Exact time-averaged conductance for small systems: Comparison between direct calculation and Green-Kubo formalism

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Exact results, in physics, play an important and useful role as a reference for other methods. For instance, they can be used to study specific features of models which are not easily accessible to approximate methods, such as computer simulations. However, non-trivial exact results are few and difficult to come by. For example, in the literature of transport phenomena there are not many exact calculations for transport coefficients based on the mechanical parameters of the systems under observation. Indeed, the calculation of transport coefficients is one of the most important goals of non-equilibrium physics.

Our present goal is to study exactly the validity, and consistency, of some methods used in the derivation of transport coefficients, namely the thermal conductivity, for small classical systems. We study exactly, via time averaging calculations, the thermal conductivity of a low dimensional system represented by two coupled massive Brownian particles, both directly and via Green-Kubo formalism. These two different approaches lead to the same result. We also obtain exactly the steady state probability distribution for that system by means of time-averaging. We would like to emphasize that this techniques based on time-averaging are very interesting since they are ensemble independent, driven only by the dynamical relations governing the interaction Brownian particle-heath bath.

The model:

A system composed by two coupled Brownian particles can be described by the Langevin equations :

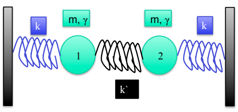
$$\dot{x}_\alpha(t) \;=\; v_\alpha(t) \qquad (1)$$

$$m_\alpha\,\dot{v}_\alpha(t) \;=\; -k\,(x_\alpha(t)-x_\beta(t)) - k'\,x_\alpha(t) - \gamma_\alpha v_\alpha(t) + \eta_\alpha(t) \qquad (2)$$

where $\alpha, \beta = 1, 2,\ \alpha \neq \beta$ and the inicial conditions are:

$$x_1(0) = x_2(0) = v_1(0) = v_2(0) = 0 \qquad (3)$$

Pictorically this system can be seen as ilustrated bellow:



Energy is injected into each particles by a heat bath. Both heat baths are white Gaussian noise terms can be defined in terms of their two lowest two cumulants:

$$\langle \eta_\alpha(t)\rangle \;=\; 0,$$
$$\langle \eta_\alpha(t)\eta_\beta(t')\rangle \;=\; 2\,\gamma\,T_\alpha(t)\,\delta_{\alpha\beta}\,\delta(t-t') \qquad (4)$$

where the modulated temperatures above are given by:

$$T_\alpha(t) = \bar{T}_\alpha\,\left[1 + A_\alpha\,\sin(\omega_\alpha\,t)\right]^2 \qquad (5)$$

for α = 1, 2 and $|A_\alpha| < 1$.

Taking the Laplace transformations of Eq.(1) and (2) yields:

$$\tilde{x}_1(s) \;=\; \Lambda(s)\,\tilde{\eta}_1(s) + \Delta(s)\,\tilde{\eta}_2(s), \qquad (6)$$

$$\tilde{v}_1(s) \;=\; s\,\Lambda(s)\,\tilde{\eta}_1(s) + s\,\Delta(s)\,\tilde{\eta}_2(s), \qquad (7)$$

$$\tilde{x}_2(s) \;=\; \Delta(s)\,\tilde{\eta}_1(s) + \Lambda(s)\,\tilde{\eta}_2(s), \qquad (8)$$

$$\tilde{v}_2(s) \;=\; s\,\Delta(s)\,\tilde{\eta}_1(s) + s\,\Lambda(s)\,\tilde{\eta}_2(s), \qquad (9)$$

where defining $\Gamma(s) \equiv m\,s^2 + \gamma\,s + k + k'$ one can write:

$$\Lambda(s) \;\equiv\; \frac{\Gamma(s)}{\Gamma^2(s) - k^2},\ \ \Delta(s) \;\equiv\; \frac{k}{\Gamma^2(s) - k^2}. \qquad (10)$$

The Laplace transformation for the independent noise variables is given by (α = 1, 2):

$$\frac{\langle \tilde{\eta}_\alpha(iq_i+\epsilon)\,\tilde{\eta}_\alpha(iq_j+\epsilon)\rangle}{2\,\gamma\,\bar{T}_\alpha} \;=\; \left[\frac{1}{i(q_i+q_j)+2\epsilon} + \frac{2\,A_\alpha\omega_\alpha}{[i(q_i+q_j)+2\epsilon]^2+\omega_\alpha^2}\right. \\ \left. +\; \frac{2\,A_\alpha^2\omega_\alpha^2}{[i(q_i+q_j)+2\epsilon]\,([i(q_i+q_j)+2\epsilon]^2+4\,\omega_\alpha^2)}\right] \qquad (11)$$

Thermal conductance:

Since the present model is effectively zero dimensional, the thermal conductance between the Brownian particles is defined simply as the energy flow per unit time per temperature difference between the particles, i.e., the conductive flow of energy (for particle 1, from particle 2) is defined as:

$$j_{1,2} = -\kappa\,(T_{1,2} - T_{2,1}) \qquad (12)$$

where κ is the inter-particle thermal conductance in first-order approximation.

As the coupling spring acts as the interaction channel between the particles, we define, for each particle, the transmitted heat flux (Energy/Time) as:

$$j_{t1} \;=\; -k\,(x_1(t) - x_2(t))\,v_1 \qquad (13)$$

$$j_{t2} \;=\; -k\,(x_2(t) - x_1(t))\,v_2 \qquad (14)$$

The local inter-particle elastic energy is defined as:

$$E_{el} = \frac{1}{2}k\,(x_1(t) - x_2(t))^2 \qquad (15)$$

The effective transfer flux j_{12} can now be defined:

$$j_{12} \;=\; \frac{1}{2}(j_{t1} - j_{t2}) = \;-k\,(x_1(t) - x_2(t))\left(\frac{v_1(t)+v_2(t)}{2}\right) \qquad (16)$$

The definition above corresponds to sharing the elastic energy, defined in Eq.(15), in equal parts between the neighboring particles.

A. Direct calculation of *κ*

The thermal conductance is:

$$\kappa \equiv \kappa(T, \Delta\,T) = \frac{\partial}{\partial\,\Delta\,T}\langle j_{12}\rangle_{\Delta\,T}, \qquad (17)$$

where $A_1 = A_2 = 0$, $T_1 = T$, $T_2 = T + \Delta T$, and $\langle\rangle_{\Delta T}$ is the average at $\Delta T > 0$.

The average heat flux is given by $\langle j_{12}\rangle_{\Delta T}$ and can be calculated exactly:

$$\langle j_{12}\rangle_{\Delta\,T} \;=\; -k\left\langle (x_1 - x_2)\left(\frac{v_1+v_2}{2}\right)\right\rangle = -\frac{k}{2}\left(\langle x_1 v_2\rangle - \langle x_2 v_1\rangle\right) \\ \;=\; -\frac{k\,(\mathcal{D}_1 - \mathcal{D}_3)}{2\,\mathcal{D}_2} \qquad (18)$$

where D_1, D_2 and D_3 are constants related to mechanical ones: k, k', m, g.

It is possible to show that Eq.(18) reduces to:

$$\langle j_{12}\rangle_{\Delta\,T} = 2\,k\,\mathcal{H}\Delta T \Rightarrow\ \kappa = \frac{k^2\,\gamma}{2\,\left[m\,k^2 + \gamma^2(k+k')\right]}, \qquad (19)$$

where κ is exact and independent of T and ΔT .

B. Green-Kubo calculation of *κ*

The exact expression for κ above can be compared with proposals in the literature where Green-Kubo formulations for the thermal conductance are given. The effective flux plays the role of the fluctuating flux j_{12} for a Green-Kubo relation proposed for obtaining the thermal conductance:

$$\kappa = \lim_{\Delta\,T\to 0}\frac{\langle\bar{j}\rangle_{\Delta\,T}}{\Delta\,T} = \frac{1}{T^2}\int_0^\infty dt\,\langle\bar{j}(t)\bar{j}(0)\rangle, \qquad (20)$$

Replacing the flux above into Eq.(21), we obtain the Green-Kubo expression for κ:

$$\kappa \;=\; \lim_{\Omega\to\infty}\frac{1}{\Omega}\int_0^\Omega dt\,\frac{1}{(T)^2}\int_0^\infty d\tau\,\langle j_{12}(t+\tau)j_{12}(t)\rangle_{\Delta T=0}, \\ \;=\; \lim_{z\to 0^+}\lim_{\theta\to 0^+}\frac{z}{(T)^2}\int_0^\infty dt\,e^{-zt}\int_0^\infty d\tau\,e^{-\theta\tau}\,\langle j_{12}(t+\tau)j_{12}(t)\rangle_{\Delta T=0}.$$

After some algebraic manipulation the expression for the thermal conductance becomes:

$$\kappa \;=\; \lim_{z\to 0^+}\lim_{\theta\to 0^+}\lim_{\epsilon\to 0^+}\frac{k^2}{16\,T^2}\int_{-\infty}^{\infty}\frac{dq_1}{2\pi}\int_{-\infty}^{\infty}\frac{dq_2}{2\pi}\int_{-\infty}^{\infty}\frac{dq_3}{2\pi}\int_{-\infty}^{\infty}\frac{dq_4}{2\pi}\times \\ \times\ \frac{z}{z - [(iq_1+\epsilon)+(iq_2+\epsilon)+(iq_3+\epsilon)+(iq_4+\epsilon)]}\ \frac{(iq_3+\epsilon)(iq_4+\epsilon)}{\theta - [(iq_1+\epsilon)+(iq_3+\epsilon)]}\times \\ \times\ \langle[(\tilde{x}_1(iq_1+\epsilon) - \tilde{x}_2(iq_1+\epsilon))\,(\tilde{x}_1(iq_3+\epsilon) + \tilde{x}_2(iq_3+\epsilon))]\ \times \\ \times\ [(\tilde{x}_1(iq_2+\epsilon) - \tilde{x}_2(iq_2+\epsilon))\,(\tilde{x}_1(iq_4+\epsilon) + \tilde{x}_2(iq_4+\epsilon))]\rangle \\ =\ \lim_{\theta\to 0^+}\lim_{\epsilon\to 0^+}\frac{k^2\gamma^2}{4}\int_{-\infty}^{\infty}\frac{dq_1}{2\pi}\int_{-\infty}^{\infty}\frac{dq_3}{2\pi}\,\frac{(iq_3+\epsilon)(-iq_3-\epsilon)}{\theta - [(iq_1+\epsilon)+(iq_3+\epsilon)]}\times \\ \times\ \frac{1}{[\Gamma(iq_1+\epsilon)+k][\Gamma(-iq_1-\epsilon)+k][\Gamma(iq_3+\epsilon)-k][\Gamma(-iq_3-\epsilon)-k]}.$$

This integration leads to exactly the same result as Eq. (19).

Conclusions

The coherence shown for the thermal conductance results for finite systems, calculated either directly, Eq.(19), or via the Green-Kubo approach, Eq.(24), seems to point to the validity of considering the microscopic work as the correct fluctuating flux variable to be used for coupled particle systems. In our case, despite the somewhat involved aspects of the algebra, the final value for is quite simple and carries the influence of both couplings, *k* and *k'*, the friction coefficient, and the inertia *m*. The program we followed in order to find is equivalent to solving the exact equations of motion of the Brownian particles system for each realization of the noise functions, and then taking the average over the noise. No approximations of any sort are necessary once the basic model is provided. For further details see **WAMM and DOSP PRE 79 (09) 051116**.