Ising chain: Thermal conductivity and first-principle validation of Fourier's law

Henrique Santos Lima[1], Constantino Tsallis[1,2,3]

[1]Centro Brasileiro de Pesquisas Físicas and National Institute of Science and Technology of Complex Systems, Rua Xavier Sigaud 150, Rio de Janeiro-RJ 22290-180, Brazil

[2]Santa Fe Institute, 1399 Hyde Park Road, Santa Fe, New Mexico 87501, USA

[3]Complexity Science Hub Vienna, Josefstädter Strasse 39, 1080 Vienna, Austria

Introduction

- Fourier's law [1] describes the heat diffusion rate through a macroscopic material in the direction of the flow ($\mathbf{J} \propto -\nabla T$);
- In this work two types of anisotropic planar rotators are studied through molecular dynamics;
- We approach, for a linear chain, the Ising limit via two different types of extremely anisotropic XY models (local and in the coupling), which allowed us to evaluate the validity of the Fourier's law;
- Furthermore, we better characterized the conductivity change for a more extended range of temperatures, resulting in the q-stretched exponential [2] instead of the q-Gaussian distribution [3] .

Models

- The Hamiltonians of the local and anisotropic coupling models are, respectively, given by

$$\mathcal{H}_{XY}^{l} = \sum_{i=1}^{L} \frac{p_i^2}{2} + \frac{1}{2} \sum_{\langle i,j \rangle} [1 - \cos(\theta_i - \theta_j)] + \epsilon_l \sum_{i=1}^{L} \sin^2 \theta_i \quad (1)$$

and

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

where $\epsilon_l \in [0, \infty)$ and $\epsilon_a \in [-1, 1]$;

- $\epsilon_a = \pm 1$ correspond to the Ising model along the y and x axes respectively, whereas $\epsilon_a = 0$ recovers the standard isotropic XY -model (see Fig. 1);
- We have considered unit momenta of inertia and unit first-neighbor coupling constant;

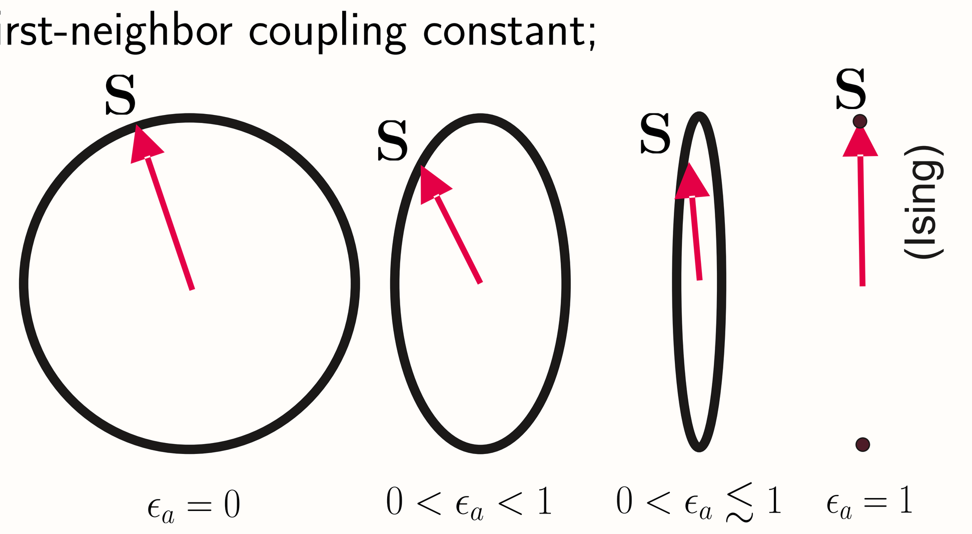

Figure 1: Schematic representation of the anisotropic XY coupling.

Methods

- The dynamical evolution were conducted using Velocity-Verlet algorithm [4] with step size $dt = 0.01$;
- The transient time : 10^{10} (10^{8} time units) ;
- After transient the average of the heat flux is realized for 4×10^{8} time steps (4×10^{6} time units) ;
- We set $T_{h/l} = T(1 \pm \Delta)$ with $\Delta = 0.125$, where T is the average temperature ;
- The average is taken over 80 experiments ($80 \times 4 \times 10^{8}$ time steps);
- The macroscopic conductivity κ is given by $\kappa = \frac{J}{(T_h - T_l)/L}$ where $J = \langle J_i \rangle$;
- The Lagrangian fluxes for local and anisotropic coupling are $J_i = \frac{1}{2}(p_i + p_{i+1}) \sin(\theta_i - \theta_{i+1})$ and $J_i = \frac{p_i + p_{i+1}}{2} \sin(\theta_i - \theta_{i+1}) + \epsilon_a \frac{p_i - p_{i+1}}{2} \sin(\theta_i + \theta_{i+1})$, respectively.

Results

- The present numerics at a wider range of T are proportional to stretched q-exponential whose definition $y(x) = e_q^{-B|x|^{\eta}}$ with $q \geq 1$, $\eta > 0$ and $B > 0$. The q-Gaussian [5] form is recovered as the $\eta = 2$ particular limit;
- Consistently with this Ansatz, we verify that, in the thermodynamic limit ($L \gg 1$), $\sigma(\epsilon_l, T) \propto \sigma(\epsilon_a, T) \propto T^{-\frac{\eta}{q-1}}$, where $(\eta, q) \approx (1.94, 1.65)$ thus yielding the slope $\eta/(q-1) \approx 3.0$ (see Figs. 2 and 3).

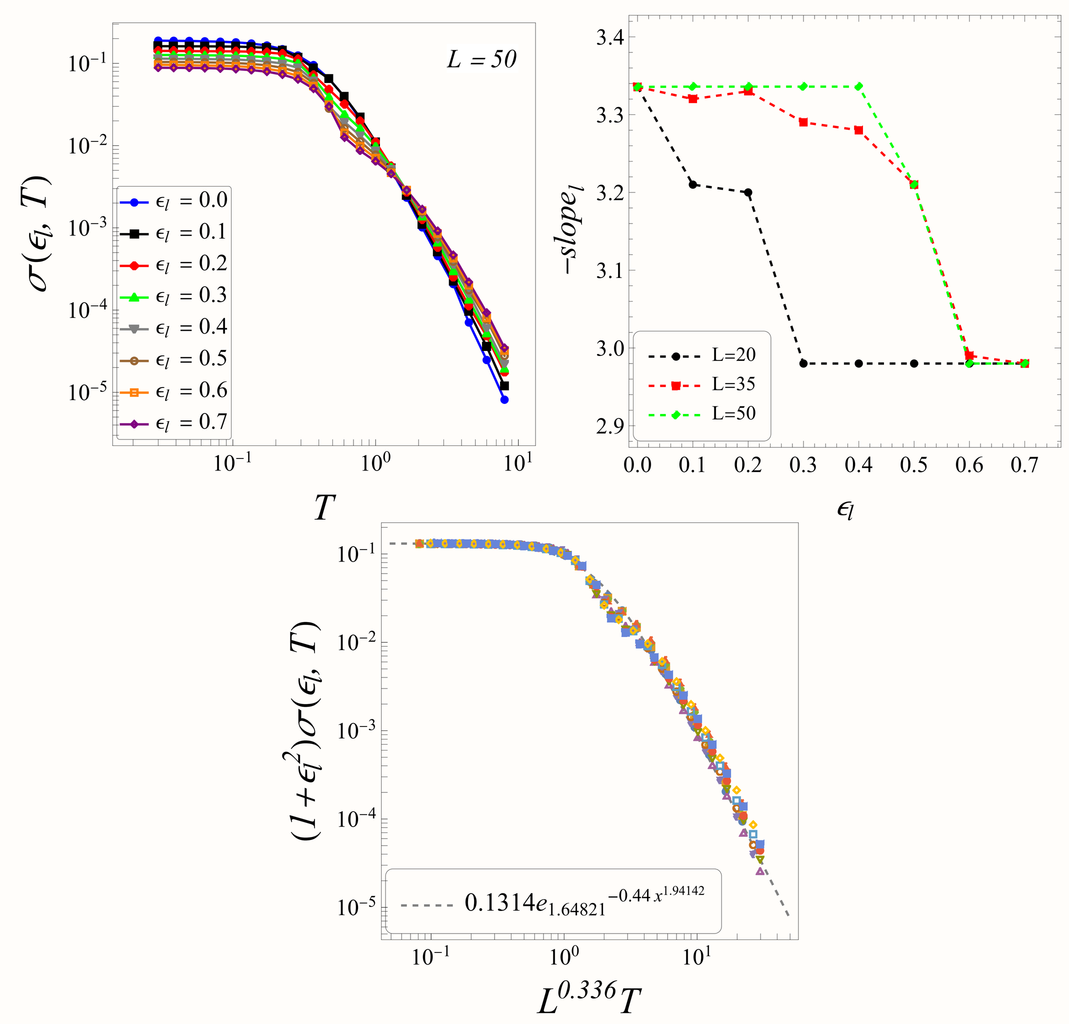

Figure 2: *Left:* Thermal conductance of the first anisotropic model as a function of temperature for one-dimensional lattice structure and the local coupling constant for $L = 50$. *Center:* Plot of -slope versus ϵ_l for $L = 20, 35, 50$. All the curves approach the same saturation value $slope_l \simeq -3.0$. *Right:* Collapse with a stretched q-exponential form, from $\epsilon_l = 0.4$ to $\epsilon_l = 0.7$ with $L = 20, 35, 50$. The values of the minimum (T_{min}) and maximum (T_{max}) temperatures are 0.03 and 8.0 respectively.

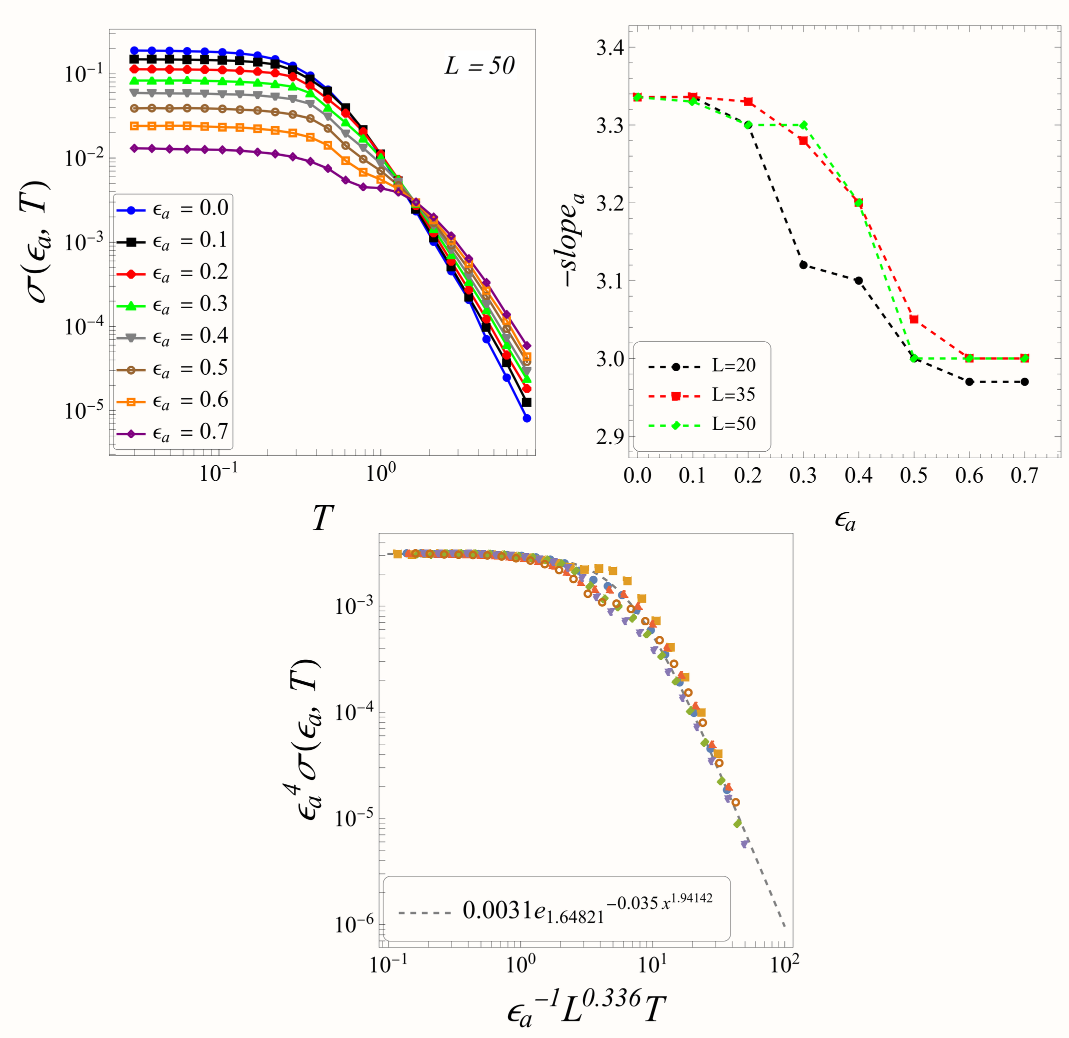

Figure 3: *Left:* Thermal conductance of the second anisotropic model as a function of temperature for one-dimensional lattice structure and the local coupling constant for $L = 50$. *Center:* Plot of -slope versus ϵ_a for $L = 20, 35, 50$. All the curves approach the same saturation value $slope_a \simeq -3.0$. *Right:* Collapse with a stretched q-exponential form, for $\epsilon_a = 0.6$ and $\epsilon_a = 0.7$ with $L = 20, 35, 50$. The values of the minimum (T_{min}) and maximum (T_{max}) temperatures are 0.03 and 8.0 respectively.

Conclusion

- Fourier's law is microscopically shown to be satisfied for the two types of anisotropic XY-models;
- A closed formula is obtained for the thermal conductivity for finite lattice sizes at arbitrary temperatures;
- In the limit of extreme anisotropy, both models approach the Ising model and its thermal conductivity κ, which, at high temperatures, scales like $\kappa \sim T^{-3}$;
- This behavior reinforces the result obtained in various d-dimensional models, namely $\kappa \propto L\, e_q^{-B(L^{\gamma}T)^{\eta}}$ where $e_q^z \equiv [1 + (1-q)z]^{\frac{1}{1-q}}$ ($e_1^z = e^z$), L being the linear size of the d-dimensional macroscopic lattice;
- The scaling law $\frac{\eta\gamma}{q-1} = 1$ guarantees the validity of Fourier's law, for all dimensions.

Acknowledgments

We acknowledge fruitful discussions with U. Tirnakli and D. Eroglu, useful remarks from U. B. de Almeida and L. M. D. Mendes, as well as partial financial support by CNPq and FAPERJ (Brazilian agencies). We also acknowledge LNCC (Brazil) for allowing us to use the Santos Dumont (SDumont) supercomputer.

References

[1] J.B.J. Fourier, *Théorie analytique de la chaleur*, (Paris, Firmin Didot Père et Fils, 1822).

[2] C. Tsallis, H.S. Lima, U. Tirnakli, and Deniz Eroglu, *First-principle validation of Fourier's law in d = 1, 2, 3 classical systems*, Phys. D: Nonlinear Phenom., 446, 133681 (2023).

[3] Y. Li, N. Li, U. Tirnakli, B. Li and C. Tsallis, *Thermal conductance of the coupled-rotator chain: Influence of temperature and size*, EPL **117**, 60004 (2017).

[4] L. Verlet, *Computer experiment on classical fluids. I. Thermodynamical properties of Lennard-Jones molecules*, Phys. Rev. **159**, 98 (1967).

[5] C. Tsallis, *Entropy*, Encyclopedia **2**, 264-300 (2022).

[6] H. S. Lima, C. Tsallis, *Ising chain: Thermal conductivity and first-principle validation of Fourier's law*, Phys. A: Stat. Mech. Appl., 129161 (2023).