Heat conduction in one-dimensional Yukawa chains

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Heat conduction in one-dimensional Yukawa chains is investigated. It is shown numerically that it has the abnormal heat conduction which is proportional to the system size. Effects of asymmetric external potential, the modified Frenkel-Kontorova one, on the heat conduction of system are also studied. It is found that the asymmetric property of external potential can induce asymmetric thermal conductivity that can be used to be a effective thermal rectifier. In certain of system parameters the heat flux are significantly different for two opposite direction. One can parametrically control the heat flux through this system by changing the potential strength and width.

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Recent years many interesting works have been addressed to the problem of heat conduction$^1$$^2$$^3$$^4$$^5$$^6$$^7$$^8$$^9$. It is well known that heat conductivity of one dimensional (1D) lattice is an important problem which is related to microscopic foundation of the Fourier law. It also provides an abundant example for the microscopic origin of the macroscopic irreversibility phenomenon. Detailed review of the problem is presented in the recent paper$^1$.

Except of extensive numerical studies focusing on the validity of Fourier law $J = -k\partial T/\partial x$ for many models such as the Fermi-Pasta-Ulam (FPU) model$^2$$^3$, the ding-a-ling model$^4$$^5$, the Frenkel-Kontorova (FK) model$^6$$^7$ and the Lorenz-gas model$^8$ and so on, some other different and important problems have also attracted people attention. For example most recently Casati et al.$^9$ investigated the possibility to control the energy transport inside a nonlinear 1D chain connecting with two thermostats at different temperatures. They emphasized that controlling heat conduction by nonlinearity opens a new possibility to design a thermal rectifier, i.e., a lattice that carries heat preferentially in one direction.

In this Letter we investigate heat conduction problem for a new type of model wherein there is a Yukawa-Coulomb interaction potential. It arises from dust-grain plasma which is extensively studied recently due to its new features with dust crystal or collective waves$^{10}$$^{11}$$^{12}$$^{13}$$^{14}$$^{15}$. Our study shows that the heat conductivity is abnormal in absence of external field as $\kappa \propto N$ as in harmonic chains. Under FK field, however, it is normal which is similar to the cases of former studies but with harmonic or/and FPU interactions$^3$. Surprisingly for the dust chains with real wake potential$^{12}$, modified FK field, the heat conduction exhibits a mixture property of normal and abnormal behaviors. It is found that the asymmetric property of external wake potential can induce asymmetric thermal conductivity that can be used to be a thermal rectifier. In a certain of system parameters, by changing the strength and width of wake potential, the heat fluxes for two opposite direction can be different remarkably.

In a general form the Hamiltonian of the considered system is written as

$$H = \sum_i h_i, \quad h_i = \frac{p_i^2}{2} + V(x_{i-1}, x_i) + U(x_i)$$

(1)

where $V(x_{i-1}, x_i)$ stands for the interaction potential of the nearest-neighbor particles and $U(x_i)$ is a external on-site potential. For dust particles system we have the interaction potential (refer to$^{12}$)

$$V(r_{ij}) = \frac{q^2}{r_{ij}} \exp(-\frac{r_{ij}}{\lambda_d}) - \alpha \frac{q^2}{r_{ij}}$$

(2)

where $\alpha$ is the parameter that ranges from 0 to 1, $\lambda_d$ is the plasma Debye length and $q$ is the dust grain charges, while $r_{ij}$ is the distance between particles $i$-th and $j$-th. For simplicity we have assumed that the masses $m_d$ and charges of all the grains $q$ are the same and constant, while for convenience we shall choose parameter $\alpha$ that makes the neighbor dust particle is located at the bottom of $V$ (see more clear in the following). Note that the plasma electrons and ions do not appear explicitly in the simulations but their effects, which result in an attractive force to dust, are taken into account in the effective interaction potential as the second term of Eq.(2). On the other hand in dusty plasma we know that there exist wake potential acting the dusts along downstream$^{12}$

$$U(r_{ti}) = \frac{qq_i}{r_{ti}} \frac{2}{1-M^{-2}} \cos(\frac{r_{ti}}{\lambda_d\sqrt{M^2-1}})$$

(3)

where $q_i$ is the upstream test dust particle charge, $M > 1$ is the Mach number of ion flow and $r_{ti}$ is the distance of
\(T_i + = 0.12\) and \(T_i - = 0.08\). The parameters are chosen as \(\gamma_1 = 1\) and \(\gamma_2 = 0.3\) (b), 2 (c). Averages are carried over a time interval \(10^7\) by dropping a transient \(10^6\).

Let us turn to the side of the motion of system. A general approach is employed here that are used by many authors like Lepri et al. and Hu et al., namely, two Nose-Hoover thermostats are put on the first and last particle, keeping the temperature at \(T_i +\) and \(T_i -\), respectively. For simplicity and convenience, firstly we need to normalize the basic physical quantities: the mass by the particle mass \(m_d\), the space distance by the dust inter-particle distance \(a_d\) and the time by the \(\sqrt{m_d a_d^2/\lambda_d^2}\) respectively. Then the equations of motion for particles are

\[
\ddot{x}_i = -\xi_+ \dot{x}_i + f_1 - f_2, \quad \xi_+ = \frac{x_i^2}{T_i^+} - 1
\]

\[
\ddot{x}_N = -\xi_- \dot{x}_N + f_N - f_{N-1}, \quad \xi_- = \frac{x_N^2}{T_-} - 1
\]

where \(f_i = -V'(x_i - x_{i-1}) - U'(x_i)\) is the force. Usually the fixed boundary conditions \(x_0 \equiv \text{const}\) and \(x_{N+1} \equiv \text{const}\) are assumed. Now the interaction potential in normalized form can be written

\[
V(x_{i-1}, x_i) = (\exp[-\chi(x_i - x_{i-1})] - \alpha)/(x_i - x_{i-1})
\]

where parameter \(\chi = a_d/\lambda_d\) is the ratio of inter-particle distance to the plasma Debye length. Many studies show that when \(\chi\) is large the nearest neighbor interaction is
appropriate instead of particle-pair interaction \[ \mathcal{F}. \] In our following numerical studies \( \chi = 5 \) is generally used. The particles are arranged initially at equilibrium positions of \( V \) and the normalized inter-distance equals to 1, therefore, it means that parameter \( \alpha \) adjusting the attraction of plasma to dust particle, must satisfy \( \alpha = (1 + \chi) \exp(-\chi) \). For the external FK-modified potential Eq. 5, we have its normalized form

\[
U(x_i) = \gamma_2 \cos(\gamma_1 x_i)/x_i,
\]

where \( \gamma_1 = \chi/\sqrt{M^2-1} \) and \( \gamma_2 = 2\beta/(1-M^{-2}) \) with \( \beta = q_i/q \) the ratio of upstream test particle charge to downstream particles charge. Now we denote \( x_i \) as the position of \( i \)-th dust particle in the chain from the origin of test dust particle \( x_\text{ref} \equiv 0 \). In correspondence for the normalized external FK potential one has \( U(x_i) = \gamma_2 \cos(\gamma_1 x_i) \). The different temperature profiles for different external potentials of field-free, FK and FK-modified are shown in Fig.1. The imposed temperature are \( T_+ = 0.12 \) and \( T_- = 0.08 \) and \( \gamma_1 = 1 \). The potential strengths are \( \gamma_2 = 0.3 \) and 2 for FK and FK-modified, respectively. Obviously the temperature gradients are constructed globally only in the FK case.

Usually the heat flux at the \( i \)-th position is given by

\[
J_i(t) = \frac{1}{2}(x_i + x_{i+1}) f_{i+1}.
\]

Numerically the time average \( J = \langle J_i(t) \rangle \) is independent of the index for long time enough. We plot in Fig.2 the heat flux \( JN \) vs the system size \( N \) for three different cases of field-free (a), FK (b) and FK-modified (c). Obviously the abnormal heat conductivity \( \kappa \propto N \) is obtained for purely Yukawa interaction chains, which is similar to the case of harmonic situation. In the Yukawa chains for standard FK external potential, although it seems unclear about whether there exists phase transition of heat conduction between normal and abnormal \[ \mathcal{F}, \] our results indicates that the normal heat conductivity exists, which support the conclusion of normal heat conduction in Ref. \[ \mathcal{F} \]. From Fig.2 (c), however, we can see that it is abnormal globally on heat conduction in the Yukawa chains under FK-modified on-site external potential while the local temperature gradient appeared in the left region of system, see Fig.1(c). The dependence of \( J_L/J_R \) on parameter \( \gamma_2 \), the strength of the FK-modified on-site external potential is plotted in Fig.3, where the power law \( J_L/J_R \propto 10^{0.24\gamma_2} \) is fitted in our numerical parameter regime. Our numerical experiments shows the validity of this power law until to \( \gamma_2 = 4 \) which indicates that the difference of two directional heat current can possessively over one order. However in practice of dusty plasmas it can only be realized by a relatively small \( \gamma_2 \) due to the test dust charge equals or less than the charge of particles in chains. For example, for given \( \chi = 5 \), \( \gamma_1 = 1 \) and \( \beta = q_i/q \approx 1 \) it corresponds to the practice ion flow Mach number \( M = \sqrt{26} \) (usually in the sheath \( M > 1 \)), and \( \gamma_2 \approx 2 \) which indicates \( J_L/J_R \approx 3 \).

In order to see how the single kicked particle transfer energy to the others, in Fig.4 we plotted the momentum excitations with different external potentials of three cases of field-free (a), FK (c), and FK-modified (f). \( p_L(0) \) and \( p_R(0) \) denote the initial momentum kick on the left 1-th particle and right 100-th particle, respectively. For (c)-(f) the parameters of \( \gamma_1 = 1 \) and \( \gamma_2 = 2 \) are given.

![FIG. 3: Dependence of \( J_L/J_R \) on parameter \( \gamma_2 \).](image1)

![FIG. 4: Momentum excitations for different types of external potentials.](image2)
three solitons in Fig.3(f) but only one in Fig.3(e). Maybe this is one reason why in this case the left-directional heat flux, $J_L$, is larger than that of right directional, $J_R$.

On the other hand according to the expression of heat flux, the ratio of them of two-direction is approximately

$$\frac{J_L}{J_R} \approx \sqrt{\frac{T_+}{T_-}} \exp (r_+ - r_-)$$

where $r_+$ and $r_-$ are the average inter-particle distance in the region where the temperature is almost constant for $[T_+, T_-]$, right-direction heat-flow $J_R$, and $[T_-, T_+]$, left-direction heat-flow, respectively. In general it is shown that $r_+$ is a little larger than $r_-$ by numerical experiments. It is not surprising that the more phonons are scattered in the case of $[T_+, T_-]$ than that of vise versa. Therefore even if $r_+$ is just a very little greater than $r_-$, $J_L/J_R$ would be greatly larger than one. For example, $r_+ \approx 1.08$ and $r_- \approx 0.92$, then we have $J_L/J_R \approx 3$. However in the case of Harmonic interaction potential because of its symmetric quadratic property about equilibrium position the ratio of opposite directional heat flux is in order of $\sqrt{T_+T_-}$, for example by choosing $T_+ = 0.12$, $T_- = 0.08$, the ratio of $J_L/J_R \approx 1.23$. Our numerical results confirm this simple approximation analysis. Indeed if we instead of harmonic interaction chains the heat flux difference for two direction can not be over 23% under asymmetric potential.

Finally we calculate heat flux in different potential width $\gamma_1^{-1}$ (see Fig.5). It shows that we can also control the energy flow by changing the potential width $\gamma_1^{-1} = \sqrt{M^2 - 1/\chi}$ through adjusting the ion flow velocity, which is associated with $M$ or the plasma particles density which is associated with $\chi$. Obviously the great difference of heat flux at low temperature caused by the width of potential smear out as the temperature increases to over 0.3. It is noted that the ratio of heat flux $J_R(\gamma_1 = 1)/J_R(\gamma_1 = \pi)$ is about over two orders difference.

In summary we have studied the heat conduction problem in the system of 1D Yukawa interaction chains with asymmetric on-site modified FK in the Yukawa chains, thus we provide a simple method to change the properties of the system, from a normal conductor obeying Fourier law, down to an almost perfect insulator. Some theoretical consideration has also been attempted to understand for our results and it is found that in the case of Yukawa interaction potential, the asymmetric property about equilibrium position has played a crucial role to improve the ratio of opposite directional heat flux. It seems that there exist some modes which are combinations of solitary-like and scattering phonons. Certainly more formidable theoretical works is still challenging our research on this problem in the future.

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