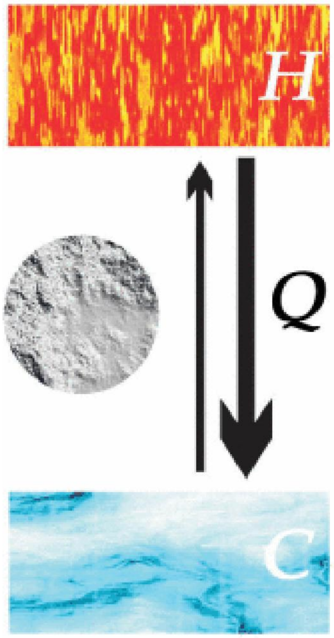

Thermostatistical idiosyncrasies of small non-linear mechanical systems

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Plan

- Introduction

- Model and analytic approach

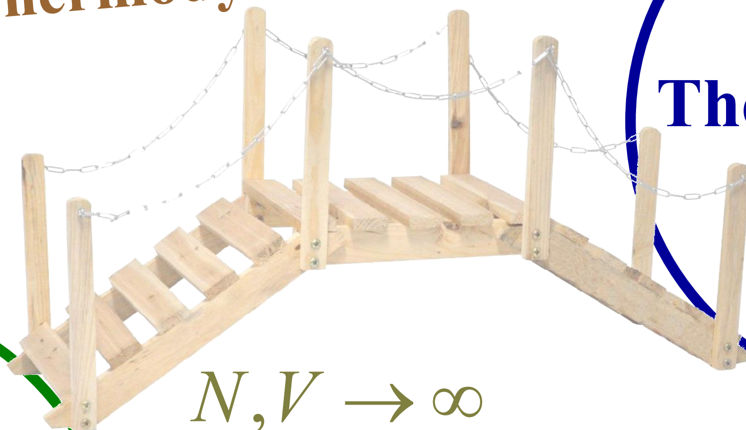
- Business (almost) as usual: the Gaussian case

- Introducing Poissonian reservoirs;

-Concluding Remarks.

Introduction

Thermodynamic Limit



Thermodynamics

Equilibirum Statistical Mechanics

$$N, V \to \infty$$

$$n \equiv \frac{N}{V} = const.$$

observable $\mathscr{O}_N \equiv \mathscr{O}(N; V, \ldots)$

$$\lim_{N\to\infty} \frac{\sqrt{\langle \mathscr{O}_N^2 \rangle - \langle \mathscr{O}_N \rangle^2}}{\langle \mathscr{O}_N \rangle} = 0.$$ 'Corollary':

We can get rid of the average notation in formulae and simply use quantitative relations between observables *tout court*.

Examples:

The first of thermodynamics,

$$\Delta U = Q + \sum_i W_i \qquad (U_0 = 0)$$

Work done during an irreversible process (proxy for the second law),

$$W_{A \to B} \le F_A - F_B \qquad (F = U - T\,S)$$

but what if the system does not hold the thermodynamic limit?

For a mammoth system undergoing an irreversible transformation from state *A* to *B* one will get, without a shadow of a doubt,

$$W_{A\to B} < F_A - F_B$$

However, if the system is rather small, although,

$$\langle W_{A\to B}\rangle \leq F_A - F_B$$

there will be a number of times that in performing a change alike one will measure,

$$W_{A\to B} \geq F_A - F_B \qquad !!!!$$

Thence: for small systems we need a probabilistic approach.

For the present case solved by the Jarzynski equality,

$$\langle \exp[-\beta W]\rangle = \exp\left[\beta\left(F_A - F_B\right)\right]$$

previous approaches by Bochkov and Kuzovlev

The model

Following* C. Jarzynski *when we study the thermostatistical behaviour of a small system there is a need to detail the equations governing its evolution.

Classical 1-D massive particle the dynamics of which is ruled by,

$$\dot{x}(t) = v(t),$$

$$m\,\ddot{x}(t) = -k_1\,x(t) - k_3 x^3(t) - \gamma \dot{x}(t) + \eta(t).$$

Dissipation

(Pseudo) Force representing the interaction of the system with a reservoir

Confining potential (permits stationary solutions)

A statistical mechanics problem aims at making predictions by computing probabilities and cumulants, often in the steady state.

How can we do it?

I – Hammering away at the "Kramers equation" and get the PDFs (which can be a pain in the bottom of the back).

II – Considering a time averaging approach (which easily turns into a pain in the neck)

Redundant with the Kramers equation approach for Brownian reservoirs

BUT

Outperforms the "Kramers equation" for non-Brownian reservoirs as Fokker-Planck methods are generally poor approximations to the actual solution.

Other 'pain prone' methods might be chosen as well, *e.g.*, Cáceres & Budini (1997) and Kanazawa, Sagawa & Hayakawa (2012).

Average steady state

$$p_{ss}(x,v) = \lim_{z\to 0} z \int_0^\infty dt\, e^{-zt} < \delta(x - x(t))\delta(v - v(t)) > .$$

Or

$$p_{ss}(x,v) = \sum_{n,m=0}^{\infty} \int_{-\infty}^{+\infty} \frac{\mathrm{d}Q}{2\pi} \frac{\mathrm{d}P}{2\pi} \mathrm{e}^{\mathrm{i}(Qx+Pv)} \frac{(-\mathrm{i}Q)^n}{n!} \frac{(-\mathrm{i}P)^m}{m!} \overline{\langle x^n v^m \rangle}$$

$$= \int_{-\infty}^{+\infty} \frac{\mathrm{d}Q}{2\pi} \frac{\mathrm{d}P}{2\pi} \mathrm{e}^{\mathrm{i}(Qx+Pv)} \exp\left\{ \sum_{n,m=0:(m+n>0)}^{\infty} \frac{(-\mathrm{i}Q)^n}{n!} \frac{(-\mathrm{i}P)^m}{m!} \overline{\langle x^n v^m \rangle_c} \right\}.$$

Business as usual: Gaussian reservoirs

$$< \eta(t_1) \dots \eta(t_n) >_c = 0 \quad (\text{if } n \neq 2),$$

$$< \eta(t_1)\, \eta(t_2) >_c = 2\, \gamma\, T\, \delta(t_1 - t_2)$$

In this case the thermostatistical approach must be consistent with equilibrium at temperature T,

$$p_{ss}(x,v) \propto \exp\left[-\frac{1}{T}\left(m\frac{v^2}{2} + k_1 \frac{v^2}{2} + k_3 \frac{v^4}{4} \right) \right]$$

average

$$\mathcal{E} = \underbrace{Q_I}_{\text{injected heat}} + \underbrace{Q_D}_{\text{dissipated heat}} = T$$

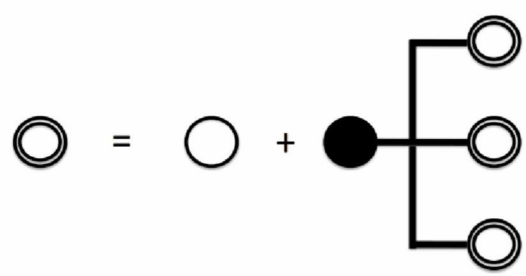
In the time averaging approach we use a Laplace transforming of the dynamical equations

$$\begin{cases} \tilde{x}(s) = \frac{\tilde{\eta}(s)}{R(s)} - \frac{k_3}{R(s)} \lim_{\epsilon \to 0^+} \int_{-\infty}^{+\infty} \frac{dq_1}{2\pi} \int_{-\infty}^{+\infty} \frac{dq_2}{2\pi} \int_{-\infty}^{+\infty} \frac{dq_3}{2\pi} \frac{\tilde{x}(\mathrm{i}\, q_1+\epsilon)\, \tilde{x}(\mathrm{i}\, q_2+\epsilon)\, \tilde{x}(\mathrm{i}\, q_3+\epsilon)}{s-(\mathrm{i}\, q_1+\mathrm{i}\, q_2+\mathrm{i}\, q_3+3\epsilon)}, \\ \tilde{v}(s) = s\, \tilde{x}(s), \end{cases}$$

$$R(s) \equiv m\, s^2 + \gamma s + k_1 = m\,(s-\zeta_+)(s-\zeta_-).$$

$$< \tilde{\eta}(s_1) \tilde{\eta}(s_2) >_c = \frac{2\,\gamma\, T}{s_1 + s_2},$$

Diagrammatically,



For the kinetic energy we read,

$$\overline{\mathcal{K}} = \frac{m}{2} \lim_{z,\epsilon\to 0} \int_{-\infty}^{\infty} \frac{dq_1}{2\pi} \int_{-\infty}^{\infty} \frac{dq_2}{2\pi} \frac{z}{z-(\mathrm{i}\,q_1+\mathrm{i}\,q_2+2\epsilon)} \langle \tilde{v}(\mathrm{i}\,q_1+\epsilon)\,\tilde{v}(\mathrm{i}\,q_2+\epsilon)\rangle\,.$$

$$= \frac{m}{2} \lim_{z,\epsilon\to 0} \int_{-\infty}^{\infty} \frac{dq_1}{2\pi} \int_{-\infty}^{\infty} \frac{dq_2}{2\pi} \frac{z}{z-(\mathrm{i}\,q_1+\mathrm{i}\,q_2+2\epsilon)} \times$$

$$\times(\mathrm{i}\,q_1+\epsilon)\,(\mathrm{i}\,q_2+\epsilon)\,\langle \tilde{x}(\mathrm{i}\,q_1+\epsilon)\,\tilde{x}(\mathrm{i}\,q_2+\epsilon)\rangle\,.$$

The calculations show that the terms arising from the non-linear contribution vanish.

$$\overline{\mathcal{K}} = \frac{m}{2} \lim_{z,\epsilon\to 0} \int_{-\infty}^{\infty} \frac{dq_1}{2\pi} \int_{-\infty}^{\infty} \frac{dq_2}{2\pi} \frac{z}{z-(\mathrm{i}\,q_1+\mathrm{i}\,q_2+2\epsilon)} \times$$

$$\times \frac{(\mathrm{i}\,q_1+\epsilon)\,(\mathrm{i}\,q_2+\epsilon)}{R(\mathrm{i}\,q_1+\epsilon)\,R(\mathrm{i}\,q_2+\epsilon)} \langle \tilde{\eta}(\mathrm{i}\,q_1+\epsilon)\,\tilde{\eta}(\mathrm{i}\,q_2+\epsilon)\rangle$$

$$= \frac{T}{2}.$$

$$\overline{\mathcal{V}} = \frac{k_1}{2} \lim_{z\to 0}\lim_{\epsilon\to 0} \int_{-\infty}^{\infty} \frac{dq_1}{2\pi} \int_{-\infty}^{\infty} \frac{dq_2}{2\pi} \frac{z}{z-(\mathrm{i}\,q_1+\mathrm{i}\,q_2+2\epsilon)} \langle \tilde{x}(\mathrm{i}\,q_1+\epsilon)\,\tilde{x}(\mathrm{i}\,q_2+\epsilon)\rangle +$$

$$+\frac{k_3}{4} \lim_{z\to 0}\lim_{\epsilon\to 0} \int_{-\infty}^{\infty} \frac{dq_1}{2\pi} \cdots \int_{-\infty}^{\infty} \frac{dq_4}{2\pi} \frac{z}{z-(\mathrm{i}\,q_1+\mathrm{i}\,q_2+\mathrm{i}\,q_3+\mathrm{i}\,q_4+4\epsilon)} \times$$

$$\times \langle \tilde{x}(\mathrm{i}\,q_1+\epsilon)\,\tilde{x}(\mathrm{i}\,q_2+\epsilon)\,\tilde{x}(\mathrm{i}\,q_3+\epsilon)\,\tilde{x}(\mathrm{i}\,q_4+\epsilon)\rangle\,,$$

$$= \frac{1}{2}T - \frac{3}{4}\frac{k_3\,T^2}{k_1^2} + 6\frac{k_3^2\,T^3}{k_1^4} + O\left(\left(\frac{k_3\,T}{k_1^2}\right)^3\right)$$

Making use of further statistical moments one can obtain the steady (equilibrium state) distribution,

$$p_{ss}(x,v) \propto \exp\left[-\frac{1}{T}\left(m\frac{v^2}{2} + k_1\frac{v^2}{2} + k_3\frac{v^4}{4}\right)\right]$$

Importing the *greeks* to a physical problem…

$$\nu \equiv \frac{\partial \overline{\mathcal{E}}}{\partial T} \approx 1 - \frac{3}{2}\frac{k_3}{k_1^2}T + 18\frac{k_3^2}{k_1^4}T^2$$

$$\rho \equiv \frac{\partial \overline{\mathcal{E}}}{\partial k_1} \approx \frac{3}{2}\frac{k_3}{k_1^3}T^2 - 24\frac{k_3^2}{k_1^5}T^3 + \frac{891}{2}\frac{k_3^3}{k_1^7}T^4,$$

$$\varrho \equiv \frac{\partial \overline{\mathcal{E}}}{\partial k_3} \approx -\frac{3}{4}\frac{T^2}{k_1^2} + 12\frac{k_3}{k_1^4}T^3 - \frac{891}{4}\frac{k_3^2}{k_1^6}T^4,$$

$$\upsilon \equiv \frac{\partial \overline{\mathcal{E}}}{\partial \gamma} = 0,$$

$$\Gamma \equiv \frac{\partial \overline{\mathcal{E}}}{\partial m} = 0,$$

$$\alpha \equiv \left(\overline{x^2}\right)^{-\frac{1}{2}} \frac{\partial \sqrt{\overline{x^2}}}{\partial T} = \frac{1}{2T} - \frac{3}{2}\frac{k_3}{k_1^2} + \frac{39}{2}\frac{k_3^2}{k_1^4}T$$

And what about the power?

$$\mathcal{E}(\Theta) \equiv \mathcal{J}_I(\Theta) + \mathcal{J}_D(\Theta) = \int_0^{\Theta} \eta(t)\, v(t)\, dt - \gamma \int_0^{\Theta} v(t)^2\, dt.$$

Because the system attains an equilibrium steady state we must verify,

$$\lim_{\Theta \gg \theta} \langle \mathcal{J}_I(\Theta) + \mathcal{J}_D(\Theta) \rangle = \langle \mathcal{E} \rangle = \overline{\mathcal{E}},$$

Analysis of the average injected power

$$\langle \mathcal{J}_{I,0}(\Theta) \rangle = \lim_{\Theta \gg \theta} \lim_{\epsilon \to 0} \int_{-\infty}^{\infty} \frac{dq_1}{2\pi} \int_{-\infty}^{\infty} \frac{dq_2}{2\pi} \frac{\exp\left[(\mathrm{i}\, q_1 + \mathrm{i}\, q_2 + 2\epsilon)\, \Theta\right]}{(\mathrm{i}\, q_1 + \mathrm{i}\, q_2 + 2\epsilon)} \times$$
$$\times\, (\mathrm{i}\, q_1 + \epsilon) \frac{1}{R(\mathrm{i}\, q_1 + \epsilon)} \langle \tilde{\eta}(\mathrm{i}\, q_1 + \epsilon)\, \tilde{\eta}(\mathrm{i}\, q_2 + \epsilon) \rangle,$$

$$= \frac{\gamma}{m} T\, \Theta$$

The non-linearity does not influence the long term behaviour of the injected power!

Analysis of the avegare dissipated power,

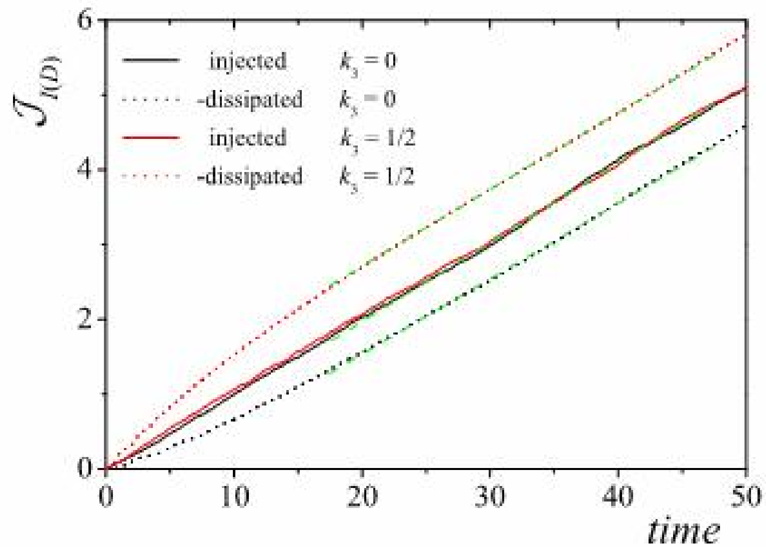
$$\langle \mathcal{J}_{D,0}(\Theta) \rangle = - \lim_{\Theta \gg \theta} \lim_{\epsilon \to 0} \gamma \int_{-\infty}^{\infty} \frac{dq_1}{2\pi} \int_{-\infty}^{\infty} \frac{dq_2}{2\pi} \frac{\exp[(\mathrm{i}\, q_1 + \mathrm{i}\, q_2 + 2\epsilon)\,\Theta] - 1}{(\mathrm{i}\, q_1 + \mathrm{i}\, q_2 + 2\epsilon)} \times$$
$$\times \frac{(\mathrm{i}\, q_1 + \epsilon)\,(\mathrm{i}\, q_2 + \epsilon)}{R(\mathrm{i}\, q_1 + \epsilon)\, R(\mathrm{i}\, q_2 + \epsilon)} \langle \tilde{\eta}(\mathrm{i}\, q_1 + \epsilon)\, \tilde{\eta}(\mathrm{i}\, q_2 + \epsilon) \rangle$$

$$= -\frac{\gamma}{m} T\,\Theta + T,$$

first order,

$$\langle \mathcal{J}_{D,1}(\Theta) \rangle = \lim_{\Theta \gg \theta} \lim_{\epsilon \to 0} \lim_{\epsilon' \to 0} \frac{2\,\gamma\, k_3}{m^5} \int_{-\infty}^{\infty} \frac{dq_1}{2\pi} \cdots \int_{-\infty}^{+\infty} \frac{dq_5}{2\pi} \times \frac{\exp[(\mathrm{i}\, q_1 + \mathrm{i}\, q_2 + 2\epsilon)\,\Theta] - 1}{(\mathrm{i}\, q_1 + \mathrm{i}\, q_2 + 2\epsilon)}$$
$$\times \frac{1}{R(\mathrm{i}\, q_1 + \epsilon)\, R(\mathrm{i}\, q_2 + \epsilon)\, \prod_{l=3}^{5} R(\mathrm{i}\, q_l + \epsilon')} (\mathrm{i}\, q_1 + \epsilon)\,(\mathrm{i}\, q_2 + \epsilon)$$
$$\times \frac{\langle \tilde{\eta}(\mathrm{i}\, q_2 + \epsilon)\, \tilde{\eta}(\mathrm{i}\, q_3 + \epsilon')\, \tilde{\eta}(\mathrm{i}\, q_4 + \epsilon')\, \tilde{\eta}(\mathrm{i}\, q_5 + \epsilon') \rangle}{(\mathrm{i}\, q_1 + \epsilon) - (\mathrm{i}\, q_3 + \mathrm{i}\, q_4 + \mathrm{i}\, q_5 + 3\epsilon')}$$

$$= -\frac{3}{4} \frac{k_3\, T^2}{k_1^2}.$$

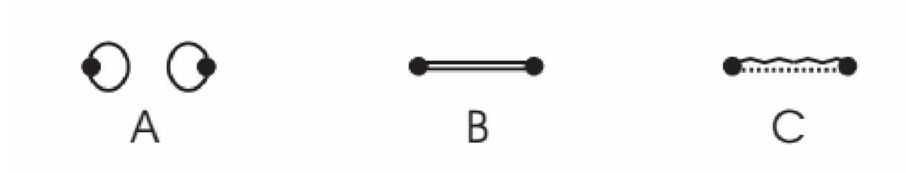


Injected and dissipated heats vs time. The parameters used are the following $k_1 = 1$, $m = 1$, $\gamma = 1/10$ and $T = 1$ and $k_3 = 0$ or $k_3 = 1/2$, *i.e.*, significantly non-linear. It is clear that after the transient both heats grow at a rate $\gamma T/m = 1/10$, which agrees with the slopes of the dashed green lines. N.B.: In order to obtain a greater separation between the curves we have set slightly different initial conditions, namely $x = 1$.

W.A.M. Morgado and SMDQ (2013)

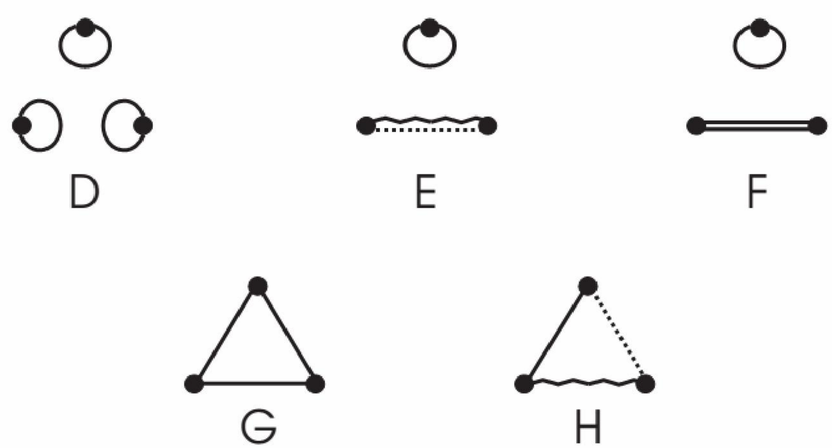
Long-term average values concur, but are the distributions equal?

$$\left\langle \mathcal{J}_I^2(\Theta) \right\rangle = \lim_{\Theta \gg \theta} \lim_{\epsilon \to 0} \int_0^\Theta dt \int_0^\Theta dt' \int_{-\infty}^{\infty} \frac{dq_1}{2\pi} \cdots \int_{-\infty}^{\infty} \frac{dq_4}{2\pi} \exp\left[(\mathrm{i}\, q_1 + \mathrm{i}\, q_2 + 2\epsilon)\, t + (\mathrm{i}\, q_3 + \mathrm{i}\, q_4 + 2\epsilon)\, t' \right] \times$$
$$\times \frac{(\mathrm{i}\, q_2 + \epsilon)\, (\mathrm{i}\, q_4 + \epsilon)}{\prod_{l=1}^{2} R(\mathrm{i}\, q_{2l} + \epsilon)} \left\langle \tilde{\eta}(\mathrm{i}\, q_1 + \epsilon)\, \tilde{\eta}(\mathrm{i}\, q_2 + \epsilon)\, \tilde{\eta}(\mathrm{i}\, q_3 + \epsilon)\, \tilde{\eta}(\mathrm{i}\, q_4 + \epsilon) \right\rangle, \qquad (26)$$



$$= \left\langle \mathcal{J}_I(\Theta) \right\rangle^2 \qquad\qquad = 0$$

For the third-order moment,



Computing further moments (and with the help of the `on-line encyclopaedia of integers and series`) we are able to find the moment generating function,

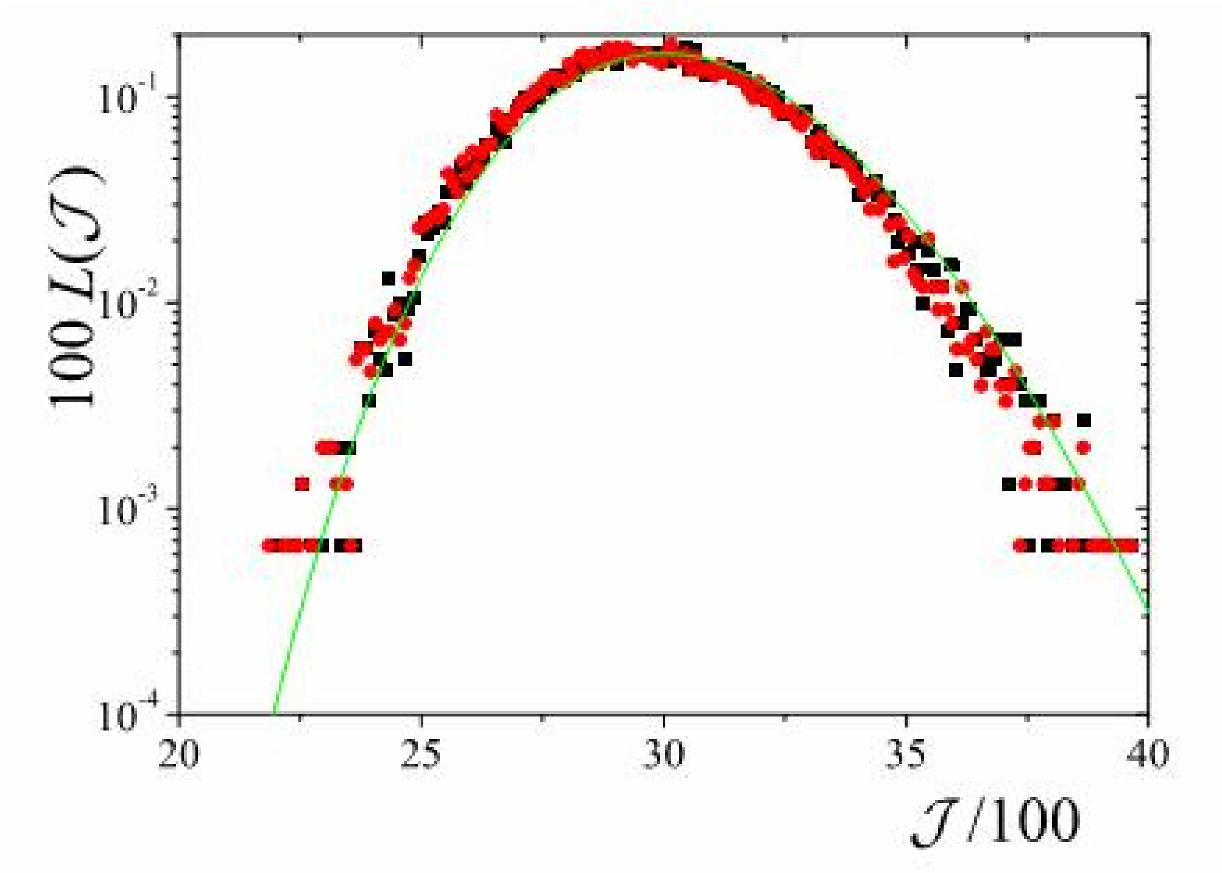
$$\mathcal{M}_{\mathcal{J}_I(\Theta)}(\lambda) \equiv \langle \exp [\lambda \, \mathcal{J}_I (\Theta)] \rangle$$
$$= \exp \left[\frac{\gamma \, \Theta}{2 \, m} \left(1 - \sqrt{1 + 4 \, T \, \lambda} \right) \right]$$

Heeding that the injected energy corresponds to the integral of the injected power with respect to time, we can use large deviation theory and obtain the distribution of the total injected energy imposing the Gartner-Ellis theorem which yields,

$$L(\mathcal{J}_I) \sim \exp \left[- \frac{(\mathcal{J}_I - \gamma \, T \, \Theta / m)^2}{4 \, T \, \mathcal{J}_I} \right] H(\mathcal{J}_I)$$

matching Farago's solution who does the computation for a harmonic system.

Moreover, the computation of higher moments of the dissipated power shows that both distributions actually have the same distribution.



W.A.M. Morgado and SMDQ (2013)

The concentration of the measure is the same, the injected and dissipated power are likely to have different distributions,

$$j_I \equiv \eta\, v \qquad\qquad j_D \equiv -\gamma\, v^2$$

The dissipated power PDF is easily computed using the conservation of the probability,

$$p\left(|j_D|\right) = \sqrt{\frac{m}{2\pi\,\gamma\,T\;|j_D|}}\exp\left[-\frac{m}{2\gamma T}\,|j_D|\right],$$

Injected power is more complex because the velocity and the "noise" are correlated,

$$\begin{aligned} C_{\eta v}\left(\tau\right) &\equiv \overline{\langle\eta\left(t\right)v\left(t+\tau\right)\rangle} - \overline{\langle\eta\left(t\right)\rangle\langle v\left(t\right)\rangle} \\ &= 2T\frac{\gamma}{m}\exp\left[-\frac{\gamma}{2\,m}\tau\right]\left\{\cos\left[\sqrt{\frac{k}{m}-\left(\frac{\gamma}{2\,m}\right)^2}\tau\right]\right. \\ &\quad \left. -\frac{\gamma}{m}\left[4\frac{k}{m}-\left(\frac{\gamma}{m}\right)^2\right]^{-\frac{1}{2}}\sin\left[\sqrt{\frac{k}{m}-\left(\frac{\gamma}{2\,m}\right)^2}\tau\right]\right\}, \end{aligned}$$

$$\overline{\langle\eta\left(t\right)v\left(t+\tau\right)\rangle} = 0, \qquad \left(\tau<0\right).$$

Thus we define the velocity as the sum of to variables,

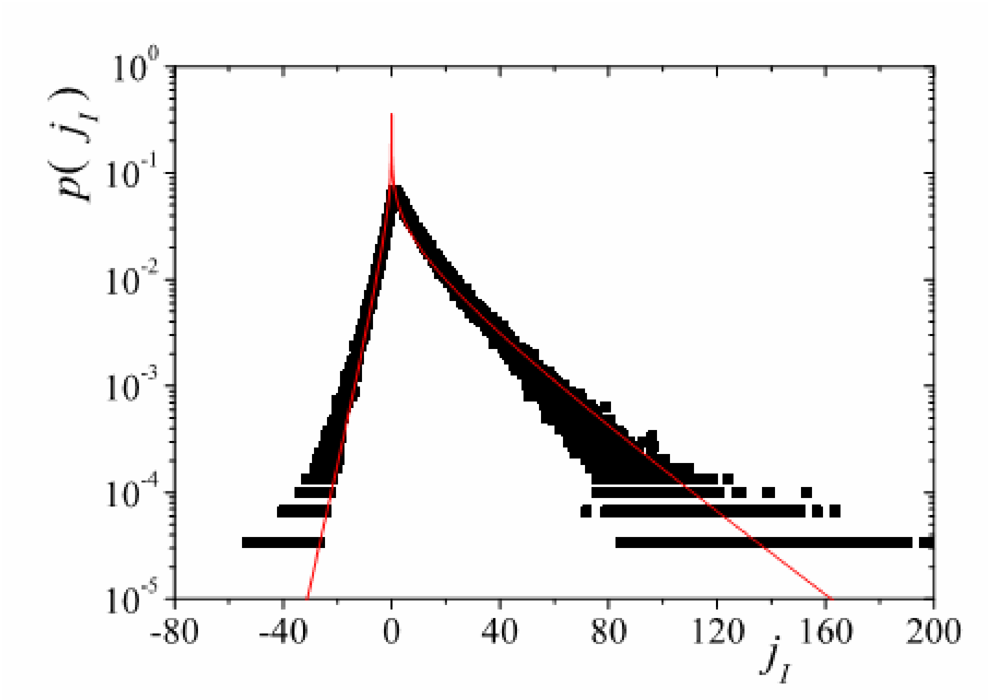
$$v = c\,\eta + f\,\xi$$

$$c = C_{\eta\,v}\,(0) = T\frac{\gamma}{m} \qquad f = \sqrt{1 - \frac{\gamma}{2\,m}} \qquad \langle \xi^2 \rangle = \omega^2 = \frac{T}{m}$$

Under this assumptions the injected power PDF reads,

$$p\,(j_I) = \int\!\!\int \frac{1}{2\,\pi\,\sigma\,\omega} \exp\left[-\frac{\eta^2}{2\sigma^2} - \frac{\xi^2}{2\,\omega^2}\right] \delta\,(j_I - \eta\,v)\;\delta\,(v - c\,\eta - f\,\xi)\;d\eta\,d\xi,$$

$$= \frac{2\,c}{\pi\,f\,\sigma\,\omega} \exp\left[\frac{c}{f^2\omega^2} j_I\right] K_0 \left[\frac{\sqrt{(c\,\sigma)^2 + f^2\omega^2}}{f^2\omega^2\,\sigma}\,|j_I|\right],$$



Beware that ηv is a pulse which is not numerically reproducible. To obtain minimally reliable results we had to use Savitzky-Golay filter.

W.A.M. Morgado and SMDQ (2013)

The PDF allows making explicit the fluctuation relation of the injected power,

$$\lim_{\Theta \to \infty} \frac{p(|j_I|)}{p(-|j_I|)} = \exp\left[2\frac{c}{f^2\omega^2}|j_I|\right]$$

A non-equilibrium Gaussian model

Classical 1-D massive particles the dynamics of which is ruled by,

$$v_i(t) = \frac{d\,x_i(t)}{dt}$$

$$m\frac{d\,v_i(t)}{dt} = -k\,x_i(t) - \gamma v_i(t) - \sum_{l=1}^{2} k_{2l-1}\left[x_i(t) - x_j(t)\right]^{2l-1} + \eta_i(t)$$

$$k_{2l-1} = 0 \quad \forall_l \Rightarrow \text{decoupled} \quad \text{particles}$$

Confining potential
(permits stationary solutions)

Dissipation

Coupling between particles

(Pseudo) Force representing the interaction of the system with a reservoir

After a transient this 2-particle system with T_1 different to T_2 yields a steady state.
A relevant thermal quantity is the heat flux between particles,

$$J_{1\to 2} = \frac{dW_{1\to 2} - dW_{2\to 1}}{2\,dt} = \frac{F_{1\to 2}v_2 - F_{2\to 1}v_1}{2}$$

that written in Laplace space reads,

$$J_Q = -k_1 \lim_{z\to 0} \lim_{\epsilon\to 0} \int_{-\infty}^{\infty} \frac{dq_1}{2\pi} \int_{-\infty}^{\infty} \frac{dq_2}{2\pi} \frac{z}{z-(\mathrm{i}\,q_1 + \mathrm{i}\,q_2 + 2\epsilon)} \times$$
$$\times\, (\mathrm{i}\,q_2 + \epsilon)\, \langle \tilde{r}_D(\mathrm{i}\,q_1 + \epsilon)\, \tilde{r}_S(\mathrm{i}\,q_2 + \epsilon)\rangle$$

where r_S refers to the CoM position and r_D the relative position.

Here we highlight its average value,

$$J_Q = \langle J_{1\to 2}\rangle \equiv \kappa_T (T_2 - T_1)$$

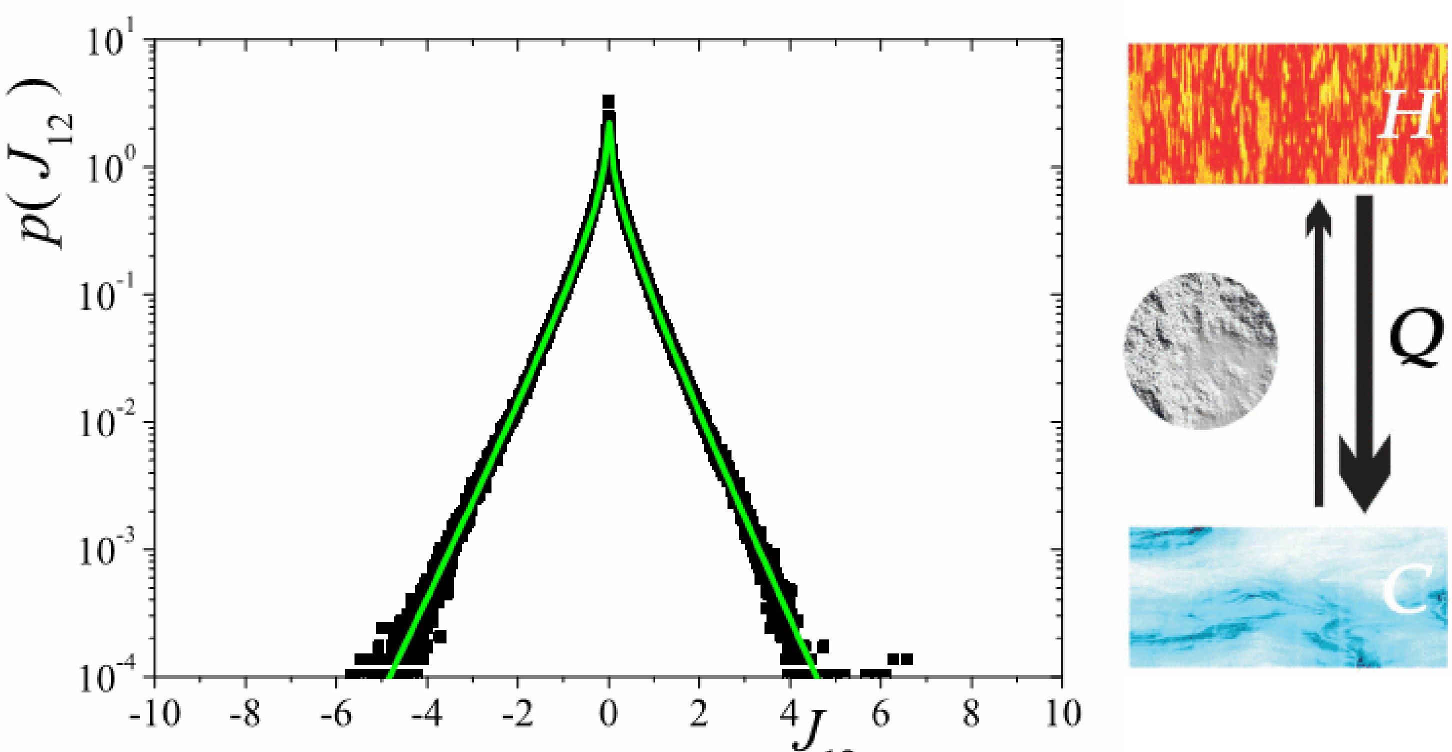
Heat conductance

which gives in the linear case,

$$\kappa = \frac{\gamma\, k^2}{2\,\left(\gamma^2(k_l + k) + k^2 m\right)}$$

The moment generating function of the heat flux is,

$$\mathcal{M}_{J_{1\to 2}}(\lambda) = \frac{1}{\sqrt{\left[1 - \left(A + \sqrt{B}\right)\lambda\right]\left[1 - \left(A - \sqrt{B}\right)\lambda\right]}}$$



W.A.M. Morgado and SMDQ (2013)

Applying the Edgeworth expansion using the equilibrium case PDF as the reference distribution, we obtain another fluctuation relation, namely,

$$\lim_{|J_{1\to2}|\to\infty} \frac{p\left(|J_{1\to2}|\right)}{p\left(-|J_{1\to2}|\right)} = \exp\left[2\frac{\overline{J_{1\to2}}}{\sigma^2_{J_{1\to2}}}|J_{1\to2}|\right]$$

In equilibrium we have, $p_0\left(J_{1\to2}\right) = \frac{1}{\pi\sqrt{B}} K_0\left[\frac{|J_{1\to2}|}{\sqrt{B}}\right]$

A rush of fresh air: Poissonian reservoirs

$$\eta(t) = \sum_{\ell} \Phi(t)\delta(t - t_{\ell}), \quad \lambda(t) = \lambda_0[1 + A\cos(\omega t)], \quad (0 \leq A < 1).$$

$$\langle \eta(t_1) \ldots \eta(t_n) \rangle_c = \lambda(t_1)\, \overline{\Phi^n}\, \delta(t_1 - t_2) \ldots \delta(t_{n-1} - t_n).$$

Why is this relevant?

I – Theoretical relevance

Poisson noise is the quintessential stochastic process with singular measure.

The *Lévy-Itô theorem* states that every white noise is represented by a superposition of Brownian and Poisson noises.

II – Factual relevance

Physical-Chemical problems using Anderson thermostats;

Landsberg engine systems

RLC circuits

Nano-technological and nano-bio-technological problems

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Line Shape Broadening in Surface Diffusion of Interacting Adsorbates with Quasielastic He Atom Scattering

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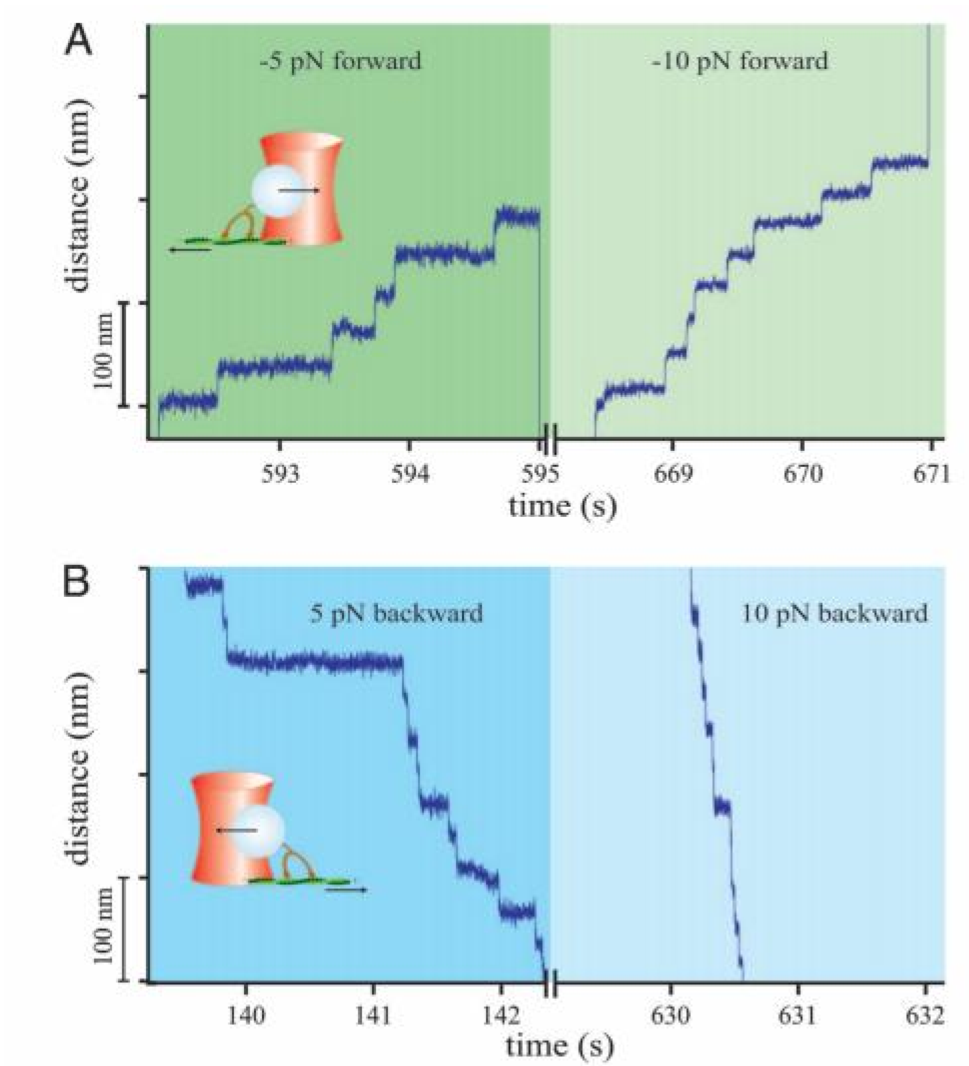
The experimental line shape broadening observed in adsorbate diffusion on metal surfaces with increasing coverage is usually related to the nature of the adsorbate-adsorbate interaction. Here we show that this broadening can also be understood in terms of a fully stochastic model just considering two noise sources: (i) a Gaussian white noise accounting for the surface friction, and (ii) a shot noise replacing the physical adsorbate-adsorbate interaction potential. Furthermore, contrary to what could be expected, for relatively weak adsorbate-substrate interactions the opposite effect is predicted: line shapes get narrower with increasing coverage.

Molecular motors (Kinesin and Myosin-V) **We utterly depend on these mechanisms!**



J Christof *et al*, PNAS **103**, 8680 (2006)

1-Particle steady state probabilistcs (linear potentials)

[Morgado, DQ, Soares-Pinto, JSTAT P06010 (2011)]

After a raft of humdrum calculations,

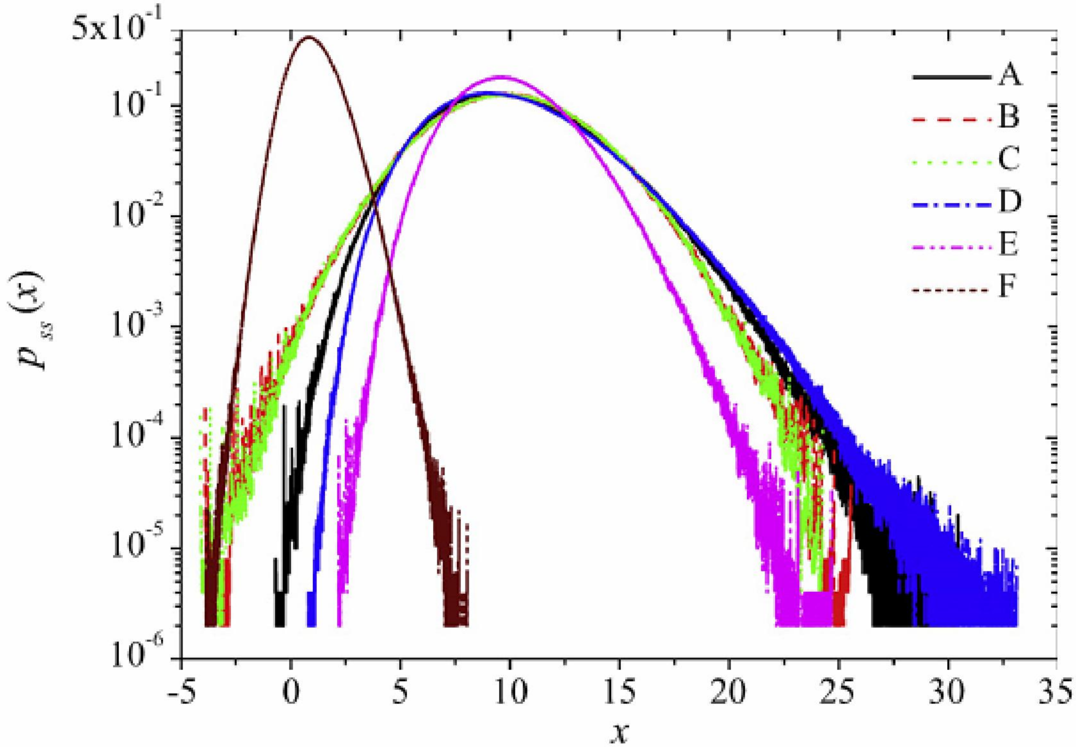
$$p_{ss}(x,v) = \mathcal{F}_{x,v}\left[\exp\left\{\sum_{n,m=0:(m+n>0)}^{\infty} \lambda_0 (n+m)! \frac{Q^n}{n!}\frac{P^m}{m!}(\mathrm{i}\bar{\Phi})^{n+m} \times \left(\Psi_{1x}\,\delta_{m,0} + \Psi_{1v}\,\delta_{n,0} + \Psi_2\,\delta_{m,1} + \sum_{m=2}^{n+m-1}\Psi_3(m)\right)\right\}\right]$$

a little more understandable for the marginal steady state distributions …

$$p_{ss}(x) = \mathcal{F}_x\left[\exp\left\{\sum_{n>0}^{\infty}\lambda_0 Q^n\,\bar{\Phi}^n\,\Psi_{1x}\right\}\right], \qquad \kappa_n \equiv \overline{\langle x^n\rangle_c} = n!\lambda_0\,(\mathrm{i}\bar{\Phi})^n\,\Psi_{1x}.$$

and thus,

$$\kappa_n^{(x)} = \lambda_0\left(\frac{\bar{\Phi}}{M}\right)^n(-1)^{n-1}\frac{(n!)^2}{D_n} \qquad (n \geq 1).$$



$$\overline{\langle x \rangle} = \bar{\Phi}\,\frac{\lambda_0}{k_0},$$

$$\overline{\langle x^2 \rangle} - \overline{\langle x \rangle}^2 = \bar{\Phi}^2\frac{\lambda_0}{\gamma\,k_0}.$$

Figure 1. Numerically obtained probability density function $p_{ss}(x)$ versus position x for various cases with $\lambda_0 = 10$, $\bar{\Phi} = 1$ and the noise defined by equation (4) with $\omega = \pi$. Following the legend in the figure we have the respective cases, A: $M = 1, k_0 = 1, \gamma = 1, A = 0$, B: $M = 10, k_0 = 1, \gamma = 1, A = 0$, C: $M = 10, k_0 = 1, \gamma = 1, A = 1/2$, D: $M = 0.1, k_0 = 1, \gamma = 1, A = 0$, E: $M = 1, k_0 = 1, \gamma = 2, A = 0$ and F: $M = 1, k_0 = 10, \gamma = 1, A = 0$.

Morgado,DQ, Soares-Pinto (2011)

For the velocity,

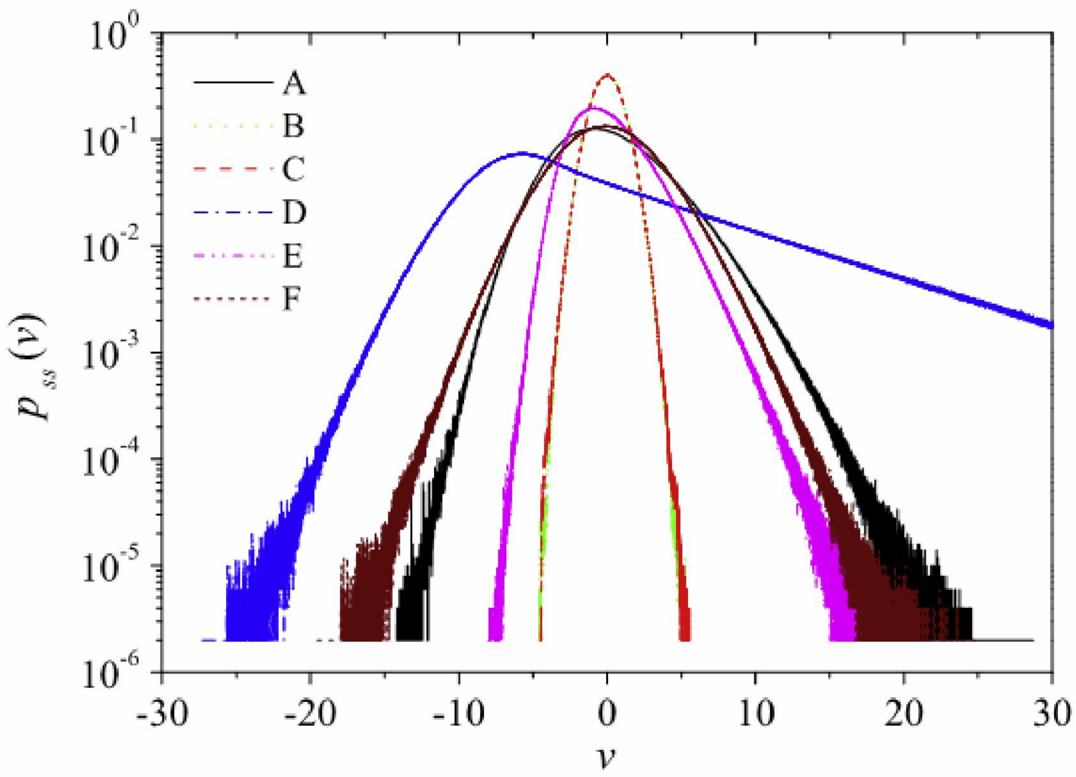
$$p_{ss}(v) = \mathcal{F}_v\left[\exp\left\{\sum_{m>0}^{\infty} \lambda_0\, P^m\, \bar{\Phi}^m\, \Psi_{1v}\right\}\right],$$

and thus,

$$\kappa_m^{(v)} \equiv \overline{\langle v^m\rangle_c} = m!\,\lambda_0\,(\mathrm{i}\bar{\Phi})^m\,\Psi_{1v}.$$

with,

$$\Psi_{1v} = \sum_{j=0}^{m-1} \binom{m-1}{j} \frac{\mathrm{i}^m(-1)^{m-j} k_+^j k_-^{m-j-1}[j,(m-j-1)]}{[1,-1]^{m-1}[j,(m-j)][(j+1),(m-j-1)]}$$



$$\kappa_1^v \equiv \overline{\langle v \rangle} = 0,$$

$$\kappa_2^v \equiv \overline{\langle v^2 \rangle} = \frac{\lambda_0 \, \bar{\Phi}^2}{M \, \gamma}.$$

Figure 2. Numerically obtained probability density function $p_{ss}(v)$ versus scalar velocity v for the same parameter sets of figure 1.

Morgado,DQ, Soares-Pinto (2011)

Neither $p_{ss}(x)$ nor $p_{ss}(v)$ are Gaussians.

2-Particle steady state heat transport (linear potentials)

[Morgado, DQ, PRE **86**, 041108 (2012)]

$$J_Q = \langle J_{1\to 2}\rangle \equiv \kappa_T\,(T_2 - T_1)$$

Using the average trick of Laplace transforming, the calculations boil down to evaluating,

$$\overline{\mathcal{J}_{rs}} = \lim_{z\to 0}\lim_{\varepsilon\to 0}\int \frac{dq_1}{2\pi}\frac{dq_2}{2\pi}\frac{z}{z - \mathrm{i}\,(q_1 + q_2 + 2\varepsilon)} \times \langle \tilde{x}_r\,(\mathrm{i}\;q_1 + \varepsilon)\;\tilde{v}_s\,(\mathrm{i}\;q_2 + \varepsilon)\rangle\,.$$

Assuming the temperature of a Poissonian particle as,

$$T_i = \lambda_0 \frac{\overline{\Phi_i}^2}{\gamma}$$

the integration renders up,

$$\kappa = \frac{1}{2}\frac{k_c^2\gamma}{m\,k_c^2 + \gamma^2\,(k + k_c)}$$

The exact same result of coupled Brownian particles!

In fact, for Poissonian particles, one gets the same thermal properties as those featured by if Brownian particles.

$$\int_0^\tau \left[\eta(t)\, v(t) - \gamma v(t)^2\right] \mathrm{d}t = \tfrac{1}{2} M v(t)^2 \Big|_{t=0}^{t=\tau} + \tfrac{1}{2} k_0 x(t)^2 \Big|_{t=0}^{t=\tau}.$$

$$E_M^c = \tfrac{1}{2} M \overline{\langle v(t)^2 \rangle_{asy}} + \tfrac{1}{2} k_0 \overline{\langle x(t)^2 \rangle_{asy}} = \lambda_0 \frac{\bar{\Phi}^2}{\gamma} + \frac{{\lambda_0}^2 \bar{\Phi}^2}{2\, M\, \omega_0^2} + \frac{{\lambda_0}^2 \bar{\Phi}^2 A^2 \left(\omega^2 + \omega_0^2\right)}{4\, M \left[\left(\omega_0^2 - \omega^2\right)^2 + 4\, \theta^2 \omega^2\right]}.$$

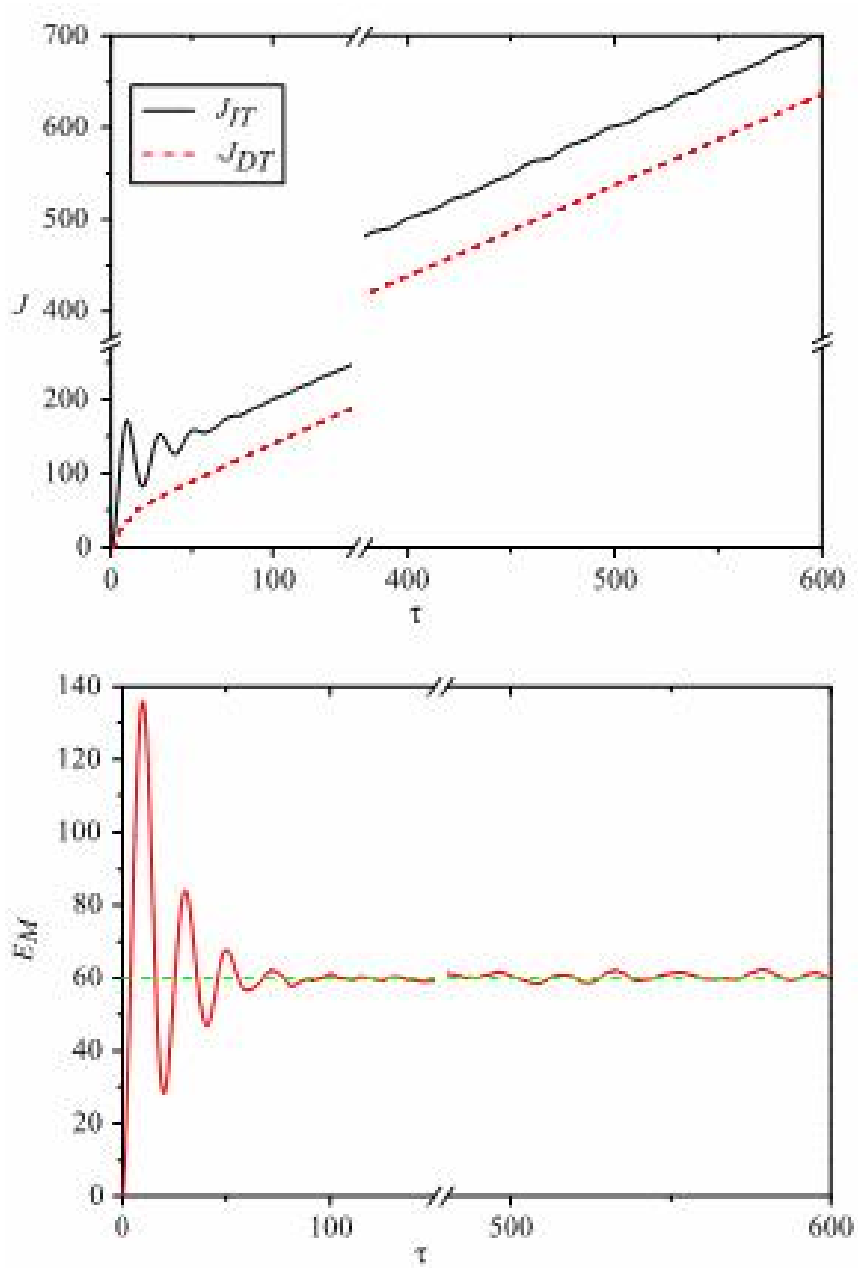
$$J_{\mathrm{I}} = v(t)\, \eta(t), \qquad J_{\mathrm{D}} = -\gamma\, v^2(t).$$

$$J_{\mathrm{IT}} = \int_0^\tau \mathrm{d}t\, v(t) \eta(t), \qquad J_{\mathrm{DT}} = -\gamma \int_0^\tau \mathrm{d}t\, v^2(t).$$

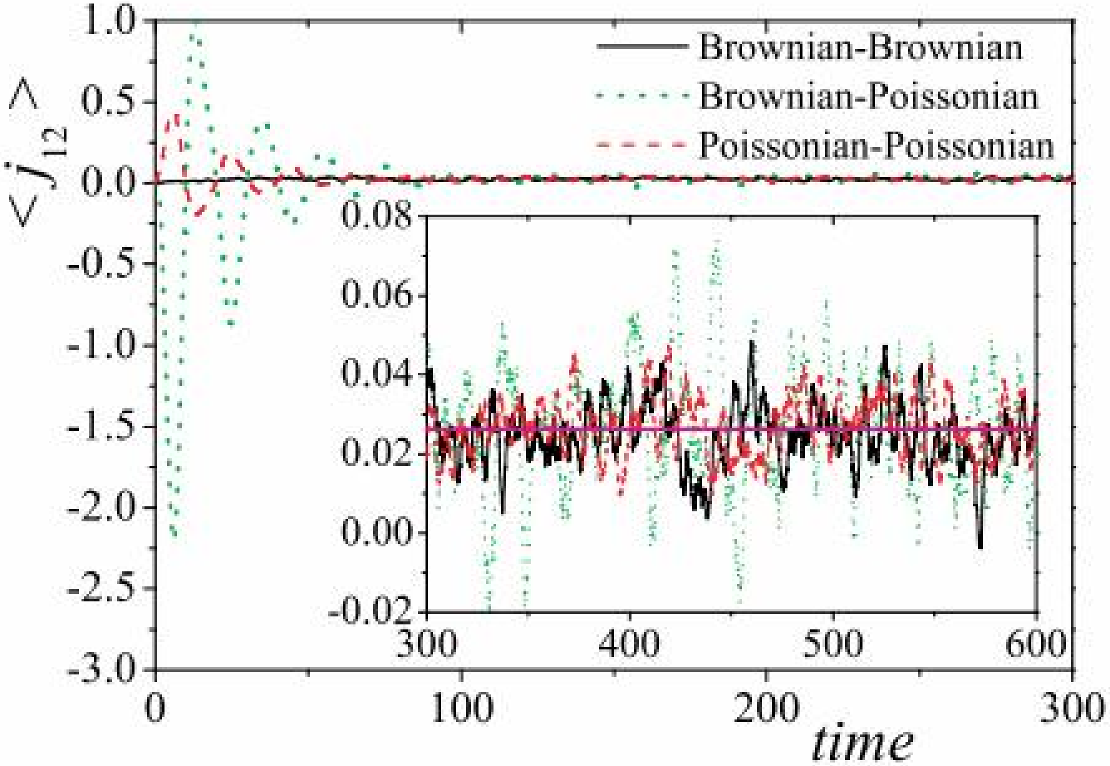
Both asymptotic linear parts equal to $\dfrac{\lambda_0 \overline{\Phi}^2}{M} \tau$.

The non-oscillating part of the total energy flux $J_E = J_{IT} + J_{DT}$ equals to $E_M{}^c$,

$$J_{\mathrm{E}}^{\mathrm{no}} = \frac{\bar{\Phi}^2 \lambda_0 \left(2\, M {\omega_0}^2 + \lambda_0 \gamma\right)}{2\gamma\, M \omega_0^2} + \frac{\left(\omega^2 + \omega_0^2\right) A^2 \bar{\Phi}^2 {\lambda_0}^2}{4\, M\, \left[\omega^2 \left(\omega^2 - 2\, \omega_0^2 + 4\, \theta^2\right) + \omega_0^4\right]}$$



Morgado,DQ, Soares-Pinto (2011)



W.A.M. Morgado and SMDQ (2012)

CONCLUSION:

THE SINGULAR NATURE OF THE MEASURE OF A POISSONIAN PARTICLE IS IRRELEVANT FOR THERMAL PURPOSES.

THENCE

IN ANALYTICALLY TREATING THE THERMOSTATISTICS OF SUCH PARTICLES ONE CAN HEDGE ALL THOSE NASTY CALCULATIONS BY USING BROWNIAN PROXIES!

A brand new day: non-linear systems [Morgado, DQ, PRE **86**, 041108 (2012)]

$$m\frac{dv_i(t)}{dt} = -k\,x_i(t) - \gamma\,v_i(t) - \sum_{l=1}^{2} k_{2l-1}\,[x_i(t) - x_j(t)]^{2l-1} + \eta_i(t)$$

$$\overline{\langle j_{12}\rangle} = \overline{\left\langle j_{12}^{(0)}\right\rangle} + \overline{\left\langle j_{12}^{(1)}\right\rangle} + \overline{\left\langle j_{12}^{(s)}\right\rangle} + \mathcal{O}\left(k_3^2\right)$$

$$\begin{cases} \overline{\left\langle j_{12}^{(0)}\right\rangle} = -\frac{k_1^2}{4}\frac{[\mathcal{A}_1(2)-\mathcal{A}_2(2)]}{m\,k_1^2+\gamma^2(k+k_1)} \\ \overline{\left\langle j_{12}^{(1)}\right\rangle} = -\frac{3}{8}\gamma\,k_1\,k_3\frac{(2\,k+k_1)\left[\mathcal{A}_1(2)^2-\mathcal{A}_2(2)^2\right]}{(k+2\,k_1)\left[\gamma^2(k+k_1)+m\,k_1^2\right]^2} \end{cases}$$

$$\overline{\left\langle j_{12}^{(s)}\right\rangle} = -\frac{27}{2}\gamma^2\frac{k_1\,k_3}{\lambda}\frac{\mathcal{N}}{\mathcal{D}}\left(\left[\mathcal{A}_1(2)^2 - \mathcal{A}_2(2)^2\right]\right)$$

THERMOSTATISTICS DOES CARE ABOUT THE NATURE OF THE RESERVOIRS

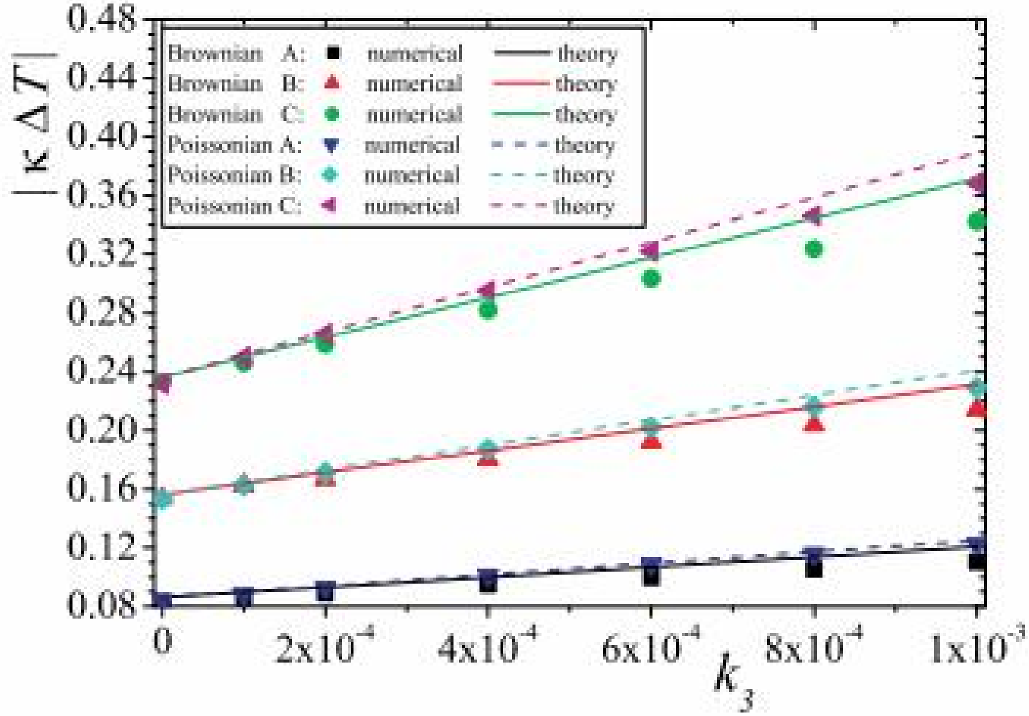


FIG. 2. (Colour on-line) Comparison between numerically obtained values (symbols) and the first order approximation of thermal conductance from Eqs. (9)-(11) for different temperatures pairs, namely A $= \left\{10, \frac{169}{10}\right\}$, B $= \left\{10, \frac{225}{10}\right\}$, C $= \left\{10, \frac{289}{10}\right\}$ with $m = 10$, $\gamma = k = 1$, $k_1 = 1/5$ and $\lambda = 1$ for Poissonian particles.

W.A.M. Morgado and SMDQ (2012)

Ulterior evidences of our result

PHYSICAL REVIEW E **87**, 052124 (2013)

Heat conduction induced by non-Gaussian athermal fluctuations

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We study the properties of heat conduction induced by non-Gaussian noises from athermal environments. We find that new terms should be added to the conventional Fourier law and the fluctuation theorem for the heat current, where its average and fluctuation are determined not only by the noise intensities but also by the non-Gaussian nature of the noises. Our results explicitly show the absence of the zeroth law of thermodynamics in athermal systems.

PHYSICAL REVIEW E **87**, 052126 (2013)

Fourier's law from a chain of coupled anharmonic oscillators under energy-conserving noise

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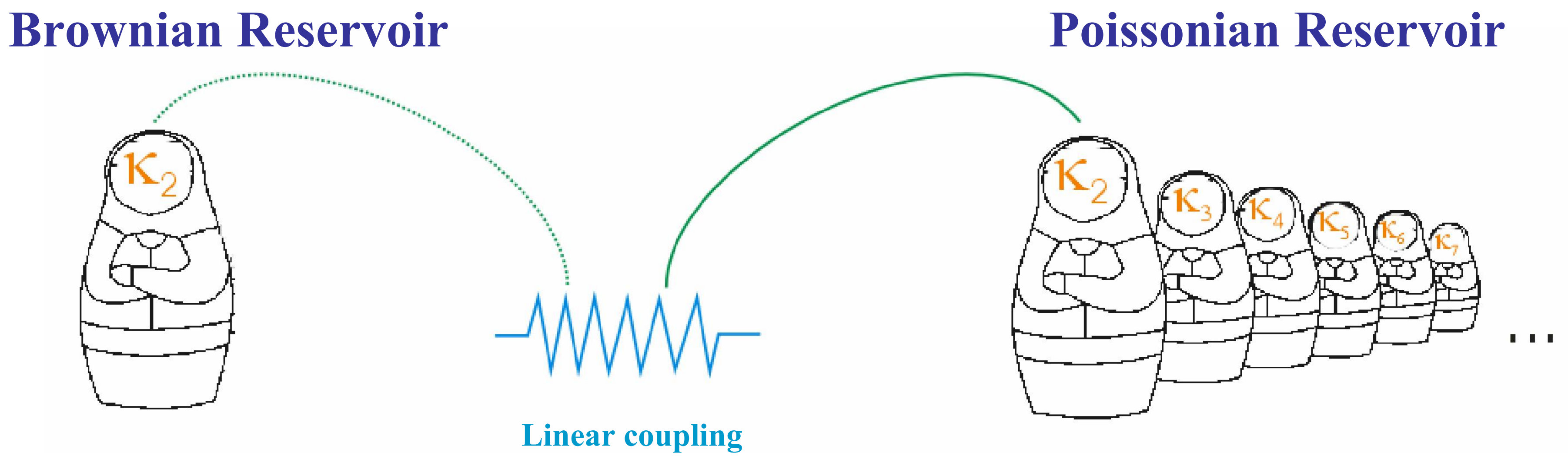
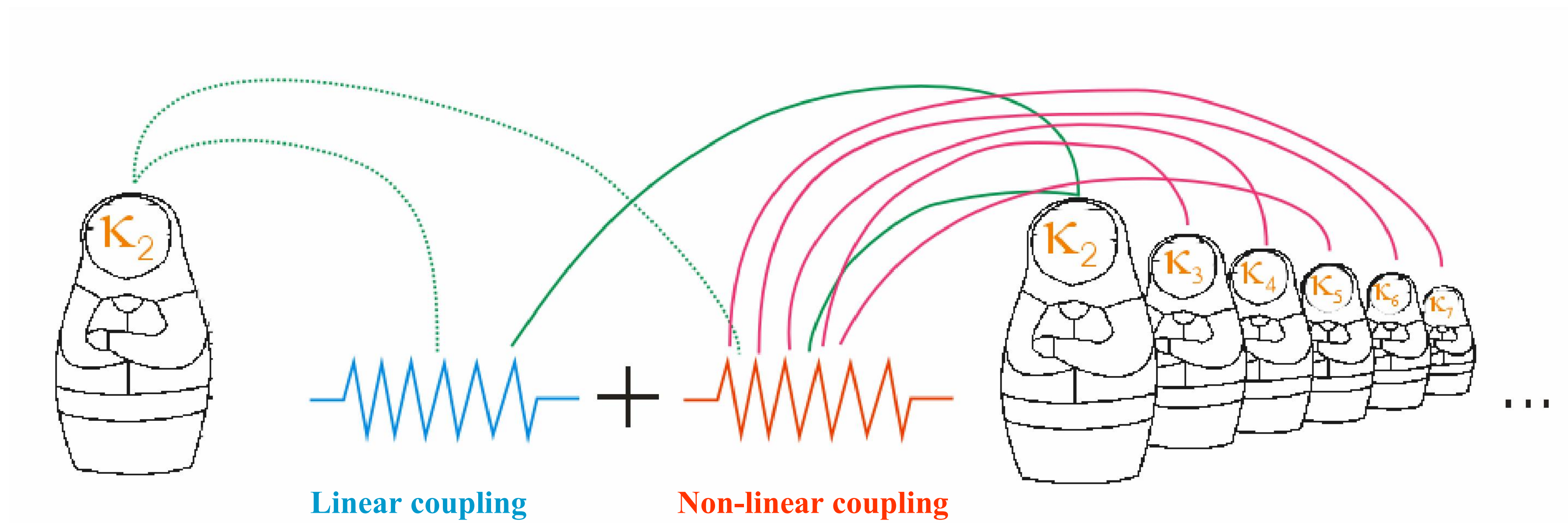
We analyze the transport of heat along a chain of particles interacting through anharmonic potentials consisting of quartic terms in addition to harmonic quadratic terms and subject to heat reservoirs at its ends. Each particle is also subject to an impulsive shot noise with exponentially distributed waiting times whose effect is to change the sign of its velocity, thus conserving the energy of the chain. We show that the introduction of this energy-conserving stochastic noise leads to Fourier's law. The behavior of the heat conductivity for small intensities of the shot noise and large system sizes is found to obey a finite-size scaling relation. We also show that the heat conductivity is not constant but is an increasing monotonic function of temperature.

DOI: 10.1103/PhysRevE.87.052126 PACS number(s): 05.70.Ln, 05.10.Gg, 05.60.−k

Conclusions (this time for real)





Consequence: The zeroth law of thermodynamics is not universal because for non-Gaussian heat reservoirs it depends on the mechanical trait of the system.