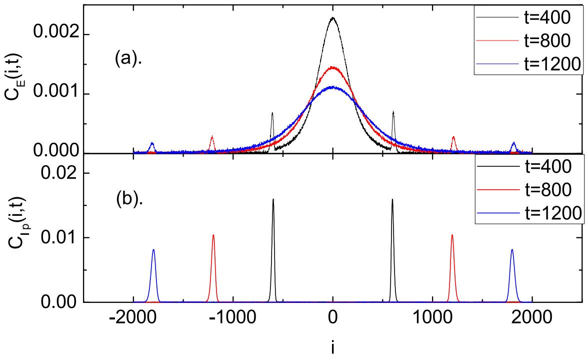

Fig. 3. Distribution functions $C_E(i,t)$ and $C_{I_p}(i,t)$ for energy and new conserved quantity I_p which is momentum-like at three different correlation times $t = 400$, 800 and 1200 for the inverse-coupling model. Lattice length is $N = 4001$. The energy density $e = \langle H_i \rangle = 1$ and corresponding temperature is $T = \langle p_i^2 \rangle \approx 1.16$.

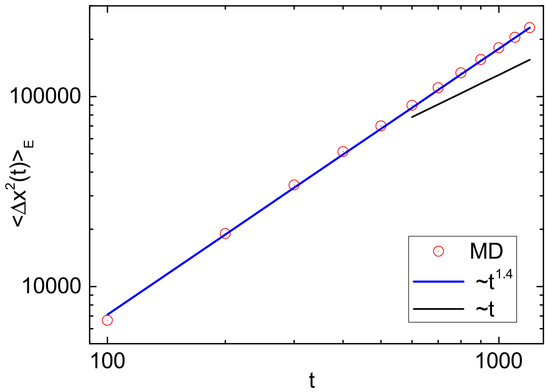

Fig. 4. The MSD $\langle \Delta x^2(t) \rangle_E$ of energy diffusion for the inverse-coupling model. The same parameters are used as in Figure 3. The energy diffusion is super-diffusion as $\langle \Delta x^2(t) \rangle_E \propto t^{1.4}$. The curve $\sim t$ is shown for comparison.

which is a conserved quantity. The $L = \sum_{i=1}^{N}(\dot{x}_i^2/2 - V(x_i + x_{i-1}))$ with $V(x) = x^2/2 + x^4/4$ is the Lagrangian of the inverse coupling model and $p_i = \dot{x_i}$.

Therefore, although the 1d inverse coupling model does not conserve the total momentum $\sum_i p_i$ with the standard definition, it does conserve the new introduced parity-momentum $I_p = \sum_i (-1)^i p_i$. We should expect that the 1d inverse coupling model without momentum conservation has the same energy diffusion behavior with the 1d FPU-β model with momentum conservation.

We then numerically study the energy diffusion behavior for the 1d inverse coupling model. The numerical energy diffusion method in equilibrium is proposed to calculate the spatio-temporal distribution of the energy fluctuation correlation function $C_E(i,t)$ which is defined as [21]:

$$C_E(i,t) = \frac{\langle \Delta H_i(t) \Delta H_0(0) \rangle}{\langle \Delta H_0(0) \Delta H_0(0) \rangle} + \frac{1}{N-1}, \tag{13}$$

where $\Delta H_i(t) = H_i(t) - \langle H_i(t) \rangle$ is the real-time energy density fluctuation at site i and $\langle \cdot \rangle$ means ensemble average or time average in equivalence. Here the site index i is chosen from $i = -(N-1)/2$ to $(N-1)/2$ for simplicity. The extra term of constant $1/(N-1)$ is a result of energy conservation in the microscopic simulations. From definition, the initial distribution is a Kronecker δ function as $C_E(i, t = 0) = \delta_{i,0}$ in the thermodynamical limit $N \to \infty$. The distribution $C_E(i,t)$ describes the spatio-temporal energy spreading from the center site $i = 0$ and initial correlation time $t = 0$.

In Figure 3a, the distribution functions $C_E(i,t)$ has been plotted for an inverse-coupling model with length $N = 4001$ at three different correlation times $t = 400, 800$ and 1200. The energy density e is set as $e = 1$ which corresponds to a temperature $T = 1.16$. The energy distributions $C_E(i,t)$ exhibit Levy walk distribution with two side peaks indicates anomalous diffusion, rather than normal diffusion with the Gaussian normal distribution. It is clear that these distributions are almost the same as that of FPU-β lattice [21,37]. However, it should be emphasized that the side peaks obtained for 1d inverse coupling model represent the energy carried by the short-wave length phonons with $k \to \pi$, which is different from the side peaks of 1d FPU-β model where energy are carried by the long-wave length phonons with $k \to 0$. Since the non-vanishing side peaks are responsible for the anomalous super-diffusion of energy, the underlying physical mechanism behind the same energy super-diffusion behavior for 1d inverse coupling model and 1d FPU-β model is different.

To identify the exact diffusion behavior, the MSD $\langle \Delta x^2(t) \rangle_E = \sum_i i^2 C_E(i,t)$ has been plotted in Figure 4. The fitted time behavior of $\langle \Delta x^2(t) \rangle_E \propto t^{\beta=1.40}$ indicates that the energy diffusion in the 1d inverse coupling model is super-diffusion where the exponent $\beta = 1.40$ is also same as that of 1d FPU-β model [21,38]. Although the translational symmetry and momentum conservation are broken in the 1d inverse coupling model, its energy diffusion does exhibit an anomalous energy super-diffusion behavior.

With this new parity-momentum conserved quantity I_p, we can also calculate the distribution correlation function $C_{I_p}(i,t) = \langle (-1)^i p_i(t) p_0(0) \rangle / T$ as we did the momentum distribution for 1d FPU-β lattice [21,37]. The spatio-temporal spreading of the I_p is plotted in Figure 3b which is also the same as that for FPU-β lattice. The new conserved quantity I_p might be the reason for energy super-diffusion behavior. It suggests that when discussing the conserved quantities in 1D nonlinear lattices, the consideration of total momentum with standard definition is incomplete. The total momentum and this new total parity-momentum I_p together constitute one complete conserved quantity.

3 Summary

In conclusion, we have studied the phonon transport properties for a 1d inverse coupling model. With the standard definition of momentum, this 1d inverse coupling model does not conserve the total momentum. We also derived the renormalized phonon dispersion relation for this 1d inverse coupling model and verified it with numerical simulations. Although the 1d inverse coupling model has different physical properties from the 1d FPU-β model, they can be connected by a parity transformation. As a result, the 1d inverse coupling model without momentum conservation has the same energy super-diffusion behavior as that of 1d FPU-β model with momentum conservation. In contrary to the 1d FPU-β model where long-wave length phonons with $k \to 0$ are responsible for the super-diffusion of energy, the short-wave length phonons with $k \to \pi$ contribute to the super-diffusion of energy in 1d inverse coupling model. Our results also indicate that total momentum with the standard definition is an incomplete concept when dealing with conserved quantities in 1D nonlinear lattices. Total momentum $\sum_i p_i$ and the parity-momentum $I_p = \sum_i (-1)^i p_i$ together constitute one complete conserved quantity.

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Author contribution statement

The present research stemmed from fruitful discussions between H. Y., J. R. and N. L. H. Y. prepared all the figures. All authors H. Y., J. R. and N. L. contributed to the writing of the manuscript.

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