Thermal gradients and Energy equipartition - numerical and theoretical

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Scientific context

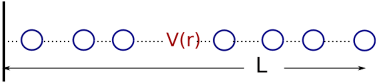
Framework developed during RareNoise project, which comprised a large team over the years:
L. Conti, L. Rondoni, M. Bonaldi, M. Borrielli, C. Lazzaro, G. Karapetyan, M. Pegoraro, P. Adamo, R.-K. Takhur, R. Belousov.
R. Hajj, C. Poli, A.B. Gounda, S. Longo, M. Saraceni

FP7 - IDEAS - ERC grant agreement n. 202680
INFN Padova - INFN Torino - CNR Trento

Outline

- A deterministic, dynamical simulation model of a 1d rod.
- Realistic equilibrium "canonical" thermoelastic properties.
- Nonequilirbium thermoelastic properties.
- Vibrational modes in and out of equilibrium: failure of the vibrational "thermometer"?

Modelling hard rods with one-dimensional chains - equilibrium



L=L(t) is the observable

Defined a variation of the celebrated FPUT chain:

$$V_t(x) \quad = \quad h\left[(x-1)^2 - \lambda(x-1)^3 + \mu(x-1)^4\right]$$

and compared it to a more 'phenomelogical' interaction potential

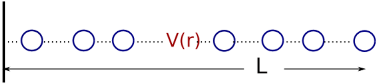
$$V_{LJ}(x) = \epsilon\left(x^{-12} - 2\,x^{-6}\right) \qquad x = r/r_0$$

$$m\ddot{r}_i \quad = \quad -\frac{\partial V(|r_i - r_{i+1}|)}{\partial r_i} - \frac{\partial V(|r_i - r_{i-1}|)}{\partial r_i} - \chi\dot{r}_i$$

deterministic dynamics

$$\dot{\chi} \quad = \quad \frac{m}{\tau^2}\left(\frac{K}{k_B T} - 1\right); \qquad K(t) = \frac{m}{N}\sum_{j=1}^{N}\dot{r}_j(t)^2; \qquad i = 1,\cdots,N,\ \ r_{N+1} \equiv r_N + R_0$$

Modelling hard rods with one-dimensional chains - equilibrium



$L = r_N$ as the observable

In a second variation, only the two ends are in contact with a thermostat.
$T_{Left} = T_{Right} = T$ at equilibrium.

$$m\ddot{r}_i = -\frac{\partial V(|r_i - r_{i+1}|)}{\partial r_i} - \frac{\partial V(|r_i - r_{i-1}|)}{\partial r_i}$$

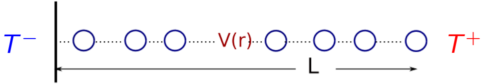
$$i = 2, \cdots, N-1$$

$$m\ddot{r}_i = -\frac{\partial V(|r_i - r_{i+1}|)}{\partial r_i} - \frac{\partial V(|r_i - r_{i-1}|)}{\partial r_i} - \chi_i \dot{r}_i$$

$$\dot{\chi}_i = \frac{m}{\tau^2}\left(\frac{K_i}{k_B T} - 1\right); \qquad K_i(t) = m\dot{r}_i(t)^2;$$

$$i = 1, N.$$

Modelling hard rods with one-dimensional chains - nonequilibrium



$T_{Left} = T^-$, $T_{Right} = T^+$. A linear T profile forms.

$$m\ddot{r}_i = -\frac{\partial V(|r_i - r_{i+1}|)}{\partial r_i} - \frac{\partial V(|r_i - r_{i-1}|)}{\partial r_i}$$

$$i = 2, \cdots, N-1$$

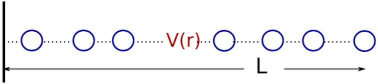
$$\begin{aligned}
m\ddot{r}_i &= -\frac{\partial V(|r_i - r_{i+1}|)}{\partial r_i} - \frac{\partial V(|r_i - r_{i-1}|)}{\partial r_i} - \chi_i \dot{r}_i; \qquad i = 1, N \\
\dot{\chi}_1 &= \frac{m}{\tau^2}\left(\frac{K_1}{k_B T^-} - 1\right); \qquad K_1(t) = m\dot{r}_1(t)^2; \\
\dot{\chi}_N &= \frac{m}{\tau^2}\left(\frac{K_N}{k_B T^+} - 1\right); \qquad K_N(t) = m\dot{r}_N(t)^2;
\end{aligned} \tag{1}$$

Modelling hard rods with one-dimensional chains

For technical reasons (stability of the chain and so on), in some instances the interaction is also with second-neighbors, and two particles at each end are thermostatted.

We should not be concerned with such modification in any important sense.

Modelling hard rods with one-dimensional chains - equilibrium

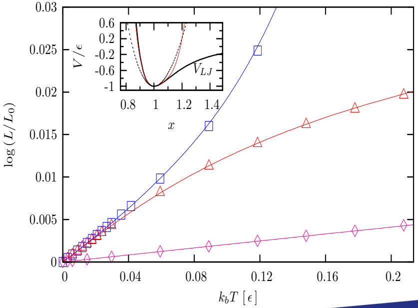


$L = r_N$ as the observable

Symbols for simulations, solid line for theory.

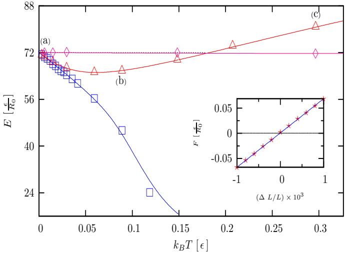
Derived the theoretical results exploiting the canonical distribution.
$\psi_i = e^{-V(|r_{i+1} - r_i|)/k_B T}$

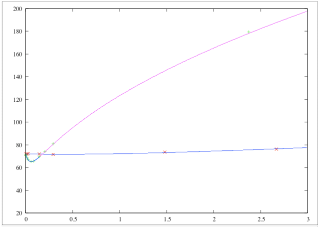
PDG, L RONDONI, M BONALDI, L CONTI, PRB 84, 224103 (2011)

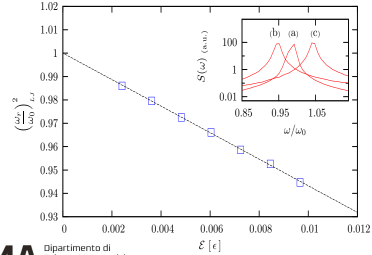


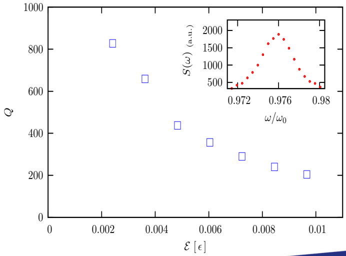
Modelling hard rods with one-dimensional chains - equilibrium

E, the elastic modulus: $F \simeq E\,(\Delta L/L)$, if $\Delta L \ll L$. ω_0 resonance frequency of 1st mode. $Q = \omega_0/\Delta\omega_{1/2}$

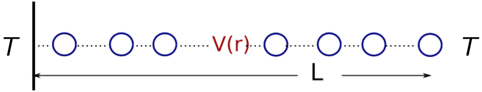


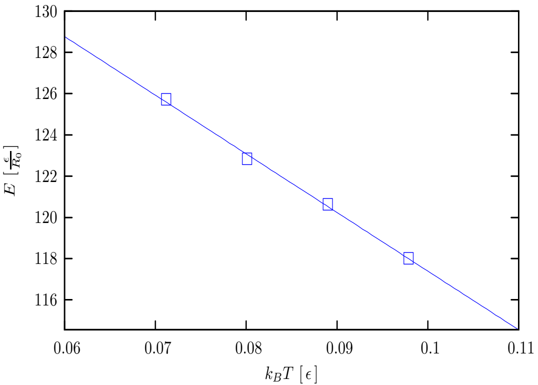




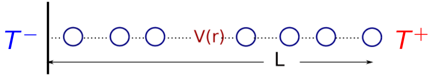


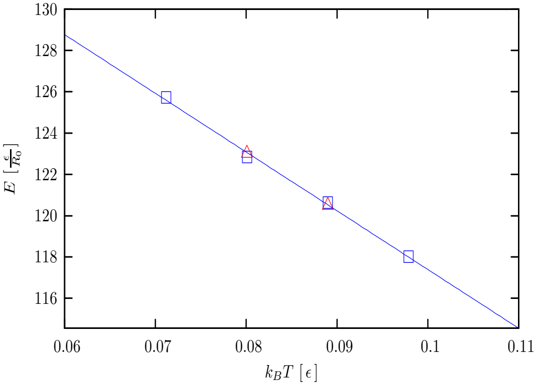
Elastic constant LJ model - equilibrium





Elastic constant LJ model - nonequilibrium





From simulations, and from theory assuming configurations are locally canonical

$$\psi_i = e^{-V(|r_{i+1}-r_i|)/k_B T_i} \quad \Rightarrow \quad E^{-1} = \sum_i E_i^{-1} L_i/\overline{L} \quad \underset{\Delta E \ll \overline{E}}{\Rightarrow} \quad E \lesssim \overline{E}$$

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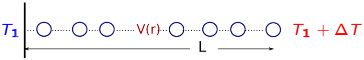
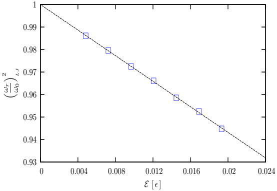
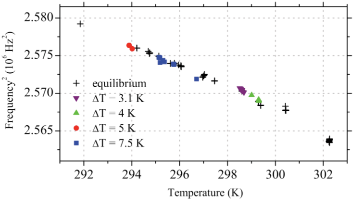
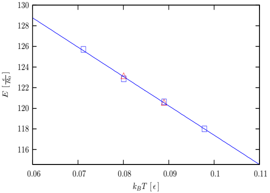
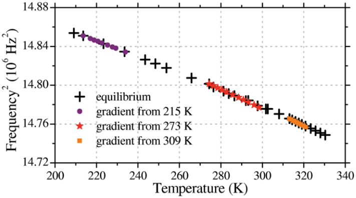
Elasticity - nonequilibrium simulations and RareNoise experiments











L. CONTI, PDG, M. BONALDI, A. BORRIELLI et al., PRE 85, 066605 (2012)

DISMA Dipartimento di Scienze Matematiche G. L. Lagrange
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Nonequilibrium thermo-elastic properties

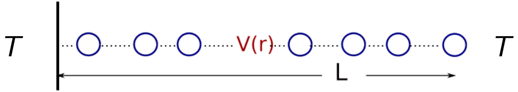
Elasticity and temperature

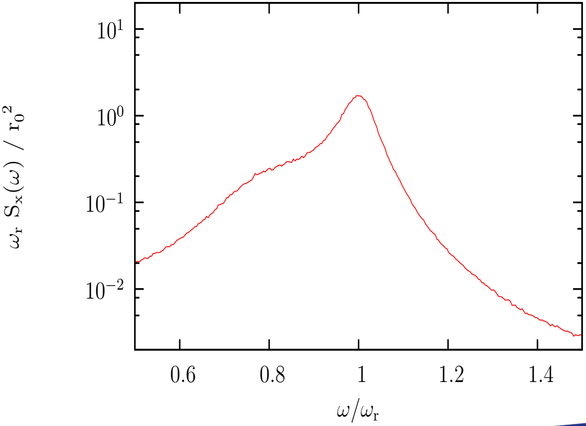
1. 1D model reproduces nice (real) thermo-elastic properties at equilibrium, e.g. linearity of elastic modulus E or of ω_{res}^2 with T.
2. It does so also (for not too large ΔT's) out of equilibrium.
3. It also agrees with experiments that out of equilibrium $\omega_r = \omega_r(\overline{T})$, with average temperature $\overline{T} = (T_1 + T_2)/2$ and $\omega_r(T)$ the equilibrium resonance frequency. (one possible explanation is that local equilibrium applies)
4. I.e., the resonance frequency is a good "thermometer" also out of equilibrium.

Vibrational modes

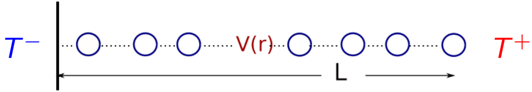
1. While thermo-elastic quantities are obtained after integrating over all degrees of freedom, a vibrational mode is one single degree of freedom.
2. Is the energy associated to any vibrational mode also a good thermometer?

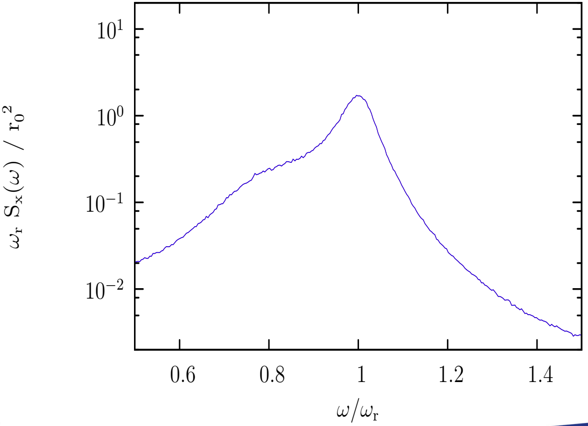
Simulations - Power spectrum of $L(t)$ around first resonance





Effects of growing gradients: $\nabla T \uparrow$ at same $\overline{T}$





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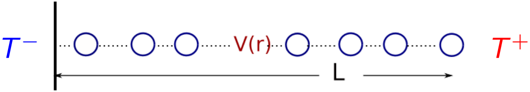

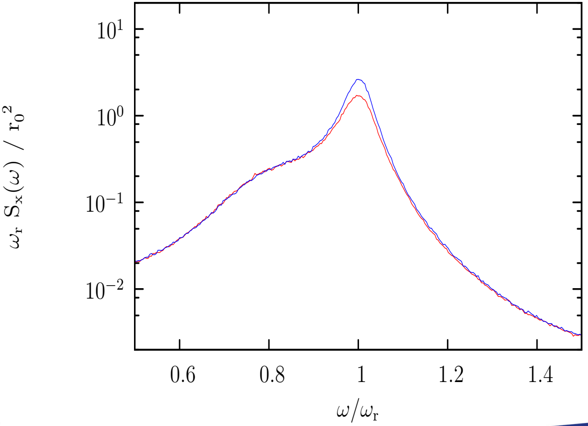

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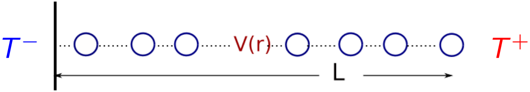

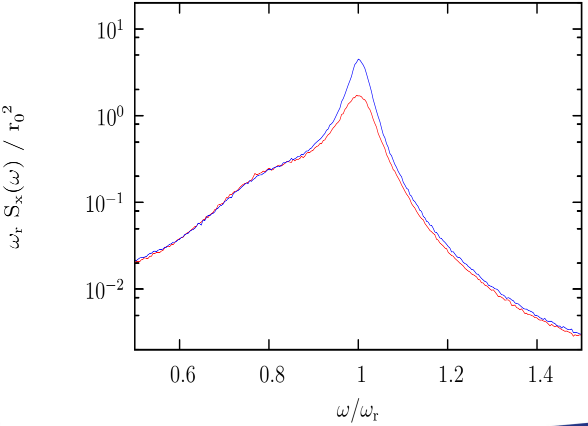

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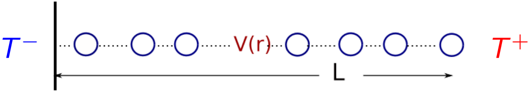

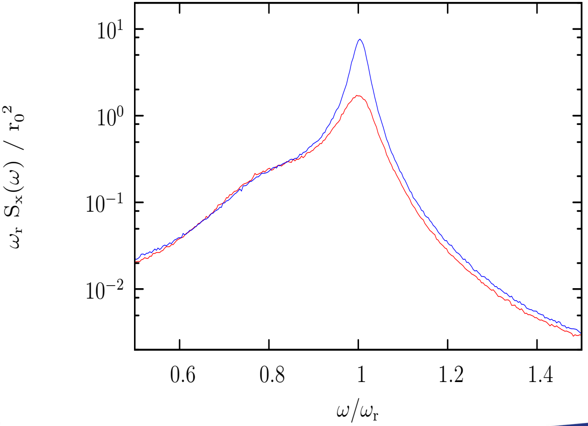

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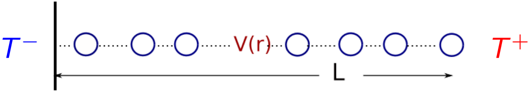
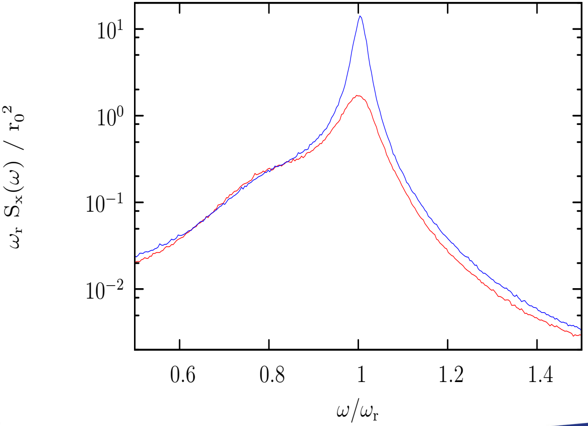
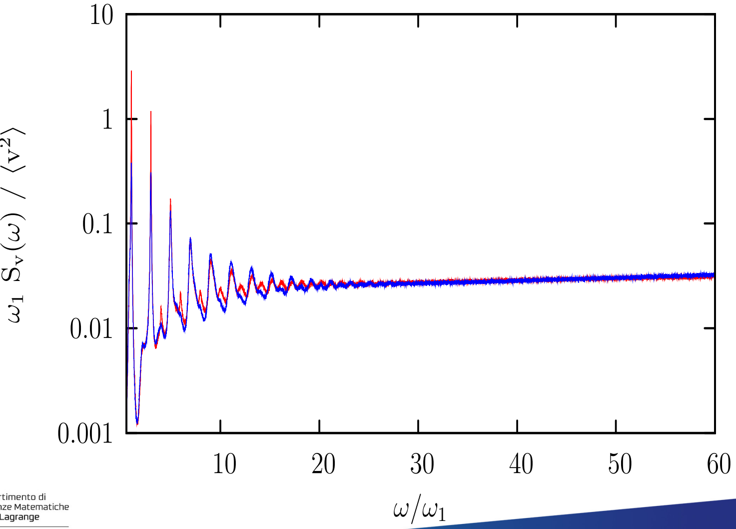




Moving body thermostatted at T^+, effect must fade out at high freq.



Normal mode expansion and canonical distribution

High Q-factor $\Rightarrow$ Dynamics as if the sum of independent damped oscillators forced by thermal noise ($S_v(\omega)$ the sum of Lorentzian curves).

The equilibrium distribution is canonical and independent of the damping, think of e.g. Langevin, Fokker-Planck.

$\Rightarrow$ H appearing in the Boltzmann weight is diagonal in the normal mode variables, like if we had independent harmonic oscillators.

$$P(\mathbf{x}, \mathbf{v}) = \frac{\exp\left[-H(\mathbf{x}, \mathbf{v})/k_B T\right]}{Z}; \qquad H = \frac{1}{2}\sum_i \mu_i(\omega_i^2 x_i^2 + v_i^2)$$

Notice: x's and v's here are not the positions and velocities of the particles in the chain. They are the variables obtained from them after a rotation.

Normal mode expansion as an equilibrium ‘thermometer’

Therefore we can actually average the modes separately

$$P(\mathbf{x},\mathbf{v}) = \frac{\exp -H(\mathbf{x},\mathbf{v})/k_B T}{Z}; \qquad H = \frac{1}{2}\sum_i \mu_i(\omega_i^2 x_i^2 + v_i^2)$$

$$\Downarrow$$

$$\langle x_1^2 \rangle = \frac{k_B\, T}{\mu_1\, \omega_1^2} \qquad \omega_1 = \omega_{res}$$

T ideally is the actual physical temperature, and approximately so in the experiment. μ_1 the reduced mass.

Can we plugin $\overline{T}$ for T out of equilibrium?

One possible explanation - mode-mode correlations

Not yet really a comprehensive theory (it does not account for T-profiles).

(In search of a comprensive theory that accounts for both local equilibrium and correlations due to energy fluxes)

In 1D models, a current $J \neq 0$ means $\langle x_i v_j \rangle \neq 0$ for some i, j.
(it applies to both NN coordinates and **therefore** normal-modes variables)

Hyp.: Suppose we have $\boxed{H/k_B T \to H/k_B T + \gamma J}$ in Boltzmann factor, which implies $\langle x_i v_j \rangle \neq 0$, and apply same rotation as before.

Miller, Larson, PRA 20, 1717 (1979) Kato, Jou, PRE 64, 052201:1 (2001)

$$J = -\frac{1}{N} \sum_{i \neq k}^{1,N} j_{ik}\, x_i v_k$$

One possible explanation - mode-mode correlations

We make a simpler assumption, implied by it, but more general.

$$P_{NEQ}(x_1, w) = \exp\left(-\mu_1\omega_1^2\ x_1^2/2k_BT - \mu^*\ w^2/2k_BT + \lambda\mu_1\omega_1^2\ x_1 w\right)$$

The correction carried by the mode-mode correlations

$$\langle x_1^2 \rangle = \frac{\eta}{\eta - \lambda(\phi)^2} \langle x_1^2 \rangle_{eq}; \qquad \eta = \frac{\mu^*}{\mu_1 \omega_1^2 (k_B T)^2}$$

$$\lambda(\phi) = \frac{1}{2\phi}(1 - \sqrt{1 + 4\eta\phi^2})$$

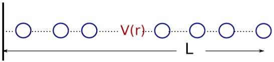
$$\langle x_1^2 \rangle \simeq \langle x_1^2 \rangle_{eq} (1 + \eta\,\phi^2); \qquad |\phi| \ll 1/\sqrt{\eta}$$

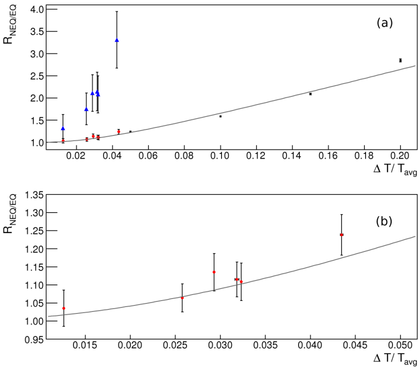
$$\langle x_1^2 \rangle \simeq \langle x_1^2 \rangle_{eq} \sqrt{\eta}\,|\phi|; \qquad |\phi| \gg 1/\sqrt{\eta}$$

ϕ the mode-mediated heat rate. If $\phi \propto \Delta T$, then

$$\frac{\langle x_1^2 \rangle}{\langle x_1^2 \rangle_{eq}} - 1 \propto (\Delta T)^2 \qquad \Delta T \ll T$$

Agreement theory+simulations+experiment





L CONTI, PDG, G KARAPETYAN, C LAZZARO, M PEGORARO, M BONALDI, L RONDONI, J.Stat.Mech. 1312 (2013), P12003

Thank you for the attention

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