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Thermal conductance of the coupled-rotator chain: Influence of temperature and size

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Abstract – The thermal conductance of a homogeneous 1D nonlinear lattice system with neareast-neighbor interactions has recently been computationally studied in detail by Li *et al.* (*Eur. Phys. J. B*, **88** (2015) 182), where its power-law dependence on temperature T for high temperatures is shown. Here, we address its entire temperature dependence, in addition to its dependence on the size N of the system. We obtain a neat data collapse for arbitrary temperatures and system sizes, and numerically show that the thermal conductance curve is quite satisfactorily described by a fat-tailed q-Gaussian dependence on $TN^{1/3}$ with $q \simeq 1.55$. Consequently, its $T \to \infty$ asymptotic behavior is given by $T^{-\alpha}$ with $\alpha = 2/(q-1) \simeq 3.64$.

Introduction. – The breakdown of Fourier's law in low-dimensional lattices has attracted much attention in recent years due to its fundamental importance within non-equilibrium thermodynamics and statistical mechanics [1–6]. In the 1D Fermi-Pasta-Ulam (FPU-β) lattice, the thermal conductivities κ diverge with system sizes N as $\kappa \propto N^{\gamma}$, where $0 < \gamma < 1$; consequently its thermal conductance $\sigma \equiv \kappa/N$ vanishes in the $N \to \infty$ limit. However, there is still no clear conclusion about the physical ingredient responsible for this kind of anomalous heat conduction. It is believed that momentum conservation is the crucial reason for the anomalous heat conduction [7–9], but normal heat conduction has been found in the 1D coupled rotator lattice, which also is a momentum-conserved system [10,11].

Unlike the FPU-β-like lattices, the 1D coupled rotator lattice has periodic interatomic potential which is finite. As a result, the energy diffusion as well as the momentum diffusion are normal [12]. In order to understand the effect of this finite interatomic potential, previous works focus on the temperature dependence of the thermal conductivities in the 1D coupled rotator lattice [10,11]. In both works, the thermal conductivity was proposed to have an exponential dependence on temperature. But it is argued that $\kappa(T) \propto e^{\Delta V/T}$, where ΔV is proportional to the potential barrier height in [10], while $\kappa(T) \propto e^{-T/A}$ with A a fitting parameter in [11]. It has only recently been found that the temperature dependence in the 1D coupled rotator lattice follows a power-law behavior on temperature as $\kappa(T) \propto T^{-\alpha}$ with $\alpha \simeq 3.2$ for intermediate temperatures [13]. Interestingly enough, this power-law dependence is qualitatively consistent with the theoretical prediction for the Chirikov standard map which is a single-rotator model [14,15].

On the other hand, the standard map, as well as several other dynamical complex systems, has recently been shown [16] to present non-Gaussian probability distributions for the sum of its position random variable. These distributions are approached extremely well by the q-Gaussian defined as

$$P_q(x) = A_q e_q^{-B_q x^2} \equiv \frac{A_q}{[1+(q-1)B_q x^2]^{1/(q-1)}}, \qquad (1)$$

where A_q is the normalization factor, $B_q > 0$ is a parameter which characterizes the width of the distribution, and the index $q \geq 1$ [17–19]. In the $q \to 1$ limit, this expression recovers the standard Gaussian distribution. This family of distributions optimizes the nonadditive entropy $S_q = k\frac{1-\int \mathrm{d}x[p(x)]^q}{q-1}$ with $S_1 = S_{BG} \equiv -k\int \mathrm{d}x p(x)\ln p(x)$ under appropriate constraints, where k is the Boltzmann constant, $p(x)$ is the probability distribution, and BG stands for Boltzmann-Gibbs.

Model and method. – In this letter, we study a homogeneous 1D nonlinear lattice system with nearest-neighbor interactions and try to see whether some of its properties also are consistent with q-Gaussians. For this lattice system, the Hamiltonian with the corresponding dimensionless units can be written in the general form

$$H = \sum_{i=1}^{N}\left[\frac{p_i^2}{2} + V(q_{i+1}-q_i) + U(q_i)\right], \qquad (2)$$

where p_i denotes the momentum for the i-th rotator. The set q_i are the displacements from the equilibrium position for the i-th rotator; $V(q_{i+1}-q_i)$ is the interaction potential between neighboring sites i and $i+1$, and $U(q_i)$ is the on-site potential, representing the interaction with the substrate. To focus on the momentum-conserving system, we set $U = 0$. The potential we employ is in the form

$$V(x) = V_0(1-\cos x), \qquad (3)$$

where V_0 is the interaction strength (without loss of generality we set $V_0 = 1$).

In our simulation, a Langevin form of heat bath is used. For the chain with N particles, only the first and last particles are coupled to the heat bath, with the temperature T_L and T_R, respectively. The dynamics equations of the motion read

$$\begin{aligned} \dot{q_i} &= p_i, \quad i = 1,2,3,\ldots,N, \\ \dot{p_i} &= F(q_i - q_{i-1}) + F(q_{i+1}-q_i), \quad i = 2,3,\ldots,N-1, \\ \dot{p_1} &= F(q_i) + F(q_{i+1}-q_i) - \gamma p_1 + \xi_1, \\ \dot{p_N} &= F(q_i - q_{i-1}) + F(-q_i) - \gamma p_N + \xi_N, \end{aligned} \qquad (4)$$

where $F(x) = -\partial V(x)/\partial q_i$ and γ is the friction coefficient; ξ_1, ξ_N stand for the Gaussian white noise with zero mean $\langle \xi_1(t)\rangle = 0$ and $\langle \xi_N(t)\rangle = 0$. The correlation functions are given by

$$\begin{aligned} \langle \xi_1(t)\xi_1(t')\rangle &= 2\gamma T_L \delta(t-t'), \\ \langle \xi_N(t)\xi_N(t')\rangle &= 2\gamma T_R \delta(t-t'). \end{aligned} \qquad (5)$$

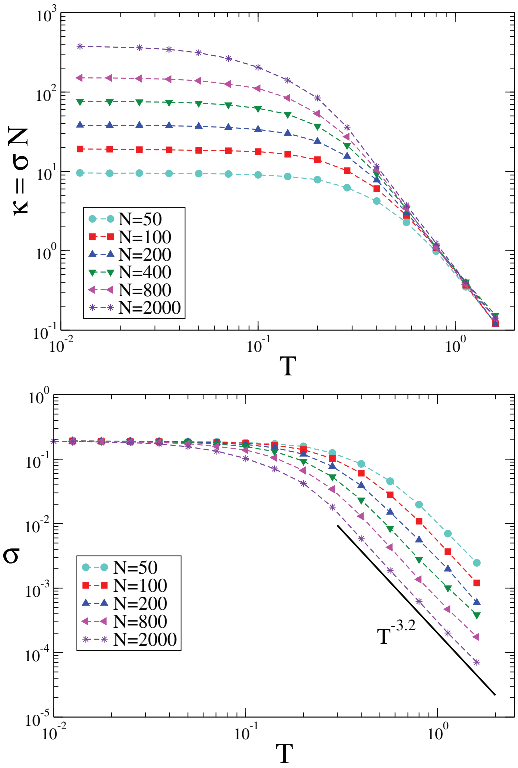

Fig. 1: (Color online) Heat flow at stationary state for typical lattice sizes. Top: thermal conductivity $\kappa \equiv \sigma N$ (notice that data collapse occurs for the high-temperature region). Bottom: thermal conductance σ (notice that data collapse occurs for the low-temperature region). Different colors correspond to the lattice lengths $N = 50$, 100, 200, 400, 800 and 2000. The slope -3.2 indicated in [13] is shown here for comparison. The dashed curves are guides to the eye.

For simplicity, the temperatures are set as $T_{L/R} = T_0(1 \pm \Delta)$, where T_0 is the average temperature and Δ is the temperature difference. Throughout our numerical simulations, $\Delta = 0.1$ is restricted to the small perturbation regime and $\gamma = 1$ is fixed. The evolution of dynamics (eqs. (4)) is integrated by the Verlet velocity algorithm and the time step $\Delta t = 0.01$, which is small enough [20]. All the results are analyzed for the time scale 10^7–10^8, after the system release to the steady state.

Results and discussion. – The thermal conductivity κ is characterized by

$$\kappa(T) = \frac{JN}{T_L - T_R}, \qquad (6)$$

where $J = \langle J_i\rangle$ is the average heat flux along the lattice and J_i is the local heat flux. As already mentioned, the thermal conductance is defined as $\sigma \equiv \kappa/N$. The temperature dependence of the thermal conductance is given in fig. 1 for six different lattice sizes. The asymptotic power-law behavior is evident with an exponent -3.2. One can easily obtain a clear data collapse as shown in fig. 2. It is evident that the temperature dependence of the

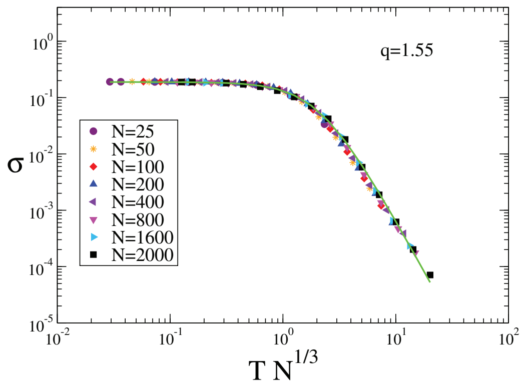

Fig. 2: (Color online) Data collapse for lattice sizes going from $N = 25$ to $N = 2000$. The continuous curve (green line) corresponds to $\sigma = A_q e_q^{-B_q\,(TN^{1/3})^2}$ with $(q, B_q, A_q) = (1.55, 0.40, 0.189)$. Notice that the maximum value 0.189 has naturally nothing to do with the normalizing factor of a q-Gaussian distribution, which for the present values $(q, B_q) = (1.55, 0.40)$ would approximately be 0.28. Indeed, q-exponential and q-Gaussian functions frequently appear in diverse physical quantities (*e.g.*, the time evolution of the nonlinear dynamical sensitivity to the initial conditions [21,22]), and not only as probability distributions. The asymptotic slope is given by $2/(1-q) \simeq -3.64$, in contrast with the intermediate slope -3.2 indicated in [13] (see fig. 1). Notice that the asymptotic slope only becomes visible several decades further down.

thermal conductance can be satisfactorily approached by a q-Gaussian with $q = 1.55$. At this point, it is worth mentioning that another system which can be considered to be similar to ours has already been shown to exhibit strong deviations from the Gaussian behavior [23]. In that contribution, the authors analytically study a Brownian particle with linear-position–dependent inverse temperature with a confining potential and show that the behavior can be well described by superstatistics [24], which includes q-Gaussians as a special case.

In conclusion, we have numerically determined that the thermal conductance for the classical one-dimensional first-neighbor coupled planar-rotator (or *inertial XY ferromagnetic*) chain (eqs. (2) and (3), with vanishing on-site potential $U(q_i)$ and unit potential strength V_0) is amazingly well described by the q-Gaussian $\sigma \propto e_{1.55}^{-0.40(TN^{1/3})^2}$ for wide ranges of temperature T and lattice size N. This result implies that, in the $(TN^{1/3}) \to \infty$ limit, we asymptotically expect $\sigma \propto [TN^{1/3}]^{-\alpha}$ with $\alpha = 2/(q-1) \simeq 3.64$, close yet different from the value 3.2 determined in [13] for intermediate temperatures. At thermal equilibrium (*i.e.*, for $T_L = T_R$), it is clear that the present short-range interacting model follows the Boltzmann-Gibbs statistical mechanics. Why then, in the nonequilibrium stationary state characterized by $T_L \neq T_R$, does such a strong suggestion of q-statistics emerge? This remains as a highly interesting and certainly intriguing open question, somewhat reminiscent of the aging and related phenomena in various systems: see for example [25] (its fig. 1), [26], and [27] (its fig. 1, for instance); see also [28] (its fig. 3). It is of course not excluded that, due to the permanent unidirectional heat flow, the phase space of the chain is visited in an incomplete manner. Such type of behavior could be related to the frequent emergence of q-statistics in hydrology [29]. As a final remark let us consider at this point why the distribution that we obtain is a q-Gaussian and not a q-exponential. This is possibly due to the fact that the heat flow occurs always from the hot source to the cold one. This fact results in a symmetry which is very reminiscent of the distribution observed in [30] where the rotation periods of asteroids are found to follow q-Gaussians, in contrast with asteroid sizes, observed to follow a q-exponential. Indeed, the periods are related to the angular velocities, which can rotate in both senses. Further understanding would of course be very welcome.

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