Non-Linear Thermal Conductance and Noise Dependence
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References:

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Abstract

- Simple small models can be quite illustrative about the way biological and molecular systems behave.
- We show how the couplings between the model's non-linearities and non-equilibrium properties of thermal noise lead to new properties of transport coefficients.

Why are we interested in this problem?

- Under certain conditions, there might be non-equilibrium energy feeding into a system (mostly small), i.e, non-gaussian noises will act upon these systems. For instance, Poisson noise.
- We might be able to solve small system models with arbitrary noise properties.
- What happens when non-linearities couple with the non-gaussian (higher cumulants) properties of noise?

Equilibrium noise

- An equilibrium thermal reservoir interacts with a system, say a Brownian particle, by an effective interaction that may be well represented by white gaussian noise.
- That form of noise ensures the Boltzmann-Gibbs equilibrium distribution for the system.
- Only the mean and variance of the noise exists.
- For non-equilibrium noise, higher order cumulants may exist.

Non-Equilibrium Stationary State - NESS

- A system in out-of equilibrium conditions might reach a NESS.
- This can be done by submitting the system to contact with distinct temperature reservoirs, or by submitting the system to a non-equilibrium noise, e.g. Poisson noise.
- We shall see that the distinction above is less than it seems.

Poisson noise & Brownian particles

A Brownian particle under Poisson noise is a paradigmatic NESS for $t \to \infty$.
The model is

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

$$M\,\dot{v}(t) = -k_0 x(t) - \gamma v(t) + \eta(t),$$

where η is a Poisson noise,

$$\eta\,(t) = \sum_{\ell} \Phi\,(t)\;\delta\,(t - t_\ell)\,.$$

It is interesting to chose a variable rate

$$\lambda(t) = \lambda_0\,[1 + A\cos(\omega\,t)]\,,$$

Noise Cumulants

- Poisson noise has infinite number of cumulants:

$$\left\langle \eta_{i_1}(t_1)\,\eta_{i_2}(t_2)\,\ldots\,\eta_{i_n}(t_n)\right\rangle_c = \overline{\Phi^n}\,\lambda(t_1)\,\delta_{i_1 i_2}\,\ldots\,\delta_{i_{n-1} i_n} \times \delta(t_1 - t_2)\ldots\delta(t_{n-1} - t_n)\,.$$

- The general Laplace transform for noise reads:

$$\langle \tilde{\eta}_1(s_1)\ldots\tilde{\eta}_n\rangle_c = \frac{A_n}{s_1 + \ldots + s_n},$$

where A_n is the n-th order cumulant

- Energy injection, dissipation, and the received heat ($x_0 = v_0 = 0$):

$$Q = \int_0^{\tau}\left[\eta(t)\;v(t) - \gamma v(t)^2\right]dt = \frac{1}{2}M\;\,v(t)^2\Big|_0^{\tau} + \frac{1}{2}k_0\;\,x(t)^2\Big|_0^{\tau}.$$

Ressonating Energy Injection

The time averaged exact NESS energy:

Then finally, we write the contributions for the injection of energy as

$$J_{\mathrm{IT0}}(\tau) = \left(\frac{\lambda_0 \bar{\Phi}^2}{M} + \frac{A^2 \omega^2 \theta \lambda_0^2 \bar{\Phi}^2}{M \left[\omega^2 (\omega^2 - 2\omega_0^2 + 4\theta^2) + \omega_0^4 \right]} \right) \tau,$$

and

$$J_{\mathrm{IT,osc}}(\tau) = \frac{\lambda_0 \bar{\Phi}^2 A \sin(\omega\tau)}{M\omega} + \frac{A \left[A ({\omega_0}^2 - \omega^2) \cos(2\omega\tau) + 4{\omega_0}^2 \cos(\omega\tau) \right] \lambda_0^2 \bar{\Phi}^2}{4M \left[\omega^2 (\omega^2 - 2\omega_0^2 + 4\theta^2) + \omega_0^4 \right]} + \frac{A \left[2\omega\theta \left(A \sin(2\omega\tau) + 4\sin(\omega\tau) \right) - 4\omega^2 \cos(\omega\tau) \right] \lambda_0^2 \bar{\Phi}^2}{4M \left[\omega^2 (\omega^2 - 2\omega_0^2 + 4\theta^2) + \omega_0^4 \right]}, \quad (47)$$

and

$$J_{\mathrm{ITc}} = \frac{\lambda_0^2 \bar{\Phi}^2}{M\omega_0^2} + \frac{A \lambda_0^2 \bar{\Phi}^2 (\omega_0^2 - \omega^2)}{M \left[\omega^2 (\omega^2 - 2\omega_0^2 + 4\theta^2) + \omega_0^4 \right]} + \frac{\left[\omega^4 (\omega^2 - 12\theta^2) + \omega_0^2 (3\omega_0^4 - 5\omega_0^2 \omega^2 + \omega^4 - 4\theta^2) \right] A^2 \lambda_0^2 \bar{\Phi}^2}{4M \left[\omega^2 (\omega^2 - 2\omega_0^2 + 4\theta^2) + \omega_0^4 \right]^2}. \quad (48)$$

For the total energy flux $J_E = J_{\mathrm{IT}} + J_{\mathrm{DT}}$ it can be easily seen that the linear term on τ cancels out, while the constant term becomes exactly the average energy of equation (40). The non-oscillating part of the energy is

$$J_{\mathrm{E}}^{\mathrm{no}} = \frac{\bar{\Phi}^2 \lambda_0 (2M{\omega_0}^2 + \lambda_0 \gamma)}{2\gamma M \omega_0^2} + \frac{(\omega^2 + \omega_0^2) A^2 \bar{\Phi}^2 {\lambda_0}^2}{4M \left[\omega^2 (\omega^2 - 2\omega_0^2 + 4\theta^2) + \omega_0^4 \right]}, \quad (49)$$

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Ressonating Energy Injection 2

Injected - Dissipated Energy = Heat

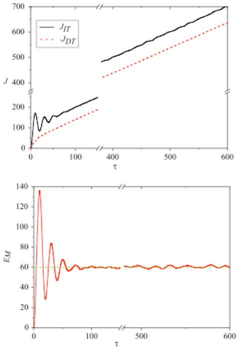

Figure 4. Upper panel: total injected and (symmetric) dissipated power, $J_{\rm IT}(-J_{\rm DT})$ versus time, τ, according to the definitions in the legend. Lower panel: total energy, E_M, versus time, τ. The dashed (green) line represents the asymptotic limit given by equation (40). In both cases we have used the following values: $M = 10$, $k_0 = 1$, $\gamma = 1$ $\bar{\Phi} = 1$, $\lambda_0 = 10$ and $A = 0$. Note: the difference between the values of $J_{\rm IT}$ and $-J_{\rm DT}$ in the upper panel are exactly equal to the total energy, E_M, which is shown in the lower panel and equals the theoretical value given by equation (40) as well.

The oscillation amplitude is modulated by the resonance between the natural frequency $\omega_0 = \sqrt{\frac{k}{m}}$ and the poisson frequency ω.

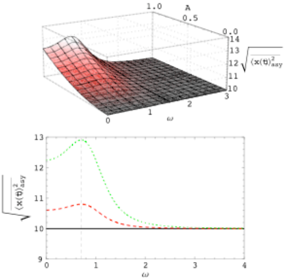

Figure 3. Upper panel: $\sqrt{\langle x(t)\rangle^2_{asy}}$ versus amplitude of the heterogeneous part, A, and frequency, ω, with $M = 1$, $\gamma = 1$, $k_0 = 1$, $\lambda_0 = 10$, $\bar{\Phi} = 1$. The maximum, characterizing a stochastic resonance phenomenon, occurs at $\omega_{res} = \sqrt{\omega_0^2 - 2\,\theta^2}$ that defines the grey dashed line in the lower panel containing the plane cuts for $A = 0$ (black line), $A = \frac{1}{2}$ (dashed red line) and $A = 1$ (dotted green line). For this case the maximum occurs at $1/\sqrt{2}$.

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Stationary Distributions

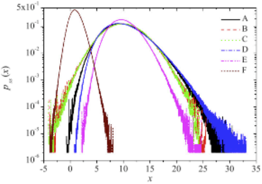

Figure 1. Numerically obtained probability density function $p_{ss}(x)$ versus position x for various cases with $\lambda_0 = 10$, $\bar{\Phi} = 1$ and the noise defined by equation (4) with $\omega = \pi$. Following the legend in the figure we have the respective cases, A: $M = 1, k_0 = 1, \gamma =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

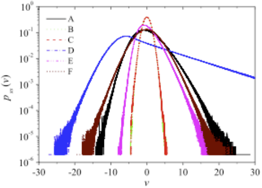

Figure 2. Numerically obtained probability density function $p_{ss}(v)$ versus scalar velocity v for the same parameter sets of figure 1.

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Linear Poisson model and energy

- We did not explore fully the Poisson model due to its linearity.
- We could not couple the energy with the higher order Poisson cumulants.
- The stationary state is a NESS one: the probability distribution is not Boltzmann-Gibbs, hence NE.

Time average

- We start from (1D Brownian Particle)

$$p(x, v, t) = \langle \delta(x - x(t))\, \delta(v - v(t)) \rangle,$$

  where $x(t)$ and $v(t)$ are solutions for the equations of motion given a realization of the noise.

- Time averaging:

$$p^{ss}(x, v) = \lim_{s \to 0} s \int_0^\infty dt\, e^{-st} \, \langle \delta(x - x(t))\, \delta(v - v(t)) \rangle \, .$$

After a straightforward calculation...

$$
\begin{aligned}
p^{ss}(x,v) &= \lim_{s\to\infty}\lim_{\epsilon\to\infty}\int_{-\infty}^{\infty}\frac{dQ}{2\pi}\,e^{iQx}\int_{-\infty}^{\infty}\frac{dP}{2\pi}\,e^{iPv}\;\times \\
&\times \;\sum_{n=0}^{\infty}\sum_{l=0}^{\infty}\frac{(-iQ)^n}{n!}\,\frac{(-iP)^l}{l!}\;\times \\
&\times \;\int_{-\infty}^{\infty}\frac{dq_1}{2\pi}\cdots\int_{-\infty}^{\infty}\frac{dq_n}{2\pi}\int_{-\infty}^{\infty}\frac{dp_1}{2\pi}\cdots\int_{-\infty}^{\infty}\frac{dp_l}{2\pi}\;\times \\
&\times \;\frac{s}{s-(iq_1+\epsilon+\ldots+iq_n+\epsilon+ip_1+\epsilon+\ldots+ip_l+\epsilon)}\;\times \\
&\times \;\langle\tilde{x}(iq_1+\epsilon)\ldots\tilde{x}(iq_n+\epsilon)\,\tilde{v}(ip_1+\epsilon)\,\ldots\,\tilde{v}(ip_l+\epsilon)\rangle\,.
\end{aligned}
$$

Cumulant-energy coupling

- Due to the linearity of the model ($\tilde{v}(s) = s\,\tilde{x}$)

$$\tilde{x,v}(s) = \frac{\tilde{\eta}(s)}{R(s)}.$$

- The exchanged heat Q is quadratic in $\tilde{\eta}$, hence

$$Q \propto \langle \tilde{\eta}(s_1)\,\tilde{\eta}(s_2) \rangle\,.$$

- We see that heat can only be a function of the variance, and average, of the noise
$\langle \tilde{\eta}(s_1)\,\tilde{\eta}(s_2) \rangle = \langle \tilde{\eta}(s_1)\,\tilde{\eta}(s_2) \rangle_c + \langle \tilde{\eta}(s_1) \rangle_c\,\langle \tilde{\eta}(s_2) \rangle_c$

Non-linear Interactions

- For a model with non-linear springs (non-linear force $= -k_3 x^3$) we can write:

$$R(s)\,\tilde{x}(s) + k_3 \int_{-\infty}^{\infty} \frac{dq_1}{2\pi}\,\frac{dq_1}{2\pi}\,\frac{dq_1}{2\pi}\,\frac{\tilde{x}(iq_1)\tilde{x}(iq_2)\tilde{x}(iq_3)}{s - i(q_1+q_2+q_3)} = \tilde{\eta}(s).$$

- The recurrence relation above shows that we can now couple the non-linearity with the higher order cumulants.
- In first order on k_3:

$$\langle \tilde{x}(s_1)\,\tilde{x}(s_2)\rangle \to k_3 \int_{-\infty}^{\infty} \frac{dq_1}{2\pi}\,\frac{dq_1}{2\pi}\,\frac{dq_1}{2\pi}\,\frac{\langle \tilde{x}(s_1)\,\tilde{x}(iq_1)\tilde{x}(iq_2)\tilde{x}(iq_3)\rangle}{s_1 - i(q_1+q_2+q_3)}$$

where we can express $\langle \tilde{x}(s_1)\,\tilde{x}(iq_1)\,\tilde{x}(iq_2)\,\tilde{x}(iq_3)\rangle$ as noisy combinations of averages, variances, skewness and kurtosis!

Higher order cumulants as distinct reservoirs

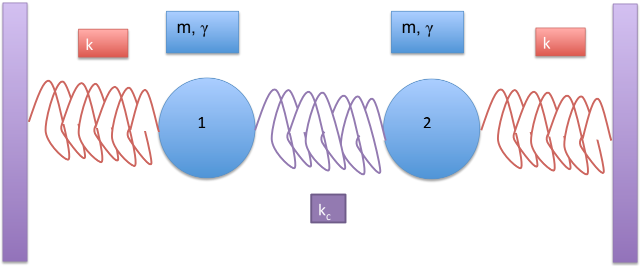
- Assuming the odd cumulants to be zero, we can express:

$$\begin{aligned}\langle \tilde{x}(s_1)\,\tilde{x}(iq_1)\,\tilde{x}(iq_2)\,\tilde{x}(iq_3)\rangle &= \langle \tilde{x}(s_1)\,\tilde{x}(iq_1)\,\tilde{x}(iq_2)\,\tilde{x}(iq_3)\rangle_c + \\ &+ \langle \tilde{x}(s_1)\,\tilde{x}(iq_1)\rangle_c \,\langle \tilde{x}(iq_2)\,\tilde{x}(iq_3)\rangle_c + \\ &+ \langle \tilde{x}(s_1)\,\tilde{x}(iq_2)\rangle_c \,\langle \tilde{x}(iq_1)\,\tilde{x}(iq_3)\rangle_c + \\ &+ \langle \tilde{x}(s_1)\,\tilde{x}(iq_3)\rangle_c \,\langle \tilde{x}(iq_2)\,\tilde{x}(iq_1)\rangle_c \,.\end{aligned}$$

- The received heat term has the (usual) contributions from the gaussian part (variance), but also the extra (unusual) kurtosis contribution.
- Thus, variance and kurtosis act as if distinct energy reservoirs are coupled to the system.

Small systems: our model

Two connected Brownian particles; non-linear springs; two thermal reservoirs.



Equations to be solved

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

with

$$\frac{dx_i(t)}{dt} = v_i(t)$$

where $(i, j) \in \{1, 2\}$ and k_1 and k_3 are the linear and non-linear coupling constants, respectively. The system is decoupled (linear) for $k_{1,3} = 0$.

Heat flux between particles

- We define the energy flux as

$$j_{12} = \frac{1}{2}(P_{21} - P_{12}) = \frac{1}{2}(F_{21} \cdot v_2 - F_{12} \cdot v_1),$$

where $F_{21} = -k_1(x_2 - x_1) - k_3(x_2 - x_1)^3$.

- We have

$$j_{12}(t) \equiv -\sum_{l=1}^{2} \frac{k_{2l-1}}{2} \left[x_1(t) - x_2(t)\right]^{2l-1} \left[v_1(t) + v_2(t)\right].$$

Thermal conductance

We are finally in the position to compute the thermal conductance,

$$\begin{aligned} \kappa &\equiv -\frac{\partial}{\partial \Delta T} \langle j_{12} \rangle_{\Delta T}, \\ \kappa &= -\frac{\overline{\langle j_{12} \rangle}}{T_1 - T_2}, \qquad (\text{for small } T_1 - T_2) \end{aligned}$$

Resorting to the single particle results and the equipartition theorem, we relate the cumulant features of the noise and the proper temperature, T_i, namely, $\mathcal{A}_i(2) = 2\,\gamma\, T_i$, yielding the thermal conductance, $\kappa = \kappa^{(0)} + \kappa^{(1)} + \mathcal{O}\left(k_3^2\right)$

- For linear systems, the higher order cumulants do not contribute. thus, the time averaged heat flux is simple and is given by

$$\overline{\left\langle j_{12}^{(B)} \right\rangle} = \overline{\left\langle j_{12}^{(0)} \right\rangle} = -\frac{k_1^2}{4} \frac{(\mathcal{A}_1(2) - \mathcal{A}_2(2))}{m\, k_1^2 + \gamma^2\,(k + k_1)},$$

where $\mathcal{A}_2(2) - \mathcal{A}_1(2) = 2\,\gamma\,\Delta\,T$.

- The linear contribution for the conductance is thus

$$\kappa_0 = \frac{k_1^2\,\gamma}{2\,\left(m\,k_1^2 + \gamma^2\,(k + k_1)\right)},$$

Conductance: non-linear systems and gaussian noises

- The reservoirs are equilibrium ones
- First order on k_3

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

where $\mathcal{A}_1(2)^2 - \mathcal{A}_2(2)^2 = -4\,\gamma^2\,\Delta T\,(T_1 + T_2)$.

- Thus, for the non-linear model and gaussian noise we have the conductance:

$$\kappa_{0,1} = \frac{k_1^2\,\gamma}{2\,\left(m\,k_1^2 + \gamma^2\,(k + k_1)\right)} +$$

$$+\frac{3}{2}\,k_1\,k_3 \frac{(2\,k + k_1)\,\gamma^3\,(T_1 + T_2)}{(k + 2\,k_1)\left[\gamma^2\,(k + k_1) + m\,k_1^2\right]^2}.$$

Conductance: non-linear systems and general noises

- The reservoirs are non-equilibrium ones
- The variance contribution still holds. however there is a new flux originating from the kurtosis in first order on k_3

$$\overline{\left\langle j_{12}^{(1,Poisson)} \right\rangle} = -\frac{27}{2}\,\frac{\gamma^2\,k_1\,k_3}{\lambda}\,\frac{\mathcal{N}}{\mathcal{D}}\left[\mathcal{A}_1(2)^2 - \mathcal{A}_2(2)^2\right],$$

where $\mathcal{A}_1(2)^2 - \mathcal{A}_2(2)^2 = -4\,\gamma^2\,\Delta T\,(T_1 + T_2)$, and

$$\mathcal{N} \equiv \gamma^2\,(5\;k + 3\,k_1) + m\left(3\,k_1^2 + 4\,k^2 + 11\,k\,k_1\right),$$

$$\mathcal{D} \equiv \left[\gamma^2\,(k + k_1)\right]\left[m\,(4\,k + 9\,k_1)^2 + 6\,\gamma^2\,(2\,k + 3\,k_1)\right]\times$$

$$\times\left[3\,\gamma^4 + m^2\,k_1^2 + 4\,m\,\gamma^2\,(k + k_1)\right]$$

Thus, for the non-linear model and general (Poisson) noise we have the conductance:

$$\kappa_{1,Poisson} = 54\, \frac{\gamma^4\, k_1\, k_3}{\lambda} \frac{\mathcal{N}}{\mathcal{D}} \left(T_1 + T_2\right).$$

Thus, for the non-linear model and general (Poisson) noise we have the total conductance:

$$\kappa_{0,1} = \frac{k_1^2\, \gamma}{2\, \left(m\, k_1^2 + \gamma^2 \left(k + k_1\right)\right)} +$$

$$+\frac{3}{2}\gamma\, k_1\, k_3 \frac{\left(2\, k + k_1\right)\, \gamma^2\, \overline{T}}{\left(k + 2\, k_1\right) \left[\gamma^2 \left(k + k_1\right) + m\, k_1^2\right] +^2}.$$

$$+54\, \frac{\gamma^4\, k_1\, k_3}{\lambda} \frac{\mathcal{N}}{\mathcal{D}} \left(T_1 + T_2\right).$$

Observe that as the Gaussian limit is reached ($\lambda \to \infty$), the last contribution above vanish.

System Energy

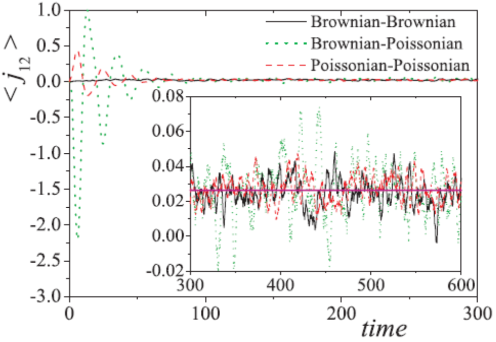


FIG. 1. (Color online) Average exchange flux $\langle j_{12} \rangle$ of a two-massive-particle system for different combinations of paradigmatic types of noise with $T_1 = 10$, $T_2 = 121/10$, $m = 10$, $\gamma = k = 1$, $k_1 = 1/5$, $k_3 = 0$, and $\lambda = 10$ for Poissonian particles. After the transient, κ agrees with the theoretical value, $\kappa = 21/800 = 0.026\,25$, with the fitting curves lying within the line thickness. The averages have been obtained by averaging over $850 \times (5 \times 10^5)$ points. The discretization used is $\delta t = 10^{-5}$ with snapshots at every $\Delta t = 10^{-3}$.

Thermal Conductance

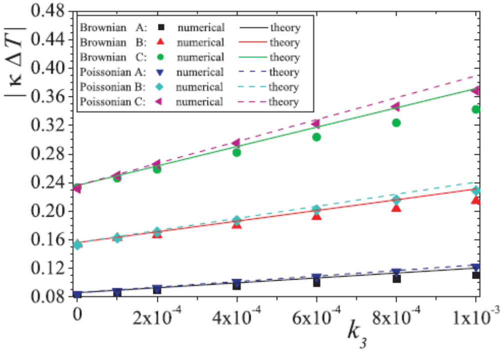


FIG. 2. (Color online) Comparison between numerically obtained values (symbols) and the first-order approximation of thermal conductance from Eqs. (8)–(10) for different temperature pairs, namely, $A = \{10, \frac{169}{10}\}$, $B = \{10, \frac{225}{10}\}$, and $C = \{10, \frac{289}{10}\}$ with $m = 10$, $\gamma = k = 1$, $k_1 = 1/5$, and $\lambda = 1$ for Poissonian particles.

Conclusions & perspectives

- We are working to systematize the case of a general potential.
- The method can be applied to a linear chain of arbitrary size, or a solid.
- Quantum version of the method.

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