Dynamics of rotator chain with dissipative boundary: energy conduction

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Abstract. Dynamical states of coupled rotator lattice are identified and their effects on energy conduction are explored. Globally synchronous rotation, clustered synchronous rotation and split synchronous rotation states are observed and the heat baths induced transitions between these states causes the reduction of overall energy flux. This result provides an explanation to the finite heat conductivity of coupled rotator lattice model.

1. Introduction

Non-equilibrium transport process is a classical yet challenging problem of non-equilibrium statistical physics. The macroscopic description of non-equilibrium transport phenomena depends on transport equations and the core of all transport equations are the linear laws that depict the amount of extensive quantities which are transferred per unit time between different regions of a system as responses to non-homogeneities in intensive quantities.

The ultimate goal of non-equilibrium statistical physics is to derive these linear laws from rigorous microscopic arguments, which is of formidable difficulty. Since the most time tested transport law in experiments is the Fourier’s law on energy transport $j(x, t) = -\kappa(T)\nabla T(x, t)$, where $j(x, t)$ is the energy flux, $T(x, t)$ is the local temperature and $\kappa(T)$ is the heat conductivity, many works have been done on the energy conduction properties. After the elementary attempt of Debye phonon gas theory, the Boltzmann-Peierls approach showed anharmonicity is necessary to give genuine diffusion of energy on a lattice through the so-called Umklapp processes[1]. However, there are more fundamental questions beyond the scope of the above theories such as the uniqueness of non-equilibrium stationary state and the sufficient condition for local equilibrium, which penetrate down to the level of dynamics. Thus great effort had been put into the investigation of transport properties on simple lattice models by simulating their dynamics in the hope of providing a more solid foundation to Fourier’s law[2–17].

Contrary to the expectation of physicists back then, Fourier’s law was found to be violated on many one dimensional lattice models by numerical simulations for heat conductivity diverges with a power law as the scale of the system increases[18, 19], i.e. $\kappa(N) \propto N^\alpha$.

These findings triggered the query of the necessary and sufficient condition for a system conforming the Fourier’s law of heat conduction(i.e. whether heat conduction on a system is normal or anomalous). Decades of observations found decisive evidences that on-site potential, which breaks the momentum conservation of a lattice, is a sufficient condition for normal conduction, provided that the temperature is sufficiently low. Numerical simulations of Ding-a-ling model and Frenkel-Konorova model support the assertion[18, 20]. On top of that,
analytical analysis even proved that for momentum conserving lattice Fourier’s law does not hold, which implies that the non-conservation of momentum is a necessary condition for normal heat conduction\cite{5}. Paradoxically, one system serves as an counter example of the above mathematically rigorous conclusion — coupled rotator lattice, without any on-site potential, exhibits normal heat conduction\cite{21, 22}. Ergo, more detailed analysis need to be performed on the coupled rotator chain model to reconcile the contradiction between the analytical and numerical results.

The study of anomalous heat conduction in one-dimensional momentum-conserving systems was based on the oscillator lattices, whose main energy carriers are phonons and solitons. But in a coupled rotator lattice, non-linear rotating modes (i.e. breathers) also exist\cite{23}. Thus the effects of rotating modes in the energy conduction on coupled rotator model were explored to probe their effects on heat conduction. Our explorations indicate that the non-linear rotating modes hamper the heat conduction, thus provide an explanation to the finite heat conductivity of coupled rotator chain model.

\section{Coupled rotator lattices}

Non-linear rotating modes could be excited by applying mechanical torque on a coupled rotator chain, which greatly facilitated our investigation, and the feasibility of this setting is grounded on the interaction potential of the model. The coupled rotator lattice model is the simplest classical 1D spin model called the Heisenberg XY model, whose interaction potential is sinusoidal coupling. Assuming the model is described by the angles \( \phi = (\phi_1, \phi_2, \ldots, \phi_N) \) and their conjugate angular momenta \( L = (L_1, L_2, \ldots, L_N) \), see FIG. 1., then the interaction potential takes the form

\[
U(\phi_k, \phi_{k+1}) = \epsilon \left[ 1 - \cos(\phi_{k+1} - \phi_k) \right],
\]  

(1)

where \( \epsilon \) is the coupling coefficient. Note that unlike the oscillator based lattice models, the interaction potential is periodic, which enables both oscillations and relative rotations among the rotators on the lattice rather than only oscillations. On top of that, applied torque can also be added to the system to artificially excite rotational modes.

Moreover, the system is homogeneous, that is, the moment of inertia of each rotator is \( I \). Therefore, the Hamiltonian of the system is

\[
\mathcal{H}(\phi, L) = \sum_k \left\{ \frac{L_k^2}{2I} + \epsilon \left[ 1 - \cos(\phi_{k+1} - \phi_k) \right] \right\}.
\]  

(2)
The total angular momentum of this system is conserved, since \( \dot{L} = \sum_k \dot{L}_k = \sum_k \partial \mathcal{H} / \partial \phi_k = 0 \). If momentum conservation was the sufficient condition for the violation of Fourier’s law, then the heat conduction on a coupled rotator lattice should be anomalous. However, independent researches concluded that the heat conduction of a coupled rotator lattice is normal when the temperature is sufficiently high\[21, 22\]. It is suggested that the excitation of stationary localized rotational modes on the coupled rotator lattice facilitate the locking of the heat flux hence render the heat conductivity finite.

The stationary localized rotational modes could be studied by adding mechanical torque to the system. Based on the previous researches one would expect Fourier’s law is also valid in this setting. Nevertheless, according to the study conducted on a coupled rotator lattice with both thermal baths and mechanical torque exist on the boundary, Fourier’s law was violated. Fourier’s law implies the stationary local temperature distribution is linear, and the heat conductivity is positive. But the temperature distribution on a coupled rotator lattice was single peaked and the heat flux was reduced when the temperature difference was increased (i.e. the heat conductivity appears to be negative). It was asserted that the two counter-intuitive phenomena were the consequence of the interaction between thermal and mechanical driving (applied torque). More specifically, the reduction of heat flux was considered to be the result of the negative flux induced by the mechanical and thermal interaction\[24\]. Since applied torque could excite non-linear rotational modes, we intent to study their effects on the thermal transport to find the mechanism behind the single peaked “temperature” distribution and the reduction of “heat flux”.

3. Propagation dynamics: energy transport

The incorporation of applied torque introduces mechanical energy flux, which is from different origin of heat flux, it is desirable to separate these two kinds of fluxes from a dynamical perspective. In order to achieve that objective, a reductionism approach was utilized: we first investigated the energy conduction properties of a coupled rotator lattice without heat baths, then the interactions of heat baths and applied torque were explored to study the effect of rotational mode on energy conduction.

3.1. Equation of motion, local temperature and energy flux

Having introduced the dimensionless time \( s = \sqrt{T}t \) and letting \( \omega_k = \frac{d\phi_k}{ds} \), the dimensionless equations of motion for a coupled rotator lattice with open boundary can be derived from (2)

\[
\begin{align*}
\frac{d\phi_k}{ds} &= \omega_k, \\
\frac{d\omega_k}{ds} &= \sin(\phi_{k+1} - \phi_k) - \sin(\phi_k - \phi_{k-1}), \quad k \neq 1, N \\
\frac{d\omega_1}{ds} &= \sin(\phi_2 - \phi_1) - \alpha \omega_1 + \tau + \sqrt{\eta_1} \xi_1, \\
\frac{d\omega_N}{ds} &= -\sin(\phi_N - \phi_{N-1}) - \alpha \omega_N + \sqrt{\eta_2} \xi_2,
\end{align*}
\]

(3)

where \( \alpha = \gamma \frac{\sqrt{T}}{\tau} \) is the effective dissipation coefficient, \( \eta = \frac{2I^2 \alpha T}{\epsilon^2} \) is the noise strength, and \( \tau = \frac{T}{\epsilon} \) is the effective torque, in which \( \gamma \) is the dissipation coefficient and \( T \) is the mechanical torque. Heat baths are modeled by Gaussian random force \( \xi \).

Local temperature and local energy flux are common observables to investigate the relationship between the temperature gradient and the energy flux in the low-dimensional system.
The definition of temperature is borrowed from classical equilibrium statistical mechanics according to Equipartition theorem

\[ E_{\text{total}} = \frac{1}{2} \sum_i m_i (v'_i + v_c)^2 = \frac{1}{2} \sum_i m_i v_i'^2 + \frac{1}{2} M v_c^2 \]

\[ = \frac{N}{2} k_B T + \frac{1}{2} M v_c^2 \Rightarrow T = \frac{1}{k_B N} \sum_i m_i (v_i - v_c)^2, \]

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where \( v_i \) is the velocity of each particle and \( v_c \) is the velocity of the center of mass. By setting \( m_i = 1 \) and \( k_B = 1 \)

\[ T = \text{var}\{v\}, \]

which is the variance of velocity. Despite the constant factor 2 its physical meaning is straightforward — the mean internal energy. The corresponding local temperature for each rotator in a coupled rotator chain is then followed naturally

\[ T_k = \text{var}\{\omega_k\} \]

\[ = \lim_{s \to \infty} \frac{1}{s} \int_0^s \omega_k^2(t)dt - \left[ \lim_{s \to \infty} \frac{1}{s} \int_0^s \omega_k(t)dt \right]^2. \]

To derive the definition of local energy flux, one notes that energy could not be created or destroyed in the rotator chain, then the continuity equation holds

\[ \frac{dh_k}{ds} = j_{k-1} - j_k, \]

where \( h_k \) and \( j_k \) are local energy and energy flux.

The expression of local energy flux could be obtained by comparing (6) with the dimensionless time derivative of effective local energy that is derived from the equation of motion. If one adopts the dimensionless coordinates introduced in (3), then the effective local energy is

\[ h_k = \frac{\omega_k^2}{2} + \frac{1}{2} \left[ 2 - \cos(\phi_{k+1} - \phi_k) - \cos(\phi_k - \phi_{k-1}) \right], \]

in which the first term on the right hand side is the effective kinetic energy and the second term is the effective interaction potential energy. Its dimensionless time derivative is

\[ \frac{dh_k}{ds} = \omega_k \frac{d\omega_k}{ds} + \frac{1}{2} \left[ (\omega_{k+1} - \omega_k) \sin(\phi_{k+1} - \phi_k) + (\omega_k - \omega_{k-1}) \sin(\phi_k - \phi_{k-1}) \right]. \]

Substituting (3) to (8)

\[ \frac{dh_k}{ds} = \frac{1}{2} \left[ (\omega_k + \omega_{k-1}) \sin(\phi_k - \phi_{k-1}) - (\omega_{k+1} + \omega_k) \sin(\phi_{k+1} - \phi_k) \right], \]
and comparing the (9) to (6) leads to the definition of energy flux
\[ j_k = \frac{1}{2}(\omega_{k+1} + \omega_k) \sin(\phi_{k+1} - \phi_k). \] (10)

Dimensionless time average is used in the numerical calculation of energy flux instead of ensemble average,
\[ \langle j_k \rangle = \lim_{s \to \infty} \frac{1}{2s} \int_0^s [\omega_k(t) + \omega_{k+1}(t)] \sin[\phi_{k+1}(t) - \phi_k(t)] dt. \] (11)

In steady states \( dh_k/ds = 0 \), hence the local energy flux on each rotator is equal. Not only is the average energy flux an important physical quantity for the properties of energy conduction, overall dynamics of rotator chain could also be reflected in the variation of energy flux.

One caution needs to be noted here, in numerical simulations we use (dimensionless) time average to calculate the quantities instead of ensemble averages. Previous study shows the ensemble averages and time averages agree with each other in weakly coupled rotator chains, thus the substitution should not raise any problem.

The system of equations (3) had been integrated numerically by Velocity-Verlet method for a chain of 1024 rotators with the time step size \( \Delta s = 0.01 \).

3.2. Dynamical states of coupled rotator lattice

To understand the mechanism behind the single peaked local temperature distribution and the reduction of energy flux, one needs to locate the dynamical states that cause the phenomena. Transitions between different dynamical states can be directly reflected in the qualitative change of averaged energy flux, thus averaged energy flux is calculated to reveal distinct dynamical states, see FIG. 3.

![Figure 3](image-url)  

**Figure 3.** Averaged energy flux of a deterministic coupled rotator lattice, three distinct dynamical states were identified.

![Figure 4](image-url)  

**Figure 4.** Averaged energy flux of a coupled rotator lattice with heat baths, the plateau was broadened.

The torque-flux curve is divided into three qualitatively different regions, which correspond to three distinct dynamical states. In region I, the local energy flux increases monotonically with driving torque; In region II, the curve plunges and exhibits a plateau; and in region III, the flux virtually vanishes. One would expect temperature gradient always enhances the energy flux, but that is not the case. The incorporation of thermal heat baths enhances the overall energy flux when applied torque is small, while reduces the flux when applied torque is large, the plateau is also broadened, see FIG. 4.
Figure 5. Averaged momenta and variance profile, see FIG. 5.

After identifying the three states, the dynamics of each state could be understood by the averaged angular momenta and momenta variance profile, see FIG. 5.

In region I, the entire lattice has the same averaged angular momentum and the variance is also identically zero, which indicates the lattice was synchronized, thus the dynamical state is called globally synchronous rotation. In region III, only the driven rotator has relatively large averaged angular momentum and non-zero variance, the other rotators are synchronized and rotates slowly, hence this state is named split synchronous rotation. The most intriguing dynamical state is II, in which the lattice is divided into three regions 1. fast rotation region 2. slow rotation region and 3. interface region. It is interesting to find that the single peaked distribution emerges even when the heat baths are absent. If heat baths can not destroy the single peaked distribution, then we can safely draw the conclusion that the distribution is of deterministic origin. The results of the simulation of a coupled rotator chain with both applied torque and heat baths confirms our hypothesis, see FIG. 6, hence the single peaked “temperature” distribution indeed results from deterministic dynamics of coupled rotator chain model.

Since the hump is located on the interface region, understanding the deterministic origin of the single peaked momenta variance distribution requires further investigations on the dynamics of interface rotators, thus the momentum distribution of interface rotators are calculated, see FIG. 7. Rotators in the interface region(450, 472 and 490) have momenta distributions extended from the slow rotation region to the fast rotation region, which implies these interface rotators

Figure 6. Comparison between a rotator chain with and without heat baths.

Figure 7. Distribution of angular momenta for $\tau = 2.2, \alpha = 1.0$.)
constantly switched between the slow rotation state and the fast rotation state, which result in large variance. This behavior leads to the name clustered synchronous rotation.

In summary, our research suggests that the mechanism of the peak in the temperature profile of a coupled rotator lattice is the torque-induced rotating interface. In the interface, rotators switch intermittently between the fast and slow rotations, which leads to the large variance of angular momenta. The local energy flux is also reduced after the system enters the region II and region III, and the incorporation of heat baths broaden the region II.

3.3. Dynamical states of coupled rotator

Since the non-linear rotation modes is induced by the applied torque on the boundary, it is desirable to reduce the system to the utmost degree to get a deeper understanding of the interaction of thermal driving and mechanical driving. Thus a coupled rotator that consists of only two rotators is investigated analytically to separate the contributions of heat baths and the applied torque to the overall energy flux and to provide insight into the mechanism behind the reduction of energy flux.

It can be proven that a deterministic coupled rotator has two dynamical states, synchronized rotation and unsynchronized rotation[25], which are divided by $\tau = 2$. The unsynchronized rotation corresponds to the non-linear rotation mode where relative rotation exist. The local energy flux can be easily calculated by

$$\langle j \rangle = \begin{cases} \frac{\tau^2}{4\alpha}, & \text{synchronized rotation} \\ \frac{\tau(\tau - \sqrt{\tau^2 - 4})}{4\alpha}, & \text{unsynchronized rotation} \end{cases}$$

which perfectly matches the numerical simulation, see FIG. 8. The local energy flux plunges immediately after the system enters the unsynchronized rotation state, which is consistent with our prediction. When heat baths is incorporated into the system, directly solving the related Fokker-Planck equation up to the first order gives the overall local energy flux in synchronized rotation state[26], see FIG. 9.

$$j = \langle j \rangle = j_w + j_h,$$

$$= \frac{\tau^2}{4\alpha} + \frac{(\eta_1 - \eta_2)\sqrt{4 - \tau^2}}{4(\sqrt{4 - \tau^2} + 2\alpha^2)} + \cdots.$$
Comparing (12) and (13) one could identify the overall energy flux is separated into the contributions of mechanical term and thermal term. More importantly, as the thermal term suggested, the mechanical and thermal contribution are not independent. More specifically, mechanical torque hampers the heat flux.

When the system is in the unsynchronized rotation state, the interaction between thermal and mechanical driving could be studied by numerical simulation.

Even with a high temperature difference between the heat baths, it is clear that the two curves of energy flux are qualitatively identical in the unsynchronized rotation state, which implies the contribution of heat baths is completely suppressed in the unsynchronized rotation state. Heat baths also broadens the transition point $\tau = 2$ to a region, in which the energy flux is reduced compare to its deterministic counterpart. This result suggests that in the transition region, the coupled rotator constantly switches between synchronized rotation and unsynchronized rotation. Thus we conclude that the reduction of local energy flux is due to the heat baths induced transition between different dynamical states.

Thus by studying a reduced model of coupled rotator lattice, we found that in the synchronized rotation state, mechanical and thermal contributions to the overall local energy flux was synergistic and in the unsynchronized (non-linear rotation modes) rotation state the contribution of heat baths is suppressed. More importantly, the reduction of heat flux is the consequence of transition between dynamical states. These results provide strong evidences that the relative rotation hampers the energy conduction, thus give an explanation to the finite heat conductivity of coupled rotator lattice.

4. Conclusion
In this paper, we have shown that the non-linear rotation mode on the coupled rotator lattice could lead to single peaked temperature profile and reduction of energy flux.

Understanding the mechanism of the energy flux reduction could lead to an understanding of the reason behind the normal heat conduction on coupled rotator lattice. It would also be interesting to explore the scaling of the energy flux plateau and the interface region in the clustered synchronous rotation state to obtain more knowledge about the non-linear rotational modes. Finally, one should take the non-linear rotational modes into consideration when investigating the heat conduction problems whenever the interaction potential permits such modes exist.

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