First-principle validation of Fourier's law: a brief study of *n*-vector models

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Introduction

Fourier's law

- Transport properties naturally emerge in macroscopic systems which are not in thermal equilibrium.
- The law for heat conduction in a given macroscopic system, where the heat flux varies linearly with the temperature gradient, $\mathrm{J} \propto -\nabla T$.
- For a simple one-dimensional system (e.g., a metallic bar along the $\hat{x}$ axis, $\mathrm{J} = J\hat{x}$), the heat flux J (rate of heat per unit area) is given by

$$J = -\kappa \frac{dT}{dx} \ , \tag{1}$$

  where κ is the thermal conductivity.
- In principle, κ may depend on temperature and pressure.

Introduction

Requirements for the validation of Fourier's law

Summarizing, κ can not be:

- dependent on temperature gradient;
- dependent on lattice size.

κ can be or must be:

- dependent on temperature and pressure (can be);
- well-behaved function of its arguments (must be).

Main goals

- We numerically investigate the thermal conductivity of n-vector models with $n = 1, 2, 3$ using molecular dynamics simulations;
- For $n = 1$, our focus is on the $d = 1$ lattice of ferromagnetically coupled planar rotators in the inertial XY model, considering both local and coupling anisotropies. In the limit of extreme anisotropy, these models approach the Ising model;
- For the classical inertial nearest-neighbor XY ferromagnet ($n = 2$) we study all feasible dimensions $d = 1, 2, 3$, with $N = L^d$ representing the total number of lattice sites;
- For the classical inertial Heisenberg model ($n = 3$), we focus on the one-dimensional lattice (chain).

n-vector models

Definition

Paradigmatic ferromagnets are in general described by a set of interacting spins in a crystalline d-dimensional lattice that contains n spin vector components such that $|\mathrm{S}| = 1$. In the absence of external fields and inertial terms, the Hamiltonian of these systems can be expressed in the following form:

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \sum_{m=1}^{n} S_i^m S_j^m \;\; (J > 0; \sum_{m=1}^{n} (S_i^m)^2 = 1)\,, \tag{2}$$

where $\langle ij \rangle$ denotes first-neighboring spins, and $n = 1, 2, 3, \infty$ correspond respectively to the Ising, XY, Heisenberg and spherical models .

Classical inertial XY model

XY model

The Hamiltonian of the d-dimensional inertial ferromagnetic XY model is given by

$$\mathcal{H} = \frac{1}{2}\sum_{\ell=1}^{L^d} p_\ell^2 + \frac{1}{2}\sum_{\langle \ell,\ell' \rangle}[1-\cos(\theta_\ell - \theta_{\ell'})]\,, \tag{3}$$

where $\langle \ell, \ell' \rangle$ denotes nearest-neighboring rotors in the d-dimensional lattice.

- Momenta of inertia and unit first-neighbor coupling constant as unit, without loss of generality;
- Periodic boundary conditions along $(d-1)$ directions, and leaving open for 1-dimensional ends. One of the ends being at a low temperature heat bath T_l and the other one at high temperature T_h.

Equations of motion: one-dimensional case

For the one-dimensional XY-model, we have:

$$\begin{aligned}
\dot{\theta}_i &= p_i \ \ (i = 1, \ldots, L) \\
\dot{p}_1 &= -\gamma_h p_1 + F_1 + \sqrt{2\gamma_h T_h}\eta_h(t) \\
\dot{p}_i &= F_i \ \ (i = 2, \ldots, L-1) \\
\dot{p}_L &= -\gamma_l p_L + F_L + \sqrt{2\gamma_l T_l}\eta_l(t)\,,
\end{aligned} \tag{4}$$

the force components being given by

$$\begin{aligned}
F_1 &= -\sin(\theta_1 - \theta_2) - \sin(\theta_1) \\
F_i &= -\sin(\theta_i - \theta_{i+1}) - \sin(\theta_i - \theta_{i-1}) \\
F_L &= -\sin(\theta_L) - \sin(\theta_L - \theta_{L-1}),
\end{aligned} \tag{5}$$

The friction coefficients are chosen $\gamma_l = \gamma_h = 1$ (for numerical convenience), and η_l and η_h represents the Gaussian white noise with zero mean value and unit variance ($\langle \eta_{h/l}(t) \rangle = 0$ and $\langle \eta_{h/l}(t)\eta_{h/l}(t') \rangle = \delta(t - t')$).

Equations of motion: two-dimensional case

For the two-dimensional XY-model, we have:

$$\begin{aligned}
\dot{\theta}_{i,j} &= p_{i,j} \;\; ((i,j) = 1, \ldots, L) \\
\dot{p}_{1,j} &= -\gamma_h p_{1,j} + F_{1,j} + \sqrt{2\gamma_h T_h}\eta_{j,h}(t) \\
\dot{p}_{i,j} &= F_{i,j} \;\; (i = 2, \ldots, L-1) \\
\dot{p}_{L,j} &= -\gamma_l p_{L,j} + F_{L,j} + \sqrt{2\gamma_l T_l}\eta_{j,l}(t)\,,
\end{aligned} \tag{6}$$

the force components being given by

$$\begin{aligned}
F_{1,j} &= -\sin(\theta_{1,j} - \theta_{2,j}) - \sin(\theta_{1,j}) \\
&\quad - \sin(\theta_{1,j} - \theta_{1,j+1}) - \sin(\theta_{1,j} - \theta_{1,j-1}) \\
F_{i,j} &= -\sin(\theta_{i,j} - \theta_{i+1,j}) - \sin(\theta_{i,j} - \theta_{i-1,j}) \\
&\quad - \sin(\theta_{i,j} - \theta_{i,j+1}) - \sin(\theta_{i,j} - \theta_{i,j-1}) \\
F_{L,j} &= -\sin(\theta_{L,j}) - \sin(\theta_{L,j} - \theta_{L-1,j}) \\
&\quad - \sin(\theta_{L,j} - \theta_{L,j+1}) - \sin(\theta_{L,j} - \theta_{L,j-1})
\end{aligned} \tag{7}$$

where $\theta_{i,1} = \theta_{i,L+1}$ and $\theta_{i,0} = \theta_{i,L}$.

Equations of motion: three-dimensional case

For $d = 3$, we have similarly :

$$\begin{aligned}
\dot{\theta}_{i,j,k} &= p_{i,j,k} \ \ ((i,j,k) = 1, \dots, L) \\
\dot{p}_{1,j,k} &= -\gamma_h p_{1,j,k} + F_{1,j,k} + \sqrt{2\gamma_h T_h}\eta_{j,k,h}(t) \\
\dot{p}_{i,j,k} &= F_{i,j,k} \ \ (i = 2, \dots, L-1) \\
\dot{p}_{L,j,k} &= -\gamma_l p_{L,j,k} + F_{L,j,k} + \sqrt{2\gamma_l T_l}\eta_{j,k,l}(t) \,,
\end{aligned} \tag{8}$$

where $\theta_{i,1,k} = \theta_{i,L+1,k}, \theta_{i,0,k} = \theta_{i,L,k}, \theta_{i,j,1} = \theta_{i,j,L+1}$ and $\theta_{i,j,0} = \theta_{i,j,L}$.

Methods

From micro to macro: heat flux

The time derivative of the Hamiltonian Eq. 3 can be written as

$$\frac{d\mathcal{H}}{dt} = -\frac{1}{2}\sum_{\ell=1}^{L^d}(J_\ell - J_{\ell'}) \tag{9}$$

where $J_\ell = (p_\ell + p_{\ell'})\sin(\theta_\ell - \theta_{\ell'})$ is the Lagrangian flux, $\ell \in \{1, \cdots, L^d\}$ is a unique label for each site and ℓ' is the nearest-neighbor of site-ℓ towards to hot reservoir.

J_ℓ is defined as the energy transfer per unit time, per transverse $(d-1)$-dimensional “area” L^{d-1}.

The heat flux remains one-dimensional $\mathrm{J} = J\hat{x}$.

The macroscopic conductivity κ is given by

$$\kappa = \frac{J}{(T_h - T_l)/L} = \frac{J}{2\Delta T/L} \tag{10}$$

Methods

- The dynamical evolution was conducted using the Velocity-Verlet algorithm with step size $dt = 0.01$;
- The transient time is carefully selected for different system sizes by considering the development of the conductivity curve for varying temperature values;
- For instance, the number of transients thrown away for the system to attain the stationary state is at least 2.6×10^{11} for $d = 1$, 8.0×10^{10} for $d = 2$ and 5.6×10^{10} for $d = 3$;
- The average of the heat flux is computed for 4×10^{8} time steps and 80 randomly initialized realizations;
- For simplicity, we set $T_h = T(1 + \Delta)$ and $T_l = T(1 - \Delta)$ with $\Delta = 0.125$, where T is the average temperature .

XY lattices

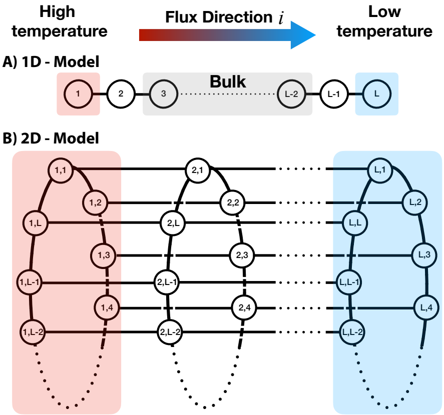


Figure: The lattice structure of the present A) $d = 1$ model (L sites) and B) $d = 2$ model (L^2 sites).

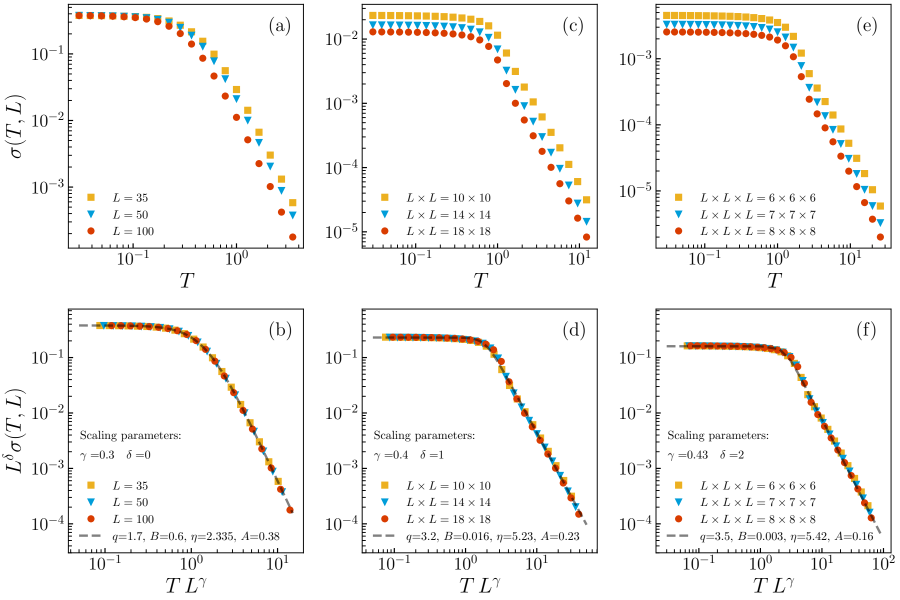


Figure: Thermal conductance as a function of temperature for d-dimensional lattice structures ($d = 1, 2$ and 3).

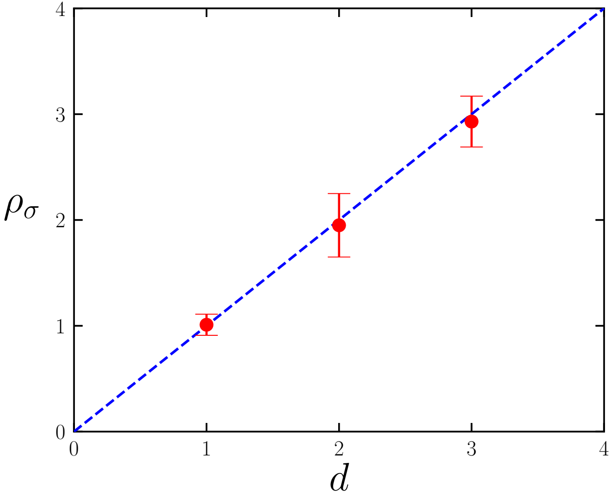


Figure: $\sigma \propto 1/L^{\rho_\sigma(d)}$ $(L \to \infty)$ and $\kappa = \sigma L^d \propto L^{d-\rho_\sigma(d)}$.

Results

q-stretched exponential

All our results for $d = 1, 2$ and 3 collapse in the following universal form:

$$\sigma(T, L)\, L^{\delta(d)} = A(d)\, e_{q(d)}^{-B(d)[T\, L^{\gamma(d)}]^{\eta(d)}}\,, \tag{11}$$

- $(A, B, q, \eta, \gamma, \delta)$ are fitting parameters ;
- Fourier's law corresponds to the $L \to \infty$ limit ;
- σ and κ decay with power laws, namely $\sigma \sim 1/L^{\rho_\sigma}$ and $\kappa \sim 1/L^{\rho_\kappa}$, where $\rho_\sigma \equiv \delta + \gamma \frac{\eta}{q-1}$ and $\rho_\kappa \equiv \rho_\sigma - d$;
- The validation of Fourier's law is confirmed if $\rho_\kappa = 0$ or, equivalently, $\rho_\sigma = d$, making the thermal conductivity independent of the lattice size.

Does it hold true for both $n = 1$ (Ising) and $n = 3$ (Heisenberg)?

Anisotropic XY models: Approaching Ising model

XY$\rightarrow$ Ising: local energy coupling

We assume that the Hamiltonian of the inertial XY model includes a local energy being proportional to a self-interaction between spins in the x-direction. This Hamiltonian can then be written as follows

$$\mathcal{H}_{XY}^{I} = \sum_{i=1}^{L} \frac{p_i^2}{2} + \frac{1}{2} \sum_{\langle i,j \rangle} \left[1 - \cos(\theta_i - \theta_j)\right] + \epsilon_I \sum_{i=1}^{L} \sin^2 \theta_i \,, \qquad (12)$$

where $\epsilon_I \in [0, \infty)$ is a coupling constant associated with this local energy. The heat flux is derived via continuity equation; the Lagrangian heat flux J_i is given by

$$J_i = \frac{1}{2}(p_i + p_{i+1}) \sin(\theta_i - \theta_{i+1}) \,. \qquad (13)$$

Anisotropic XY models: Approaching Ising model

XY→ Ising: anisotropic coupling

Let us focus now on the second possibility, namely the anisotropically coupled XY-model with L interacting spins S_i. The corresponding Hamiltonian is given by

$$\mathcal{H}_{XY}^{a} = \sum_{i}^{L} \frac{p_i^2}{2} + \frac{1}{2} \sum_{\langle i,j \rangle} [1 + \epsilon_a - \cos(\theta_i - \theta_j) - \epsilon_a \cos(\theta_i + \theta_j)] \qquad (14)$$

Notice that $\epsilon_a = \pm 1$ correspond to the Ising model along the y and x axes respectively, whereas $\epsilon_a = 0$ recovers the standard isotropic XY-model. The heat flux of the anisotropically coupled XY model is given by

$$J_i = \frac{p_i + p_{i+1}}{2} \sin(\theta_i - \theta_{i+1}) + \epsilon_a \frac{p_i - p_{i+1}}{2} \sin(\theta_i + \theta_{i+1}) \,. \qquad (15)$$

Ising chain

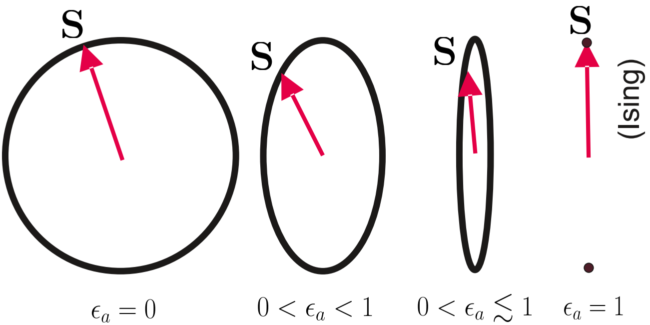
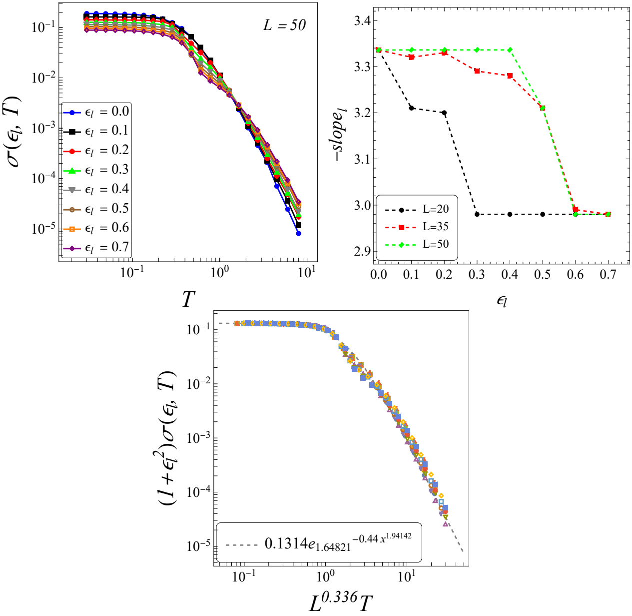
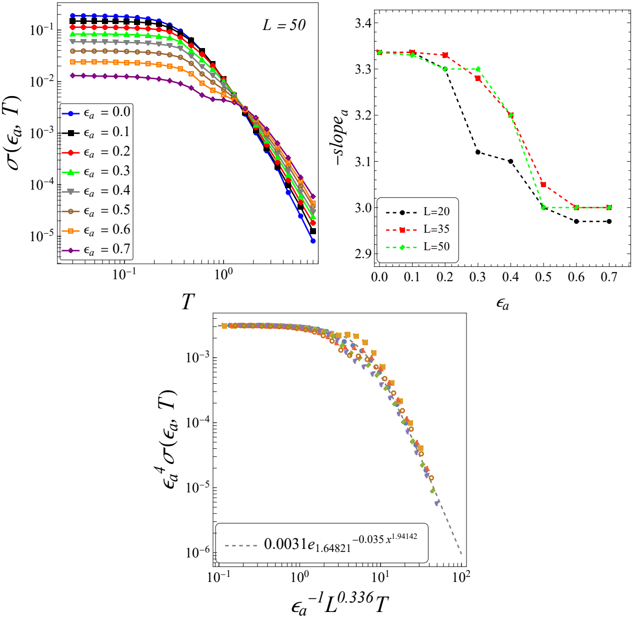


Figure: Schematic representation of the anisotropic XY coupling.



L = 50
σ(ϵl, T)
T
ϵl = 0.0
ϵl = 0.1
ϵl = 0.2
ϵl = 0.3
ϵl = 0.4
ϵl = 0.5
ϵl = 0.6
ϵl = 0.7
−slopel
ϵl
L=20
L=35
L=50
(1+ϵl2)σ(ϵl, T)
L0.336T
0.1314e1.64821−0.44 x1.94142



L = 50
ϵa = 0.0
ϵa = 0.1
ϵa = 0.2
ϵa = 0.3
ϵa = 0.4
ϵa = 0.5
ϵa = 0.6
ϵa = 0.7
σ(ϵa, T)
T
−slopea
L=20
L=35
L=50
ϵa
ϵa4σ(ϵa, T)
0.0031e1.64821−0.035 x1.94142
ϵa−1L0.336T

Results

Indeed, the same approach previously used remains true for the Ising chain, and the Fourier's law is obeyed, with $\kappa_{Ising} \sim T^{-3}$.

Heisenberg chain

Heisenberg model

The one-dimensional classical inertial Heisenberg model, for a system of L interacting rotators, is defined by the Hamiltonian,

$$\mathcal{H} = \frac{1}{2}\sum_{i=1}^{L} \boldsymbol{\ell}_i^2 + \frac{1}{2}\sum_{\langle ij \rangle} \left(1 - \mathsf{S}_i \cdot \mathsf{S}_j\right) \ , \tag{16}$$

where $\boldsymbol{\ell}_i \equiv (\ell_{ix}, \ell_{iy}, \ell_{iz})$ and $\mathsf{S}_i \equiv (S_{ix}, S_{iy}, S_{iz})$ represent, respectively, continuously varying angular momenta and spin variables at each site of the linear chain.

- Spins present unit norm, $\mathsf{S}_i^2 = 1$;
- Each site angular momentum $\boldsymbol{\ell}_i$ must be perpendicular to S_i, yielding $\boldsymbol{\ell}_i \cdot \mathsf{S}_i = 0$.

Heisenberg chain

Equations of motion

All remaining rotators ($i = 2, \cdots, L-1$) follow their usual equations of motion

$$\begin{aligned} \dot{\mathsf{S}}_i &= \boldsymbol{\ell}_i \times \mathsf{S}_i \ , \\ \dot{\boldsymbol{\ell}}_i &= \mathsf{S}_i \times (\mathsf{S}_{i+1} + \mathsf{S}_{i-1}) \ , \end{aligned} \tag{17}$$

whereas the rotators at extremities follow standard Langevin dynamics,

$$\begin{aligned} \dot{\boldsymbol{\ell}}_1 &= -\gamma_h \boldsymbol{\ell}_1 + \mathsf{S}_1 \times \mathsf{S}_2 + \boldsymbol{\eta}_h \ , \\ \dot{\boldsymbol{\ell}}_L &= -\gamma_l \boldsymbol{\ell}_L + \mathsf{S}_L \times \mathsf{S}_{L-1} + \boldsymbol{\eta}_l . \end{aligned} \tag{18}$$

Heisenberg chain

Equations of motion

The condition of a constant norm for the spin variables yields

$$\frac{dS_i}{dt} = \frac{d\left(\mathsf{S}_i \cdot \mathsf{S}_i\right)^{1/2}}{dt} = 0 \quad \Rightarrow \quad \mathsf{S}_i \cdot \dot{\mathsf{S}}_i = 0 \ , \tag{19}$$

which should be used together with $\boldsymbol{\ell}_i \cdot \mathsf{S}_i = 0$ in order to eliminate $\ddot{\boldsymbol{\ell}}_i$ and calculate $\ddot{\mathsf{S}}_i$ from Eqs. (17) and (18). One has for rotators at sites $i = 2, \cdots, L-1$,

$$\ddot{\mathsf{S}}_i = (\mathsf{S}_{i+1} + \mathsf{S}_{i-1}) - \left[\mathsf{S}_i \cdot (\mathsf{S}_{i+1} + \mathsf{S}_{i-1}) + \dot{\mathsf{S}}_i^2\right] \mathsf{S}_i \ , \tag{20}$$

whereas for those at extremities,

$$\begin{aligned} \ddot{\mathsf{S}}_1 &= -\dot{\mathsf{S}}_1 + \mathsf{S}_2 - \left[\mathsf{S}_1 \cdot \mathsf{S}_2 + \dot{\mathsf{S}}_1^2\right] \mathsf{S}_1 + \mathsf{S}_1 \times \boldsymbol{\eta}_h \ , \\ \ddot{\mathsf{S}}_L &= -\dot{\mathsf{S}}_L + \mathsf{S}_{L-1} - \left[\mathsf{S}_L \cdot \mathsf{S}_{L-1} + \dot{\mathsf{S}}_L^2\right] \mathsf{S}_L + \mathsf{S}_L \times \boldsymbol{\eta}_l \ . \end{aligned} \tag{21}$$

Heisenberg chain

Heat flux

The rotators at the bulk (i$= 2, \cdots, L-1$) follow a continuity equation,

$$\frac{dE_i}{dt} = -(J_i - J_{i-1}) \ , \tag{22}$$

therefore, the heat flux of the Heisenberg chain is given by

$$J_i = \frac{1}{2}\left(\mathsf{S}_i \cdot \dot{\mathsf{S}}_{i+1} - \mathsf{S}_{i+1} \cdot \dot{\mathsf{S}}_i\right) \ . \tag{23}$$

Heisenberg chain

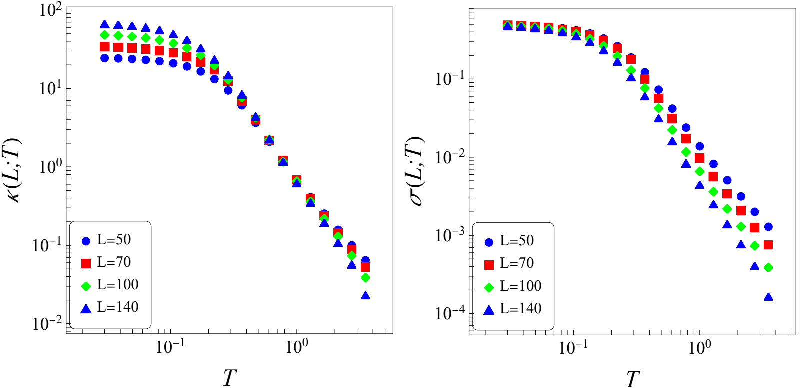


Figure: (Color online)Numerical data for the thermal conductivity [panel (a)] and thermal conductance [panel (b)] are represented versus temperature (log-log plots) for different sizes ($L = 50, 70, 100, 140$) of the one-dimensional classical inertial Heisenberg model.

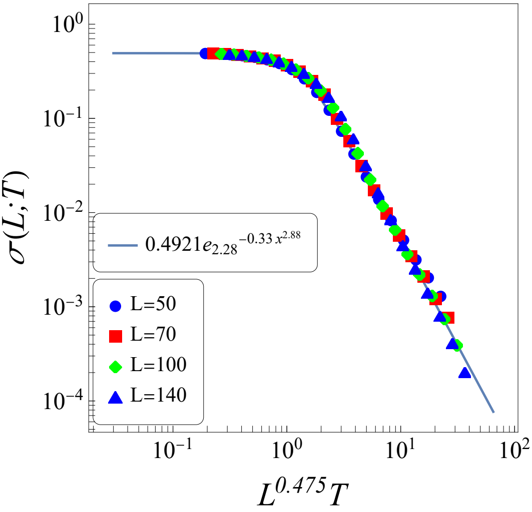


Figure: The plots for the thermal conductance of Fig. 5(b) are shown in a log-log representation, for a conveniently chosen abscissa ($x = L^{0.475}T$), leading to a collapse of data for all values of L considered.

Results

It also remains true for the Heisenberg chain, and the Fourier's law is obeyed, with $\kappa_{Heisenberg} \sim T^{-2.25}$.

Final remarks

- The Fourier's law is obeyed for $n = 1, 2, 3$ vector models;
- The q-stretched exponential provides a good explanation of all temperature regimes, mainly at high temperature regimes;
- The relation $\gamma\eta/(q-1) = 1$ is a necessary condition to this law holds;
- It opens a question about the validation of this law in systems with generic-range interactions, as α-XY model;
- Since nonextensive statistical mechanics has been used in the description of a wide variety of complex systems, one expects that the present results should be applicable to many of these systems in diverse non-equilibrium regimes.

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