Intriguing Heat Conduction of a Chain with Transverse Motions

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We study heat conduction in a one-dimensional chain of particles with longitudinal as well as transverse motions. The particles are connected by two-dimensional harmonic springs together with bending angle interactions. Using equilibrium and nonequilibrium molecular dynamics, three types of thermal conducting behaviors are found: a logarithmic divergence with system sizes for large transverse coupling, 1/3 power law at intermediate coupling, and 2/5 power law at low temperatures and weak coupling. The results are consistent with a simple mode-coupling analysis of the same model. We suggest that the 1/3 power-law divergence should be a generic feature for models with transverse motions.

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To understand microscopic dynamical origin of heat conduction is one of the long standing tasks in nonequilibrium statistical mechanics. This problem has attracted increasing attention in recent years [1–12]. The main effort has been focused on the necessary and sufficient conditions of the Fourier law of heat conduction in one-dimensional (1D) systems. With strong numerical support, it is argued that chaos (or exponential instability) is the necessary condition [1]. However, recent results in different billiard gas channels show that even linear instability, such as that found in generic polygonal billiards, is sufficient for a normal diffusion and energy transport obeying the Fourier law [2]. For some billiard gas channels, the heat conduction violates the Fourier law; it is found that the thermal conductivity, κ, changes with system size N as, $\kappa \sim N^{\alpha}$, with $\alpha = 2 - 2/\beta$ [9], where β is the exponent of the diffusion ($\Delta x^2 \sim t^{\beta}, 0 < \beta \leq 2$).

On the other hand, in 1D lattice models, it has been proved that the momentum conservation leads to an anomalous heat conduction [3]. However, its specific form of divergence with system size (the value of α) is still of considerable controversy [4–8]. Based on a renormalization group analysis for a 1D hydrodynamic fluid model, it is argued that in a generic momentum conserving system, the thermal conductivity should be $\kappa \propto N^{1/3}$ [4]. Unfortunately, most existing numerical results do not agree with this prediction for unknown reasons. A mode-coupling theory analysis for the 1D Fermi-Pasta-Ulam (FPU) model gives a divergent exponent 2/5 [5,6], which is supported by numerics from different groups [7] and confirmed recently by Pereverzev from the Peierls equation [12].

In this Letter, we would like to clarify what exponent, 1/3 or 2/5, is a generic exponent for the divergent thermal conductivity in a many-body 1D chain with momentum conservation. To this end, we consider a chain of N point particles with mass m on a 1D lattice. For the sake of generality, the particles have both longitudinal and transverse motions. The lattice fixes the connectivity topology such that only the neighboring particles interact. The Hamiltonian is given by

$$H(\mathbf{p}, \mathbf{r}) = \sum_i \frac{\mathbf{p}_i^2}{2m} + \frac{1}{2} K_r \sum_i (|\mathbf{r}_{i+1} - \mathbf{r}_i| - a)^2 + K_\phi \sum_i \cos\phi_i, \quad (1)$$

where the position vector $\mathbf{r} = (x, y)$ and momentum vector $\mathbf{p} = (p_x, p_y)$ are two dimensional; a is lattice constant. The minimum energy state is at $(ia, 0)$ for $i = 0$ to $N - 1$. If the system is restricted to $y_i = 0$, it is essentially a 1D gas with harmonic interaction. The coupling K_r is the spring constant; K_ϕ signifies bending or flexibility of the chain, while ϕ_i is the bond angle formed with two neighbor sites, $\cos\phi_i = -\mathbf{n}_{i-1} \cdot \mathbf{n}_i$, and unit vector $\mathbf{n}_i = \Delta\mathbf{r}_i/|\Delta\mathbf{r}_i|$, $\Delta\mathbf{r}_i = \mathbf{r}_{i+1} - \mathbf{r}_i$. Our model is a simplification of more realistic polymer chain models [13].

We determine the heat current in a temperature gradient by nonequilibrium molecular dynamics (MD). The system is set up with fixed leftmost and rightmost boundary. The average distance between particles is set to a, the zero-temperature equilibrium distance. A group of four particles at the two ends are subject to heat baths at temperature T_L and T_H, respectively. This is realized by Nosé-Hoover thermostats. The rest of the particles follow the equations of motion using a velocity Verlet algorithm. We use small time step sizes $h = 0.0005$ to 0.0010. Typical MD steps are 10^8 to 10^{10}.

We use the following expression for local heat current per particle:

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$$m\,\mathbf{j}_i = -\,\Delta\mathbf{r}_i((\mathbf{p}_i+\mathbf{p}_{i+1})\cdot\mathbf{G}(i)) - \Delta\mathbf{r}_{i-1}((\mathbf{p}_i+\mathbf{p}_{i-1})\cdot\mathbf{G}(i-1)) + \Delta\mathbf{r}_{i-1}(\mathbf{p}_i\cdot\mathbf{H}(i-2,i-1,i-1)) + \Delta\mathbf{r}_i(\mathbf{p}_i\cdot\mathbf{H}(i+1,i+1,i)) + \mathbf{p}_i h_i, \quad (2)$$

where $\mathbf{G}(i) = \frac{1}{4}K_r(|\Delta\mathbf{r}_i| - a)\mathbf{n}_i$, $\mathbf{H}(i,j,k) = K_\phi(\mathbf{n}_i + \mathbf{n}_k\cos\phi_j)/|\Delta\mathbf{r}_k|$, and the local energy per particle $h_i = \frac{1}{4}K_r((|\Delta\mathbf{r}_{i-1}| - a)^2 + (|\Delta\mathbf{r}_i| - a)^2) + K_\phi\cos\phi_i + p_i^2/(2m)$. This is derived from $\mathbf{J} = \sum d(\mathbf{r}_i h_i)/dt$, by regrouping some of the terms using translational invariance. It satisfies the continuity equation in the long-wave limit.

We present our main numerical results in Fig. 1. The data are obtained using 20 1GHz-Pentium PCs over six months of CPU times. We plot the average heat current multiplied by N, $jN = (T_H - T_L)\kappa$, in log-log scale [Fig. 1(a)] and linear-log scale [Fig. 1(b)]. It is clearly shown that three types of behaviors of the thermal conductivity κ are observed, the logarithmic divergence, $\log N$, power law $\kappa \propto N^\alpha$ with $\alpha = 1/3$, as well as $2/5$, depending on the model parameters. Log-log plot shows linear behavior for data set E, F, H, and J. At the parameters of set E, excellent power-law dependence is found, with an exponent of $\alpha = 0.334 \pm 0.003$ (using an error weighted least-squares fit for $N \geq 128$). Set F is also in good agreement with a slope of 1/3. On the other hand, for set H and J, we have exponent α consistent with 0.4. Set B is consistent with logarithmic divergence, $\kappa \propto \log N$ [see Fig. 1(b)]. The model has two key parameters, the temperature T, and the transverse coupling K_ϕ. We should mention that a wide range of parameters is scanned, and surprisingly, only the three scalings are found so far in this model.

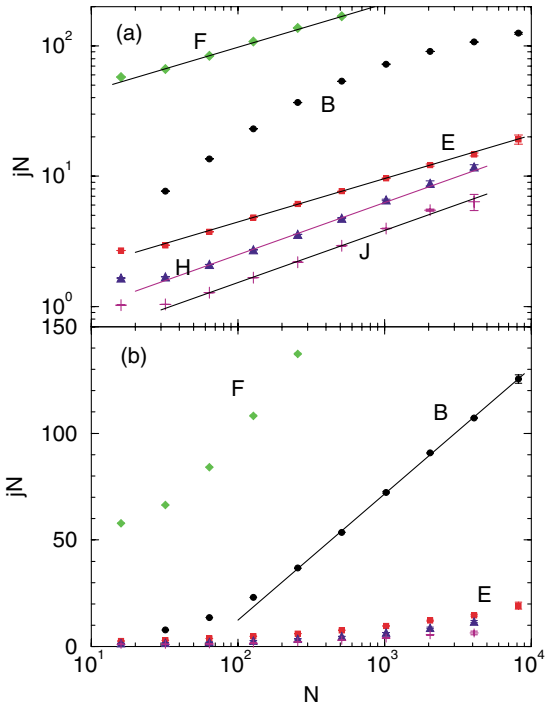

FIG. 1 (color online). jN vs N on double-logarithmic (a) and linear-log plot (b). The parameters (K_ϕ, T_L, T_H) of the model are, set B: (1, 0.2, 0.4), set E: (0.3, 0.3, 0.5), set F: (1, 5, 7), set H: (0, 0.3, 0.5), set J: (0.05, 0.1, 0.2). All of them have $K_r = 1$, mass $m = 1$, lattice spacing $a = 2$. The straight lines on F and E have slope $1/3$, while the slope on H and J is $2/5$.

To understand the simulation results, we consider a simple mode-coupling theory for the present model. The equations of motion in terms of normal-mode coordinates, $Q_k^\parallel = \sqrt{m/N}\sum_{j=0}^{N-1}(x_j - ja)e^{i2\pi jk/N}$, $Q_k^\perp = \sqrt{m/N}\sum_{j=0}^{N-1} y_j e^{i2\pi jk/N}$, for small oscillation near zero-temperature equilibrium position, keeping only leading nonlinearity, are

$$\frac{d^2Q_k^\parallel}{dt^2} = -(\omega_k^\parallel)^2 Q_k^\parallel + \sum_{k'+k''=k} c_{k',k''}^\parallel Q_{k'}^\perp Q_{k''}^\perp, \quad (3a)$$

$$\frac{d^2Q_k^\perp}{dt^2} = -(\omega_k^\perp)^2 Q_k^\perp + \sum_{k'+k''=k} c_{k',k''}^\perp Q_{k'}^\parallel Q_{k''}^\perp, \quad (3b)$$

where the bare dispersion relations are given by $\omega_k^\parallel = 2\times\sqrt{K_r/m}|\sin(\pi k/N)|$, and $\omega_k^\perp = 4\sqrt{K_\phi/a^2 m}\sin^2(\pi k/N)$. The expressions for $c_{k'k''}^{\parallel,\perp}$ are complicated, but can be simplified in the long-wave limit, as $c_{k,k'}^\perp = 2c_{k,k'}^\parallel \propto kk'(k+k')$. Instead of the integer k, we can also index the mode by its corresponding lattice momentum $p = 2\pi k/(aN)$.

A central quantity in the mode-coupling theory is the normalized correlation function, $g_p(t) = \langle Q_p(t)Q_p^*(0)\rangle/\langle|Q_p(0)|^2\rangle$. The Fourier-Laplace transform of the correlation function, $g[z] = \int_0^\infty g(t)e^{-izt}\,dt$, is given by [11,14],

$$g_p^{\parallel,\perp}[z] = \frac{-iz - p^2\nu^{\parallel,\perp}[z]}{z^2 - c_{\parallel,\perp}^2 p^2 - iz\,p^2\nu^{\parallel,\perp}[z]}. \quad (4)$$

The constants $c_\parallel$ and $c_\perp$ are effective or renormalized sound velocities for the longitudinal and transverse modes. They are defined, e.g., by $(c_\parallel p)^2\langle|Q_p^\parallel|^2\rangle = k_B T$, as $p \to 0$. The damping functions (memory kernel) are given by the coupled equations,

$$\nu^\parallel(t) = \frac{K_\parallel}{2\pi}\int_{-(\pi/a)}^{\pi/a} dp\,(g_p^\perp(t))^2, \quad (5a)$$

$$\nu^\perp(t) = \frac{K_\perp}{2\pi}\int_{-(\pi/a)}^{\pi/a} dp\,g_p^\parallel(t)\,g_p^\perp(t). \quad (5b)$$

Equations (4) and (5) form a closed system of nonlinear integral equations. This is a straightforward generalization of the strictly 1D result [6]. The above equations are derived under a number of simplification assumptions, such as long-wave approximation, mean-field type product approximation for the correlation functions, replacing

random-force correlation with true force correlation. Some of them can be removed but more complicated equations will result.

In Fourier space, for large z the solution is found from integration by part, as $\nu^{\parallel,\perp}[z] = K_{\parallel,\perp}/(iza) + O(z^{-3})$. The long-wave asymptotic decay of each mode is controlled by the small z behavior of the function $\nu^{\parallel,\perp}[z]$. We define $\delta_\parallel$ and $\delta_\perp$ by $\nu^{\parallel,\perp}[z] \propto z^{-\delta_{\parallel,\perp}}$. The dispersion relation is then given by the location of the poles in the correlation function $g[z]$. The imaginary part of the frequency gives damping, by $\gamma_p \propto p^2 \nu[z]|_{z\to cp} \propto p^{2-\delta}$. We note that three types of behaviors can be derived from the above set of equations. If $K_\parallel \approx K_\perp$ and $c_\parallel \approx c_\perp$, the two equations reduce to that of strictly 1D model; we thus expect the result of Lepri [6], i.e., $\delta_\parallel = \delta_\perp = 1/3$. On the other hand, it can be shown rigorously that in the limit of small $K_\perp$ and small $c_\perp$, we have $\delta_\perp = 0$ and $\delta_\parallel = 1/2$. Formally, when $a \to 0$, the equation possesses the scaling solution of the form $\nu[\lambda z] = \lambda^{-1}\nu[z]$; this implies $\nu[z] \propto 1/z$. These analytic results are supported by numerical solutions of the coupled equations, shown in Fig. 2. They are solved by a brute force numerical integration in Fourier space. Details of the mode-coupling calculation will be presented elsewhere.

In Fig. 2 at parameter set I, we observe very good asymptotic behavior of $\nu^\parallel[z] \propto z^{-1/2}$ and $\nu^\perp[z] \propto$ const. This corresponds to the behavior of MD results for data set E and F in Fig. 1. When $c_\parallel = c_\perp$ but $K_\parallel \neq K_\perp$ (set II), there appears to have a crossover from $\delta_\parallel = 1/3$ to $1/2$. The curve III may be related to the logarithmic divergence. We note that a meaningful, direct mapping from the simulation parameters to mode-coupling parameters is not possible, due to the qualitative nature of the theory.

The prediction of $\delta_\parallel = 1/2$ and $\delta_\perp = 0$ is checked against an equilibrium MD simulation in a microcanonical ensemble with periodic boundary condition. We compute the normal-mode correlation $\langle Q_p(t) Q_p^*(0)\rangle$ for each mode specified by the lattice momentum $p = 2\pi k/(aN)$. The functions are oscillatory with an exponential decay, $\cos(\omega t)e^{-\gamma_p t}$. The decay constants are obtained by fitting the maximum amplitude as a function of time. The results are presented in Fig. 3. Comparing with results from smaller and larger system sizes, the effect of finite sizes appears rather small at $N = 1024$. Excellent agreement with mode-coupling theory ($\gamma \propto k^{2-\delta}$) is obtained for data set E. However, for data set B and J, the slopes are not consistent with either logarithmic divergence for κ or $2/5$ law. This may be interpreted as that we are not in the asymptotic regime.

To connect the result of damping of the modes with thermal conductivity, it is noted [5,12] that each mode contributes to the thermal transport independently. Under the linear-response theory, the Green-Kubo formula relates the current-current correlation to the thermal conductivity by

$$\kappa = \frac{1}{k_B T^2 aN} \int_0^\infty \langle J(t)J(0)\rangle \, dt. \tag{6}$$

The decay rates for J are assumed to be the same as that for Q, thus $\langle J(t)J(0)\rangle \propto \sum_p \exp(-\gamma_p^\parallel t)$. The amplitude of the exponential decay is approximately independent of p. Converting the summation to integral, we have $\langle J(t)J(0)\rangle \propto t^{-1/(2-\delta_\parallel)}$. The thermal conductivity on a finite lattice is obtained by integrating over t to a time of $O(N)$, thus $\kappa_N \propto N^{1-1/(2-\delta_\parallel)} = N^\alpha$. When $\delta_\parallel = 1/2$, we have $\alpha = 1/3$, and when $\delta_\parallel = 1/3$, the exponent $\alpha = 2/5$.

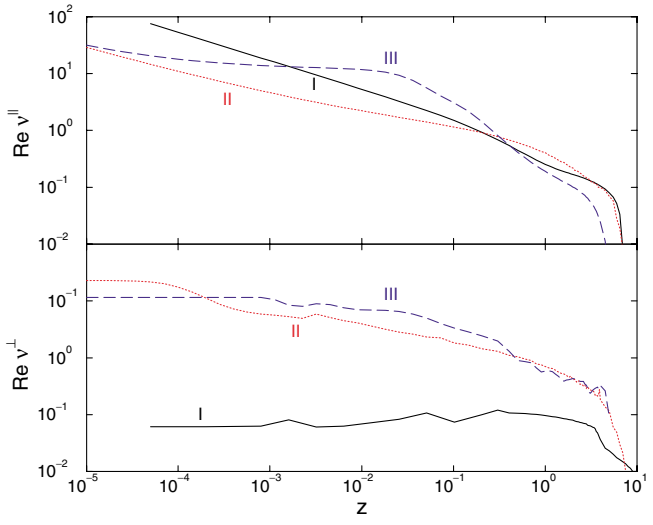

FIG. 2 (color online). Real part of $\nu^\parallel[z]$ and $\nu^\perp[z]$ vs z for parameters $a = 1$, $K_\parallel = 1$, and $(K_\perp, c_\parallel, c_\perp)$ I: (0.3, 2, 1), II: (1.8, 1, 1), III: (2, 1, 0.5).

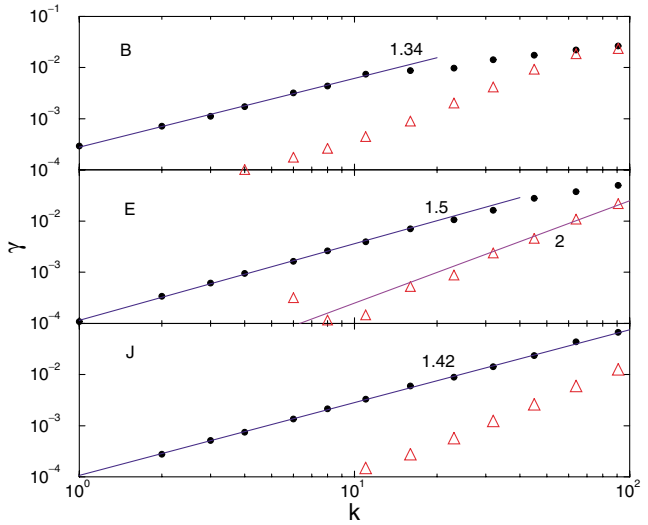

FIG. 3 (color online). The decay rate $\gamma^\parallel$ (dots) and $\gamma^\perp$ (triangles) vs k for the parameters set B, E, and J at equilibrium temperature $T = (T_L + T_H)/2$. The number on the line indicates the slope of the straight line. The system size is $N = 1024$.

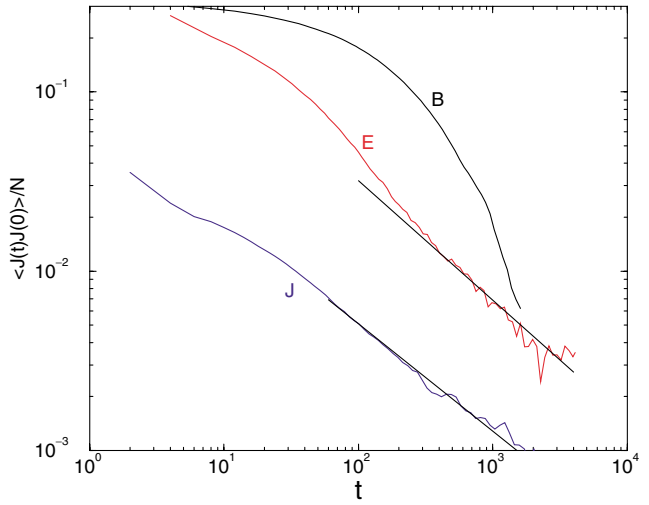

FIG. 4 (color online). The Green-Kubo integrand, $\langle J(t)J(0)\rangle/N$, vs time t. The parameters are the same as that in Fig. 3. The straight lines have slope $-2/3$ (on E) and $-3/5$ (on J).

The current-current correlation functions are presented in Fig. 4 for the parameters corresponding to data sets B, E, and J in Fig. 1. For data set J, a power-law dependence is in excellent agreement with the theoretical expectation $t^{\alpha-1}$ with $\alpha = 2/5$. For set E, the curve is a bit steeper than expected. This may be due to finite sizes. For set B, where logarithmic divergence is observed, we do not observe good power-law behavior in the correlation.

We need to clarify the relationship between the three types of observed behaviors in the nonequilibrium MD results. From a mode-coupling point of view, the $1/3$ law is generic and robust, while $\alpha = 2/5$ should eventually cross over to $1/3$ at long length scales. However, such a crossover is not observed in MD data. The crossover effect can be argued for a more general setting. More general mode-coupling equations for a generic interaction potential consistent with the symmetry would have an additional term of $(K_3/2\pi)\int_{-(\pi/a)}^{(\pi/a)} dp(g_p^{\parallel}(t))^2$ for Eq. (5a); Eq. (5b) remains the same. Such a term can appear either from cubic or quartic nonlinearity in potential. Contribution from this extra term decays in time t faster than the perpendicular component contribution. Thus, the asymptotic result of $\delta_{\parallel} = 1/2$ remains true. The same should be also true even if a chain is allowed to move in three dimensions. If the parameter K_3 is sufficiently large, we may see exponent close to 0.4. The logarithmic divergence is a bit difficult to interpret. It might be a crossover effect to other asymptotic behavior.

In summary, we have observed three different scalings in a 1D chain. When the transverse motion couples with the longitudinal motion, the thermal conductivity diverges with system size with a $1/3$ power law. This has been demonstrated with a very high precision numerical result and explained in terms of a mode-coupling theory. In the weak coupling regime, a $2/5$ power law is observed which is consistent with the results observed in the FPU model without transverse motion. In relatively large coupling regime, a logarithmic divergent law is observed.

We argue that the $1/3$ law is generic for 1D many-particle chain with momentum conservation and transverse motion. This is supported by a recent study on 1D FPU model with transverse motion [15]. If the on-site potential is considered, as in the case of Frenkel-Kontorova model [16], we expect a size-independent thermal conductivity regardless of the transverse motion.

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