

Normal heat conductivity in a periodic chain of anharmonic oscillators.

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We consider a periodic chain of coupled and pinned anharmonic oscillators subject to a non-equilibrium random forcing. Assuming that the six-point correlation functions of the stationary state factorize in terms of the two-point correlation functions, we show that the heat current going through the system is consistent with Fourier law and that the conductivity behaves as $\kappa \sim \frac{1}{\lambda^2 T^2}$ where λ is the anharmonic coupling strength.

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The analytical derivation of the Fourier's law of heat conduction in extended Hamiltonian systems remains to this day a challenging question. See [2, 5] for a review of various aspects of the problem. A qualitative explanation for Fourier law has been provided by Peierls for the case of crystalline solids. Peierls idea essentially consists in considering the lattice excitations of the crystal, the phonons, as particles interacting weakly through the nonlinear forces acting between the atoms. By analogy with the case of dilute gases, a Boltzmann equation for phonons has been derived and refined over the years, see [8] and references therein. Our aim is to provide, along Peierls ideas, a simple computational argument for the finite conductivity of periodic one-dimensional pinned anharmonic crystals. In order to do so, we derive a stationary Boltzmann-type equation for the correlations of the variables corresponding to the heat current flowing through the chain.

Crystalline solids submitted to a heat flow are often modeled by a chain of oscillators where each oscillator move around some equilibrium position located on a regular lattice. Each oscillator interact with its nearest neighbours and also possibly with some substrate. The chain is coupled to heat baths at different temperatures by some random forcing and friction acting only on the particles at the boundaries of the chain. Although mathematical properties of such systems have been extensively studied, see [6] for a review, very little is known analytically about their physical properties, except in cases where the interactions are quadratic or almost quadratic, [4, 7]. Numerous numerical simulations have been performed, see [5] and references therein, strongly supporting that Fourier law is verified in pinned anharmonic chains. The effect of the nonlinearity on the behavior of the current with respect to the size of the system is difficult to tackle in part because of the lack of translation invariance of the equations of motions. This lack of translation invariance, which has its source in the absorption and injection of energy at the boundaries of the chain, is an essential element of such non-equilibrium situations. Here, we single out the effect of the nonlinearity on the conductivity properties by considering a periodic chain submitted to a random forcing which creates, in the stationary state, a net current of heat. This drive out of equilibrium

is achieved by applying a random forcing which excites more the waves traveling in one direction than the ones traveling in the opposite direction. In the same spirit as in Evans heat flow algorithm [3], we believe that, by separating the difficulties arising from the lack of translation invariance and the ones coming from the nonlinearities, our model could prove to be useful to understand the non-equilibrium properties of chains of oscillators.

We now describe our result. The equation for the evolution of the average energy current J_k carried by the mode of wavenumber k of the chain will have the form,

$$\frac{d}{dt} J_k(t) = -\gamma J_k(t) + \lambda \mathcal{N}_k(t) + S_k. \quad (1)$$

The first term on the RHS of this equation is a damping term coming from the coupling of the chain to an external friction represented by the coefficient γ . The second term comes from the Hamiltonian evolution and vanishes when the anharmonic part of the interaction is zero, i.e., when $\lambda = 0$. The third term represents an external "creation" of current at constant rate. It models the local temperature gradient in the non-periodic chain. Equation (1) will therefore yield a balance equation for the current carried by the mode k in the stationary state. We will show that under some assumptions on the stationary state (the "closure" assumption), \mathcal{N}_k is analogous to a friction term, yielding in the end a conductivity $\kappa \sim \frac{1}{\lambda^2 T^2}$. From a mathematical point of view, there is an important difference between the part coming from the external friction and the part coming from \mathcal{N}_k . Whereas the friction acts as a diagonal operator on the vector J , we will see that $\mathcal{N}_k \sim A(J)_k$ where A is a non-diagonal linear operator. The properties of this operator are essentially governed by resonances in the four-body interactions between phonons, which we analyze in the limit of a large harmonic pinning strength μ . In particular, we show explicitly that the origin of the finite conductivity is to be found in μ -dependent resonances corresponding to *umklapp* processes. In this paper, we concentrate only on the effect of the term coming from the nonlinearity \mathcal{N}_k . In particular, the source term S_k is put by hand. However, in the non-periodic case, it should come naturally from the structure of the equations.

The Model. We consider particles located on a periodic

lattice described by their positions and momenta coordinates (q_i, p_i) with $i \in 1, \dots, N$. For the sake of notational simplicity, we assume that N is divisible by 4. The dynamics of the particles is governed by the Hamilton equations and an external random forcing. The Hamiltonian that we consider is of the form

$$H(\underline{q}, \underline{p}) = \sum_{i=1}^N \left[\frac{p_i^2}{2} + \omega^2 \mu^2 \frac{q_i^2}{2} + \frac{\lambda}{4} q_i^4 + \frac{\omega^2}{2} (q_i - q_{i-1})^2 \right]. \quad (2)$$

The anharmonic interaction is only in the on-site part of the Hamiltonian. The same analysis as found below may be carried out when the interaction between nearest neighbours contains also a quartic part. The fact that there is an on-site (large) harmonic interaction makes the distinction between the two cases irrelevant. We first consider the harmonic case $\lambda = 0$. We introduce the Fourier coordinates for the periodic linear chain by $Q_k = \frac{1}{\sqrt{N}} \sum_{j=1}^N e^{i \frac{2\pi}{N} k j} q_j$, with $-N/2 + 1 \leq k \leq N/2$. The P_k coordinates are defined in a similar fashion. We recall for further purposes that $Q_k^* = Q_{-k}$ and $P_k^* = P_{-k}$. In the complex coordinates,

$$A_k^\pm = \frac{1}{\sqrt{2\omega_k}} (P_k \pm i\omega_k Q_k), \quad (3)$$

with $\omega_k^2 = \omega^2 (\mu^2 + 4 \sin^2(\frac{\pi k}{N}))$, the Hamilton equations for the linear periodic chain read

$$dA_k^\pm = \pm i\omega_k A_k^\pm dt. \quad (4)$$

Those equations give the temporal evolution of the amplitudes of the waves with wave number k traveling through the chain in the positive or negative direction. Our (non-equilibrium) model is defined in the linear case by the system of stochastic equations

$$dA_k^\pm = \pm i\omega_k A_k^\pm dt - \frac{\gamma}{2} (A_k^+ + A_k^-) dt + dW_k^\pm, \quad (5)$$

where the Wiener processes W_k^\pm satisfy the relations

$$d(W_k^s W_{k'}^{s'}) \equiv I_{k,k'}^{s,s'} dt \equiv 2 \left[\frac{\gamma T}{\omega_k} + (s-s')\tau \alpha \left(\frac{\pi k}{N} \right) \right] \delta(k+k') dt. \quad (6)$$

In (5), the term in γ is the usual friction term acting only on the momenta P_k . The Wiener processes represent the random injection of energy in the system. In (6), α is an odd, dimensionless function of period π whose properties will be discussed below. The first term in (6) is the usual term giving the equilibrium dynamics. In terms of the original variables q, p , the second term amounts to excite also the q variables. We interpret τ as the non-equilibrium parameter of our model. When τ is zero, the periodic chain is in thermal equilibrium at temperature T . When $\tau \neq 0$, a stationary heat (energy) current proportional to τ is created in the chain.

In order to see those points, we recall first that the energy current in the periodic chain reads

$$J = \frac{\omega^2}{N} \sum_{k=-N/2+1}^{N/2} \sin(2\pi k/N) \Im(Q_{-k} P_k), \quad (7)$$

where $\Im(z)$ denotes the imaginary part of a complex z . We define the two-point correlation functions in the stationary state,

$$\Phi_{k,k'}^{s,s'} \equiv \langle A_k^s A_{k'}^{s'} \rangle, \quad (8)$$

where $\langle \cdot \rangle$ denotes the average w.r.t. the stationary measure. Since $\Im(\langle Q_{-k} P_k \rangle) = \frac{1}{2} (\Phi_{k,-k}^{+-} - \Phi_{k,-k}^{-+}) = \frac{1}{2} (\langle |A_k^+|^2 \rangle - \langle |A_k^-|^2 \rangle)$, we get

$$\langle J \rangle = \frac{\omega^2}{2N} \sum_{k=-N/2+1}^{N/2} \sin(2\pi k/N) [\langle |A_k^+|^2 \rangle - \langle |A_k^-|^2 \rangle]. \quad (9)$$

This identity expresses the fact that the energy current is the difference of the current carried by waves traveling in the positive and negative directions. From (5), we derive the equation for the two-point correlation functions,

$$i(s\omega_k + s'\omega_{k'}) \Phi_{k,k'}^{s,s'} = \gamma \Phi_{k,k'}^{s,s'} + \frac{\gamma}{2} (\Phi_{k,k'}^{-s,s'} + \Phi_{k,k'}^{s,-s'}) - \frac{1}{2} I_{k,k'}^{s,s'} \quad (10)$$

with $I_{k,k'}^{s,s'}$ given in (6). In the case where $\tau = 0$, (10) is readily solved to yield, using (6),

$$\Phi_{k,k'}^{s,s'} = \frac{T}{\omega_k} \delta(k+k') \delta(s+s'). \quad (11)$$

This is of course equivalent to $\langle |P_k|^2 \rangle + \omega_k^2 \langle |Q_k|^2 \rangle = 2T$ and $\langle P_k Q_l \rangle = 0, \forall k, l$.

When $\tau \neq 0$ and for $l = -k$, one obtains from (10) and (6),

$$J_k \equiv \Phi_{k,-k}^{+-} - \Phi_{k,-k}^{-+} = 4\tau \gamma^{-1} \alpha \left(\frac{\pi k}{N} \right), \quad (12)$$

which is the balance equation (1) in the stationary state for the harmonic case. We note that by definition, $J_k = -J_{-k}$. Using (9) and the fact that α is an odd function, we get $\langle J \rangle = 2\omega^2 \gamma^{-1} \tau \int_0^{\pi/2} \alpha(x) \sin(2x) dx$ for large N . We observe that, at this stage, we have a large freedom of choice for the function α . Indeed, as long as the above integral is non-zero, there will be a non-zero heat current flowing through the system. However, we will see at the end of the paper that the choice of physically relevant α 's is somewhat constrained by the presence of the nonlinear terms. We also remark that, as we interpret τ as a local non-equilibrium parameter, the conductivity in the harmonic case, $\kappa \equiv \langle J \rangle / \tau \sim \gamma^{-1} \omega^2$, behaves as in the harmonic chain coupled to self-consistent reservoirs [1]. It reflects the fact that when $\lambda = 0$ in the balance equation (1), the only term damping the current carried by each mode comes from the external friction. We will see below that the anharmonic interactions modify that behaviour of the conductivity. Finally, we note that there are many choices for $I_{k,k'}^{s,s'}$ that would give a current proportional to τ as in (12). However, there is basically only one which is a linear function of τ , gives the equilibrium correlation when $\tau = 0$, and does not introduce higher-order corrections (τ^2) in the correlation functions of the stationary state $\Phi_{k,k'}^{s,s'}$.

Let us now consider the anharmonic case $\lambda \neq 0$. The equations of motion (5) become

$$dA_k^\pm = \left[\pm i\omega_k A_k^\pm - \frac{\gamma}{2}(A_k^+ + A_k^-) - \frac{i\lambda}{N} R_k \right] dt + dW_k^\pm, \quad (13)$$

where

$$R_k = \sum_{k_1, k_2, k_3} \sum_{s_1, s_2, s_3} \delta(k - k_1 - k_2 - k_3) s_1 s_2 s_3 L_{kk_1 k_2 k_3} A_{k_1}^{s_1} A_{k_2}^{s_2} A_{k_3}^{s_3}, \quad (14)$$

and $L_{kk_1 k_2 k_3} = (16\omega_k \omega_{k_1} \omega_{k_2} \omega_{k_3})^{-1/2}$. Here and below, unless otherwise specified, the sums are over the k_i such that $-N/2 + 1 \leq k_i \leq N/2$ and $s_i = \pm 1$.

From (13), the equations for the n -point correlation functions in the stationary state,

$$(\Phi^{(n)})_{k_1, \dots, k_n}^{s_1, \dots, s_n} \equiv \langle A_{k_1}^{s_1} \dots A_{k_n}^{s_n} \rangle, \quad (15)$$

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$$i\bar{\omega}^{(n)} \Phi^{(n)} = \gamma \Gamma^{(n)}(\Phi^{(n)}) + i \frac{\lambda}{N} M^{(n)}(\Phi^{(n+2)}) - \frac{1}{2} I^{(n)}(\Phi^{(n-2)}), \quad (16)$$

where $\bar{\omega}^{(n)}$ is the combination of frequencies,

$$(\bar{\omega}^{(n)})_{k_1, \dots, k_n}^{s_1, \dots, s_n} = \sum_{i=1}^n s_i \omega_{k_i},$$

and

$$\begin{aligned} (\Gamma^{(n)}(\Phi^{(n)}))_{k_1, \dots, k_n}^{s_1, \dots, s_n} &= \frac{n}{2} (\Phi^{(n)})_{k_1, \dots, k_n}^{s_1, \dots, s_n} \\ &+ \frac{1}{2} \sum_{i=1}^n (\Phi^{(n)})_{k_1, \dots, k_n}^{s_1, \dots, -s_i, \dots, s_n}. \end{aligned} \quad (17)$$

$I^{(n)}$ gathers the effects of the random forcing, the special case $I^{(2)}$ being given in (6). The explicit expression of $M^{(n)}$ will be given below in the relevant cases. For $n = 2$ and $k_1 = -k_2 = k$, one gets from (16) the balance equation in the stationary state, proceeding as to obtain (12),

$$\gamma J_k + \frac{i\lambda}{N} \Psi_k = 4\tau \alpha \left(\frac{\pi k}{N} \right), \quad (18)$$

where J_k has been defined in (12) and

$$\begin{aligned} \Psi_k &\equiv (M^{(2)}(\Phi^{(4)}))_{k, -k}^{+-} - (M^{(2)}(\Phi^{(4)}))_{k, -k}^{-+} \\ &= 2i \sum_{k_1, k_2, k_3} \sum_{s_1, s_2, s_3} \delta(k + k_1 + k_2 + k_3) s_1 s_2 s_3 \\ &\quad L_{kk_1 k_2 k_3} \Im[(\Phi^{(4+)})_{k, k_1, k_2, k_3}^{+s_1 s_2 s_3}], \end{aligned} \quad (19)$$

with

$$(\Phi^{(n\pm)})_{k_1, \dots, k_n}^{s_1, \dots, s_n} \equiv (\Phi^{(n)})_{k_1, \dots, k_n}^{s_1, \dots, s_n} \pm (\Phi^{(n)})_{k_1, \dots, k_n}^{-s_1, \dots, -s_n}. \quad (20)$$

The remainder of this paper is devoted to solving equation (18) for J_k .

Closure and Linearization. In this section, we derive an explicit expression for Ψ in terms of J . The first step is to approximate the n -point correlation functions (15) by products of $\Phi^{(2)}$, turning (18) into a close but non-linear equation. This "closure" assumption on the non-equilibrium stationary measure is widely used in various forms in weak turbulence theory or in the study of dilute gases via the BBGKY hierarchy of equations. The second step is to linearize the resulting equation around the equilibrium solution (11). This is done in the spirit of taking a small temperature gradient or, in our case, a small parameter τ .

Closing as described above the expression (19) for Ψ yields zero after linearization, so that equation (18) is identical to equation (12) for the harmonic case. We thus first express $\Phi^{(4)}$ in (19) in terms of $\Phi^{(6)}$. Inverting (16) for $\Phi^{(4)}$, one can show that at lowest order in γ

$$\Im[(\Phi^{(4+)})_{k, k_1, k_2, k_3}^{+s_1 s_2 s_3}] = -\frac{\lambda}{N} (\Omega_\gamma M^{(4)}(\Re[\Phi^{(6-)}]))_{k, k_1, k_2, k_3}^{+s_1 s_2 s_3}, \quad (21)$$

where

$$(\Omega_\gamma)_{k_1, k_2, k_3, k_4}^{s_1 s_2 s_3 s_4} = \frac{2\gamma}{4\gamma^2 + (s_1 \omega_{k_1} + s_2 \omega_{k_2} + s_3 \omega_{k_3} + s_4 \omega_{k_4})^2}.$$

In (21), we have dropped a term containing $\Im[\Phi^{(6+)}]$ as well as the contribution from the Itô term $I^{(4)}$, since they vanish later in the computation. We next plug (21) into (19) and use the Wick formula to express $\Phi^{(6)}$ in terms of $\Phi^{(2)}$. Linearizing around the equilibrium solution (11) results in an expression for Ψ which depends solely on J and contains terms which may be represented graphically by 12 topologically distinct diagrams. Those diagrams are structurally similar to the usual diagrams of the equilibrium $\lambda\phi^4$ theory. The main difference comes from the presence of the quantity which is the unknown of the problem, i.e., the vector J .

For large pinning interaction μ , the result of the computation is (here and below, c denotes combinatorial positive factors),

$$\Psi_k = -\frac{cT^2}{\omega^6 \mu^6} \frac{i\lambda}{N} \sum_{l, n} (\Omega_\gamma)_{k, l, n, k+l+n}^{+-+-} [J_k + J_l + J_n - J_{k+l+n}]. \quad (22)$$

The RHS is essentially the linear operator A mentioned in the introduction. We remark that, in quantum-mechanical language, only the interactions conserving the number of phonons contribute, as the other interactions are free from resonances. We will estimate (22) in the limit of large N and for small γ , more precisely, $1 \gg \gamma/\omega \gg 1/N$. We first observe that the main contributions to the sum will arise from the resonances in Ω_γ , i.e., for lattice points (l, n) near the zeros of the function $f_x : [-\frac{\pi}{2}, \frac{\pi}{2}]^2 \rightarrow \mathbf{R}$,

$$\begin{aligned} f_x(y, z) &= \sqrt{\mu^2 + 4 \sin^2(x) + \sqrt{\mu^2 + 4 \sin^2(y)}} \\ &\quad - \sqrt{\mu^2 + 4 \sin^2(z) - \sqrt{\mu^2 + 4 \sin^2(x + y + z)}}. \end{aligned} \quad (23)$$

A careful analysis reveals that for $\mu^2 > 0$, the zeros of f_x form three smooth curves. Two of these curves are obvious and given by $x + z = 0$, and $y + z = 0$. These resonances do not contribute to the sum, however, since the combination of J 's in (22) vanishes for $k + n = 0$ or $l + n = 0$. This corresponds to the so-called *normal* processes. The third curve, corresponding to the *umklapp* processes, depends on μ and is difficult to localize explicitly. For large μ , it is given by $x + y = \frac{\pi}{2} + \mathcal{O}(1/\mu^2)$. Performing the sum over l in (22) in the above-mentioned parameter regimes thus yields at lowest order in γ and $1/\mu$ (resonances are at $l = -k + N/2$),

$$\Psi_k = -i\lambda \frac{cT^2}{\omega^7 \mu^5} \sum_n \frac{J_k^- + J_n^-}{|\sin(\frac{\pi(k+n)}{N}) \cos(\frac{\pi(k-n)}{N})|}, \quad (24)$$

where we have defined $J_k^- \equiv \frac{1}{2}(J_k - J_{k+N/2})$. Before proceeding to solving equation (18), we note that any vector J can be decomposed as $J = J^+ + J^-$ where J^- as above and $J_k^+ \equiv \frac{1}{2}(J_k + J_{k+N/2})$ have the symmetry properties $J_{k+N/2}^\pm = \pm J_k^\pm$. It then follows from (24) that J^+ does not contribute to Ψ , and that $\Psi = \Psi^-$.

Solution to the Current Equation. Recall that J is odd and periodic of period N . We first observe that J^+ does not contribute to the average current $\langle J \rangle$ given by (9). This follows from $\sum_k \sin(2\pi k/N) J_k^+ = 0$. Since, in addition, J is mapped by (24) into a vector Ψ with $\Psi = \Psi^-$ and since J^+ does not contribute to Ψ , we need only to consider in equation (18) odd forcings α and odd currents J satisfying $\alpha(\frac{\pi k}{N} + \frac{\pi}{2}) = -\alpha(\frac{\pi k}{N})$ and $J = J^-$. We denote by \mathcal{S}^- the subspace of such vectors J , in which equation (18) becomes

$$\gamma J_k + c \frac{\lambda^2 T^2}{\omega^7 \mu^5} \mathcal{L}(J)_k = 4\tau \alpha\left(\frac{\pi k}{N}\right), \quad (25)$$

where $\mathcal{L} : \mathcal{S}^- \rightarrow \mathcal{S}^-$ is given by

$$\mathcal{L}(J)_k = \frac{1}{N} \sum_{k'} \frac{J_k + J_{k'}}{|\sin(\frac{\pi(k+k')}{N}) \cos(\frac{\pi(k-k')}{N})|}. \quad (26)$$

We now proceed to analyze the linear operator \mathcal{L} . The subspace \mathcal{S}^- has dimension $N/4$, and a basis for \mathcal{S}^- is given by $\mathcal{J}_k^n = \sin(2\pi(2n+1)\frac{k}{N})$, $n = 0, \dots, N/4 - 1$. We let $\mathcal{A}^n \equiv \mathcal{L}(\mathcal{J}^n)$. A direct computation shows that the set of \mathcal{A}^n , $n = 0, \dots, N/4 - 1$, also forms a basis of \mathcal{S}^- and that \mathcal{L} is uniformly invertible (in N). This implies that the first term on the LHS of (25) is negligible for γ small. Furthermore, it follows from $\sum_k \sin(\frac{2\pi k}{N}) \mathcal{J}_k^n = 0$ for $n \neq 0$ that only \mathcal{J}_k^0 contribute to the current (9). Therefore, the only contribution of the noise α to the current is the component of α along \mathcal{A}^0 , say α^0 , where

$$\mathcal{A}_k^0 \equiv \mathcal{L}(\mathcal{J}^0)_k = 2 \operatorname{sign}(k) \left(\frac{1}{4} - \left| \operatorname{sign}(k) \frac{k}{N} - \frac{1}{4} \right| \right). \quad (27)$$

One thus finally obtains from (9),

$$\langle J \rangle \sim \frac{\omega^9 \mu^5}{\lambda^2 T^2} \alpha^0 \tau, \quad (28)$$

together with a conductivity $\kappa \equiv \langle J \rangle / \tau \sim \frac{\omega^9 \mu^5}{\lambda^2 T^2}$.

Conclusions. Not surprisingly, in terms of the original variables q, p , a forcing of the form (27) amounts to excite the variables q_i and p_{i+1} in a very correlated manner. The correlations between the other components of the external forcing corresponding to variables q_i, p_j decrease from that maximal value like $(i - j)^{-2}$.

Our computation makes precise the physical picture that the mechanism responsible for the normal conductivity in anharmonic chains is the four-body interactions between phonons. When N becomes large, the non-equilibrium stationary measure is well approximated by a system where the phonons evolve freely and interact among themselves at an average time interval given by the inverse of the conductivity found above. This interaction is solely responsible for the degradation of the current as $\gamma \rightarrow 0$.

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