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Strange Heat Flux in (An)Harmonic Networks

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We study the heat transport in systems of coupled oscillators driven out of equilibrium by Gaussian heat baths. We illustrate with a few examples that such systems can exhibit "strange" transport phenomena. In particular, *circulation* of heat flux may appear in the steady state of a system of three oscillators only. This indicates that the direction of the heat fluxes can in general not be "guessed" from the temperatures of the heat baths. Although we primarily consider harmonic couplings between the oscillators, we explain why this strange behavior persists under weak anharmonic perturbations.

KEY WORDS: Nonequilibrium statistical mechanics; entropy production; heat conduction.

1. NETWORKS OF OSCILLATORS

In this note, we consider steady states of (an)harmonic oscillators driven by heat reservoirs at different temperatures. We show, by simple examples, that "anything is possible" for such physical systems: in particular, it is basically impossible to guess in which direction energy flows. We will first describe the harmonic case and then argue why the results extend to mildly anharmonic problems.

The setup is that of n masses, all equal to 1, connected by a set of harmonic "springs," at most $n(n-1)/2$ of them. For the sake of simplicity, the position and velocity of each mass are chosen to be one-dimensional. The potential is a function $V(q_1, q_2,..., q_n)$, which is given as a positive definite quadratic form $\frac{1}{2}(\mathbf{q}, V\mathbf{q})$. The (Gaussian) heat baths interact with some (at least 2) of the n masses. Each mass is either attached to its own heat bath at temperature $T_i > 0$, with friction Γ_i, or is attached to no heat

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bath. In this case we will say that $\Gamma_i = 0$ and leave T_i undefined. The stochastic differential equations describing such a system are for $i = 1,\dots, n$:

$$dp_i = -(V\mathbf{q})_i\, dt - \Gamma_i p_i\, dt + \sqrt{2\Gamma_i T_i}\, d\omega_i(t),$$
$$dq_i = p_i\, dt,$$

where the $\omega_i(t)$ are independent Wiener processes. It will be convenient to write the problem in matrix form. Let $\mathbf{x} = (\mathbf{p}, \mathbf{q})$ denote the state of the $2n$ masses. The invariant measure of the problem (if it exists), is (up to normalization) of the form $\exp(-\frac{1}{2}(\mathbf{x}, Q^{-1}\mathbf{x}))$ with the $2n \times 2n$ matrix Q being the solution to the *Lyapunov equation*

$$QA^* + AQ = -B, \tag{1}$$

where

$$A = \begin{pmatrix} -\Gamma & -V \\ \mathbf{1} & \mathbf{0} \end{pmatrix}, \qquad B = \begin{pmatrix} 2\Gamma T & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}.$$

Here, Γ and T are the diagonal matrices whose elements are Γ_i and T_i. We denote by $\mathscr{H} = \{i: \Gamma_i \neq 0\}$ the indices of the masses in direct contact with a heat bath. The following condition assures uniqueness of the invariant measure, and can be easily derived from:[1]

Lemma 1. Consider the space $\mathscr{S}$ spanned by the vectors $\{V^k e_i, i \in \mathscr{H}, k = 0,\dots, n\}$, where e_i denotes the ith unit vector of $\mathbf{R}^n$. If $\mathscr{S} = \mathbf{R}^n$, then (1) has a unique solution. Moreover, this solution is positive definite.

When the condition of Lemma 1 is not satisfied, a change of coordinates shows that at least one mode is neither coupled to a heat bath nor to the rest of the system. The simplest example where this happens is shown in Fig. 1 (see refs. 2 and 3). The masses 1 and 2 are coupled to heat baths, while the masses 3 and 4 are only coupled to the masses 1 and 2. All the springs have the same coupling constant. Writing the equations of motion, one easily checks that the variables $q = q_3 - q_4$ and $p = p_3 - p_4$ evolve as an isolated harmonic oscillator.

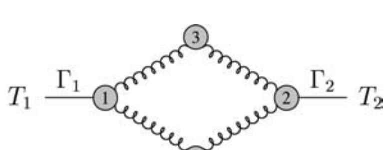

Fig. 1. Non-unique steady state.

We henceforth assume that the assumptions of Lemma 1 hold (this can be easily verified for the examples given in the sequel). Therefore, the steady state exists, is unique, and we denote by $\langle f \rangle$ the average value of an observable $f(x)$ in this state. For convenience, we shall write the matrix Q as four $n \times n$ blocks

$$Q = \begin{pmatrix} X & R \\ R^* & Y \end{pmatrix}, \tag{2}$$

where X and Y are positive symmetric matrices. As a consequence of (1), $R^* = -R$. Averages of quadratic observables are given by the elements of the matrix Q, namely $\langle p_i p_j \rangle = X_{ij}$, $\langle q_i q_j \rangle = Y_{ij}$, and $\langle p_i q_j \rangle = R_{ij}$.

2. HEAT FLUXES

We briefly recall a common definition of a heat flux between two points of the system.[4] In general, the evolution of an observable f is given by the equation $\dot{f} = \mathscr{L} f$, where $\mathscr{L}$ is the Fokker–Planck operator, in our case

$$\mathscr{L} = p \cdot \nabla_q - q \cdot V \nabla_p - p \cdot \Gamma \nabla_p + \nabla_p \cdot \Gamma T \nabla_p.$$

By definition we have $\langle \mathscr{L} f \rangle = 0$. The energy in the spring connecting points i and j is $U_{ij} = -\frac{1}{2} V_{ij} (q_i - q_j)^2$, where $V_{ij} < 0$ when the coupling is attractive. In order to obtain the heat flux between these two points, we interpret the equation $\langle \mathscr{L} U_{ij} \rangle = 0$ as a conservation equation for the energy in the spring, and identify the terms in this equation as energy fluxes. We denote the average value of the flux from i to j by $\phi_{i \to j}$, whose expression turns out to be

$$\phi_{i \to j} = V_{ij} \langle p_j (q_i - q_j) \rangle = V_{ij} \langle p_j q_i \rangle,$$

since $\langle p_i q_i \rangle = R_{ii} = 0$ by antisymmetry of the matrix R. For a point i connected to a bath, the heat flux entering the system through that point, denoted by ϕ_i, is obtained similarly, leading to

$$\phi_i = \Gamma_i (T_i - \langle p_i^2 \rangle). \tag{3}$$

Because of energy conservation, the total heat flux at every point has average zero in the steady state. In the sequel, we only consider average quantities and by *flux* we always mean *average flux in the steady state*.

Very few results are available concerning the *direction* of the heat fluxes in the system. The main one is the positivity of the global entropy production, namely

$$-\sum_{i\in\mathcal{H}}\frac{\phi_i}{T_i}>0.$$

This (strict) inequality has been proved in ref. 4 for an anharmonic chain between two baths at different temperatures. Under the conditions of Lemma 1, one can easily show that it remains valid for harmonic networks.[2] Because the matrix Q is positive definite, we can also conclude:

Lemma 2. The point(s) attached to the hottest bath(s) cannot absorb heat from the other baths. The point(s) attached to the coldest bath(s) cannot inject heat in the system.

Proof. If all the temperatures are the same, say ϑ, one easily checks that the steady state is Gibbsian, that is

$$Q=\vartheta\begin{pmatrix}\mathbf{1} & \mathbf{0}\\ \mathbf{0} & V^{-1}\end{pmatrix}. \tag{4}$$

In this equilibrium state all the fluxes vanish and the lemma is trivially verified. Consider next a system $\mathcal{S}$ with at least two different temperatures, and denote by Q the solution to the corresponding Eq. (1). Let $T_{\max}$ be the temperature of the hottest heat bath(s) of $\mathcal{S}$ and $\Theta>T_{\max}$ be an arbitrary higher temperature. We define a system $\mathcal{S}'$ as a copy of $\mathcal{S}$ but whose temperature matrix T' is given by

$$T'_i=\begin{cases}\Theta-T_i>0 & \text{for}\quad i\in\mathcal{H},\\ 0 & \text{otherwise.}\end{cases}$$

Let Q' be the solution to Eq. (1) for $\mathcal{S}'$. We note that when all the parameters but T are fixed in Eq. (1), the solution $Q(T)$ is linear in T. Therefore $Q+Q'$ is a Gibbsian matrix (4) with $\vartheta=\Theta$, in particular

$$X_{ii}+X'_{ii}=\Theta,$$

where we have used the block notation (2) for Q and Q'. Since both matrices are positive-definite, we have X_{ii} and $X'_{ii}>0$, therefore $X_{ii}<\Theta$ for any $\Theta>T_{\max}$, and finally $X_{ii}\leqslant T_{\max}$. We consider next the flux ϕ_i entering the system through a "hot" point i for which $T_i = T_{\max}$. Because of Eq. (3) we have

$$\phi_i = \Gamma_i(T_{\max} - \langle p_i^2 \rangle) = \Gamma_i(T_{\max} - X_{ii}) \geqslant 0.$$

The corresponding inequality for the cold point(s) is obtained by an equivalent construction. This concludes the proof of Lemma 2.

The two results we have mentioned give some information on how the system of oscillators exchanges heat with the baths. We are now interested in knowing how the flux propagates *within* the system of oscillators. *The main observation of this note is that "everything" is possible*, basically through superposition of elementary solutions. Indeed, by the linearity of $Q(T)$, each heat bath can be considered as an independent flux source, and the total flux at any point is simply obtained by adding the contribution of all the baths. This is how the four examples below can be found.

Remark. It should be noted that the examples we provide are not of thermodynamic nature, since they concern only a finite number of degrees of freedom. Therefore, the notion of temperature has no sharp meaning, and different definitions are possible. Thus, our results are counterintuitive only because of preconceived notions of (equilibrium) thermodynamics. On the other hand, the countercurrents of heat (energy) we illustrate below are of course really there.

Example 1. A linear chain.

Consider a linear chain composed of four equal masses, each of which is coupled to a heat bath. In the setup of Fig. 2, the heat flux is going against the (local) temperature gradient between the masses 2 and 3. Instead of defining the local temperature with the heat bath, we can also use the local kinetic energy $\langle p_i^2 \rangle$. However, we find $\langle p_2^2 \rangle = 14 < 18 = \langle p_3^2 \rangle$, thus the "backward flux" persists. This first example can be easily understood: as noted in the proof of Lemma 2, the matrix Q solving (1) is a linear function of T and so are the fluxes. Thus, we can decompose our system as the sum of two similar chains, one with temperatures (100, 0, 0, 2) and the other with (0, 2, 20, 0). The total flux in the middle

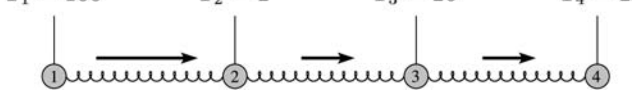

Fig. 2. The flux between 2 and 3 goes against the temperature gradient. ($\Gamma_1 = \Gamma_2 = 1$, $V_{13} = -10$, $V_{12} = V_{23} = -20$, $V_{ii} = 1 - \sum_{j \neq i} V_{ij}$ in this and all the following examples, $\phi_{3\to 1} = \phi_{2\to 3} = 0.008$, $\phi_{1\to 2} = 0.290$).

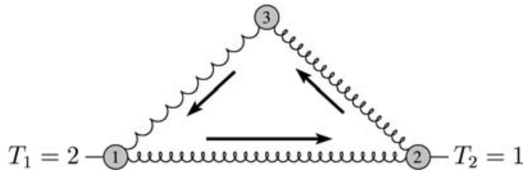

Fig. 3. A circulation of energy remains in the steady state ($\Gamma_1 = \Gamma_2 = 1$, $V_{13} = -10$, $V_{12} = V_{23} = -20$, $\phi_{3\to1} = \phi_{2\to3} = 0.008$, $\phi_{1\to2} = 0.290$).

spring still goes to the right, since temperature T_1 pushes much more energy into the chain than T_3 does.

Example 2. Circulation of heat.

In this second example, the heat injected in the system by the hot bath has two possible "channels" to reach the cold bath. What is surprising is the appearance of a "backward flux" in one of them which is not due to excess temperature as in Example 1. As a result of this, a *circulation of heat* remains in the steady state, as shown in Fig. 3. This example shows that energy fluxes between heat baths, as we understand them in this note, are *not* similar to electrical currents between potentials. Indeed, should the arrows of Fig. 3 represent electrical currents, the potentials U_i at points $i = 1$, 2, and 3 should satisfy $U_1 > U_2 > U_3 > U_1$. In other words, Fig. 3 contradicts a "Kirchoff's Law" on current loops. Such an example can also be constructed when the "triangle" is in the center of a chain connecting two heat baths.

Example 3. Three connected heat baths with different coupling constants.

The example in Fig. 4 shows that the circulation of Example 2 can also be produced when all three masses are in contact with a bath, even if two baths have the same temperature.

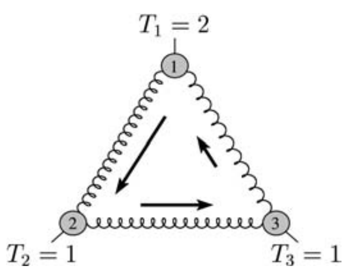

Fig. 4. Circulation in a "fully thermalized" triangle ($\Gamma_i = 1$, $V_{12} = V_{23} = -45$, $V_{13} = -30$, $\phi_{1\to2} = 0.57$, $\phi_{2\to3} = 0.35$, $\phi_{3\to1} = 0.03$).

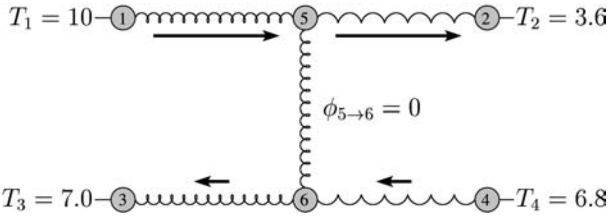

Fig. 5. The lower part of the system pumps heat from cold to hot ($\Gamma_i = 1$, $V_{15} = V_{56} = V_{36} = -40$, $V_{25} = V_{46} = -20$, $\phi_{1\to5} = 2.4$, $\phi_{6\to3} = 0.2$, $\phi_{5\to6} = 0$).

Example 4. A "heat pump."

In this last example, we construct a system that mimics a thermodynamic heat pump. Figure 5 shows two chains of three oscillators coupled through their middle point. The ends of the upper chain are connected to the hottest (T_1) and the coldest (T_2) bath, while the ends of the lower one are connected to intermediate temperatures (T_3 and T_4). Here again, the heat in the lower chain flows against the temperature gradient. The interesting point in this example is that no energy is flowing (in average) between the two chains ($\phi_{5\to6} = 0$). It is as if the upper chain was acting on the lower one through *fluctuations* only. By slightly varying the temperatures, one can even obtain $\phi_{5\to6} < 0$. This last variant is quite different from the thermodynamics of Carnot cycles, since the subsystem in which heat is pumped *releases* energy into the pump. We remark that Lemma 2 prevents us from building a pump between two baths if one of them is an extremal temperature of the system.

The situations described in these four examples are not a "far from equilibrium" behavior, because there is no such thing in harmonic systems. Indeed, because of the linearity of $Q(T)$, the fluxes in the system keep the same sign when (all) temperatures are rescaled. Moreover, fluxes are unchanged when all the temperatures are shifted by a constant. Therefore, everything we have shown can happen at arbitrary temperatures, and with arbitrarily small temperature differences. We also remark that because of the loops of heat flux, there is no possible definition of local temperature that would prevent the flux from going against the temperature gradient.

3. WEAKLY ANHARMONIC SYSTEMS

It is well-known that the heat transport in harmonic systems does not reproduce the usual macroscopic laws, in particular Fourier's law does not hold.[5] Justification is commonly seen in the fact that the modes of a harmonic system are extended, causing the heat to be transported ballistically rather than diffusively. Note however that phenomena described in this note continue to hold in a weak anharmonic limit. Indeed, consider a slight perturbation of the coupling, for instance

$$V_\varepsilon(q) = \frac{1}{2}(q, Vq) + \frac{\varepsilon}{4} \sum_{i<j} c_{ij} (q_i - q_j)^4.$$

The existence of a unique steady state for certain systems with such a potential is proved in ref. 6; since every point in our examples is reached in a simple way from a heat bath, the results of ref. 6 generalize to this case. The corresponding (smooth) invariant measure ρ_ε is not Gaussian but still decays rapidly at large energies. If ρ_ε as a function of ε is sufficiently regular around $\varepsilon = 0$, fluxes are continuous functions of this parameter. Then, for every example we have shown, one can find a small enough ε so that fluxes of the perturbed system have the same direction as those in the unperturbed system. Although a written proof of the regularity of ρ_ε does not seem to be available yet, this result is believed to be true.[7, 8] A key point is the following: as explained in ref. 9, the system in the steady state spends most of its time below a certain energy level, with only rare excursions to high energies. With sufficiently small ε, one can make sure that the anharmonicity is irrelevant in arbitrary long parts of the dynamics.

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