Fourier's law from Closure Equations

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Abstract

We give a rigorous derivation of Fourier's law from a system of closure equations for a nonequilibrium stationary state of a Hamiltonian system of coupled oscillators subjected to heat baths on the boundary. The local heat flux is proportional to the temperature gradient with a temperature dependent heat conductivity and the stationary temperature exhibits a nonlinear profile.

One of the simplest and most fundamental nonequilibrium phenomena is heat conduction in solids. It is described by a macroscopic equation, Fourier's law, which states that a local temperature gradient is associated with a flux of heat $\mathcal{J}$ which is proportional to the gradient:

$$\mathcal{J}(x) = -k(T(x))\nabla T(x) \tag{1}$$

where the *heat conductivity* $k(T(x))$ is a function only of the temperature at x.

Despite its fundamental nature, a derivation of Fourier's law from first principles, or even within a suitable approximation, such as a Boltzmann type equation, lies well beyond what can be mathematically proven (for reviews on the status of this problem, see [3], [6] and [13]). The quantities T and $\mathcal{J}$ in (1) are macroscopic variables, statistical averages of the variables describing the microscopic dynamics of matter. A first principle derivation of (1) entails a definition of T and $\mathcal{J}$ in terms of the microscopic variables and a proof of the law in some appropriate limit.

In this letter we outline a rigorous proof [4] of Fourier's law starting from a closure approximation of the equations for the nonequilibrium stationary state of a Hamiltonian system subjected to boundary heat baths. The physical situation we have in mind is a slab of crystal of linear extension N heated at the two ends by temperatures T_1 and T_2. In this case one would expect ∇T and $\mathcal{J}$ to be $\mathcal{O}(1/N)$ and (1) to hold up to corrections of order $o(1/N)$. This is indeed what we prove in our model together with a detailed description of the temperature distribution in the bulk.

Since (1) is a macroscopic law it is expected to hold for a classical system as well as for a quantum one and the quantum corrections are expected to be small except at low temperatures. A classical toy model describing the above situation which has been intensively discussed in

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recent years is given by coupled oscillators organized on a strip of width N in d-dimensional cubic lattice $\mathbb{Z}^d$. The oscillators are indexed by lattice points $x = (x_1, \ldots, x_d)$ with $0 \le x_1 \le N$ and carry momenta and coordinates (p_x, q_x). The dynamics of the oscillators consists of two parts: Hamiltonian dynamics in the bulk and noise on the boundary modelling heat baths at temperatures T_1 and T_2.

We consider a Hamiltonian of the form

$$H(q,p) = \frac{1}{2}\sum_{x\in V} p_x^2 + \frac{1}{2}(q, \omega^2 q) + \frac{\lambda}{4}\sum_{x\in V} q_x^4 \tag{2}$$

which describes a system of coupled anharmonic oscillators with coupling matrix ω^2, i.e. $(q, \omega^2 q) = \sum q_x q_y \omega^2(x-y)$. The noise is specified by the Gaussian random variables $\xi_x(t)$ at sites x on the boundary with covariance

$$< \xi_x(t)\xi_y(t') >= 4\gamma\delta_{xy}(T_1\delta_{x_1 0} + T_2\delta_{x_1 N})\delta(t-t') \equiv 2C_{xy}\delta(t-t'). \tag{3}$$

The (stochastic) dynamics is given by $\dot{q}_x = p_x$ and

$$\dot{p}_x = (-\frac{\partial H}{\partial q_x} - \gamma_x p_x) + \xi_x \tag{4}$$

where the friction is $\gamma_x = \gamma(\delta_{x_1 0} + \delta_{x_1 N})$ (more precisely, (4) is a Ito stochastic differential equation). These equations define a Markov process $(q(t), p(t))$ and we are interested in the stationary states for this process.

In the *equilibrium* case of equal temperatures, $T_1 = T_2 = T$, an explicit stationary state is given by the Gibbs state $Z^{-1}e^{-\beta H(q,p)}dqdp$ of the Hamiltonian H with inverse temperature $\beta = 1/T$. When $T_1 \neq T_2$ there is no such simple formula and, indeed, in our setup, even the existence of a stationary state is an open problem. In the $d = 1$ case of a finite chain of N oscillators the existence is proved under conditions (see [10] for a review of such results, first obtained in [5]) as well as the convergence of the Markov process to this state as $t \to \infty$.

Supposing that we have a stationary state, let us formulate the statement (1). Writing H as a sum of local terms, each one pertaining to a single oscillator: $H = \sum_{x\in\Lambda} H_x$, one has up to noise terms $\dot{H}_x = \nabla \cdot j(x)$, where the microscopic heat current $j(x)$ will depend on p_y and q_y for y near x provided the coupling matrix ω^2 is short ranged. Let also $t(x) = \frac{1}{2}p_x^2$ be the kinetic energy of the oscillator indexed by x. Then, the macroscopic temperature and heat current in eq. (1) are defined by $T(x) =< t(x) >_\mu$ and $\mathcal{J}(x) =< j(x) >_\mu$ where $< \cdot >_\mu$ denotes expectation in the stationary state.

The only rigorous results in our model as far as deriving (1) are for the harmonic case of quadratic H [11, 12]. In that case, Fourier's law *does not hold*: the current $j(x)$ is $\mathcal{O}(1)$ as $N \to \infty$ whereas $\nabla T = 0$ except near the boundary. If $\lambda \neq 0$ the law seems to hold in simulations in all dimensions [1]. In an analogous momentum conserving model conductivity seems anomalous in low dimensions: k in (1) depends on N as N^α in $d = 1$ and logarithmically in $d = 2$. It is a major challenge to explain the α which, numerically, seems to be in the interval $[1/3, 2/5]$ (see [7], [8], [9] for theories on α).

In this paper we suppose the stationary state exists and we study its properties via its correlation functions. Let us denote $(q_x, p_x) = (u_{1x}, u_{2x})$, $\Lambda(u^{\otimes 3})_{\alpha x} = -\lambda\delta_{\alpha,2}q_x^3$, $(\Gamma u)_x = (0, \gamma_x p_x)^T$ and $\eta = (0, \xi)^T$. Then (4) becomes

$$\dot{u}(t) = \Big((A-\Gamma)u + \Lambda(u^{\otimes 3})\Big) + \eta(t) \tag{5}$$

where $A = \begin{pmatrix} 0 & 1 \\ -\omega^2 & 0 \end{pmatrix}$. Applying (5) to the stationary state correlation functions

$$G_n(x_1, ..., x_n) =< u_{x_1} \otimes ... \otimes u_{x_n} >$$

these are seen to be solutions of the Hopf equations

$$(A_n - \Gamma_n)G_n + \Lambda_n G_{n+2} + \mathcal{C}_n G_{n-2} = 0. \tag{6}$$

where $A_n = \sum A_{x_i}$ and Γ_n is defined similarly. Λ_n and $\mathcal{C}_n$ are linear operators involving the quartic vertex and noise covariance C_{xy} of (3) respectively. The equations (6) have the drawback that they do not "close": to solve for G_n, we need to know G_{n+2}.

We will now introduce an approximation that will lead to a closed set of nonlinear equations for G_2. For this we note that for λ small, the equilibrium $T_1 = T_2$ measure is close to Gaussian. When $T_1 \neq T_2$ we expect this to remain true and we look for a Gaussian approximation to equation (6) for small λ by means of a *closure*, i.e. expressing the G_n in terms of G_2. Let G_4^c be the connected correlation function describing deviation from Gaussianity. Then the first equation in the hierarchy (6) reads:

$$(A_2 - \Gamma_2 + \Sigma_2)G_2 + \Lambda_2 G_4^c + \mathcal{C} = 0 \tag{7}$$

where $\Sigma_2(G_2)G_2 = \Lambda_2 \sum G_2 \otimes G_2$. The simplest closure would be to drop the $\Lambda_2 G_4^c$ from (7). This leads to a nonlinear equation for G_2. It turns out that the solution to this equation is qualitatively similar to the $\lambda = 0$ case, i.e. G_2 does not exhibit a temperature profile nor a finite conductivity. The only effect of the nonlinearity is a renormalization of ω.

The next equation in the hierarchy becomes after some some algebra

$$(A_4 - \Gamma_4 + \Sigma_4)G_4^c + b(G_2) + \Lambda_4 G_6^c = 0, \tag{8}$$

where G_6^c is the connected six point function,

$$\Sigma_4(G_2)G_4^c = \sum(\Lambda_4(G_2 \otimes G_4^c) - G_2 \otimes \Lambda_2 G_4^c).$$

and

$$b(G_2) = \sum_p \Lambda_4'(G_2 \otimes G_2 \otimes G_2),$$

where Λ_4' has Λ acting on all the three factors G_2.

(7) and (8) yield an exact equation for the two point function with the connected six point function as an input. Our closure approximation consists of dropping the G_6^c term in (8) thereby yielding a closed set of equations for G_2. For simplicity we also drop the operators Σ_2, Σ_4 and Γ_4: these could be included in our analysis, but do not change the main structure that is due to the term $b(G_2)$. Hence the closure equation we study is for $G = G_2$:

$$(A_2 - \Gamma_2)G + \mathcal{N}(G) + \mathcal{C} = 0 \tag{9}$$

with

$$\mathcal{N} = -\Lambda_2 A_4^{-1} b(G). \tag{10}$$

To write this more concretely, let us introduce the matrices $Q_{xy} =< q_x q_y >$, $P_{xy} =< p_x p_y >$ and $J_{xy} =< q_x p_y >$. Clearly $\dot{Q} = J + J^T$ so the (1,1)-component of (9) says $J_{xy} = -J_{yx}$ and we can write $G = \begin{pmatrix} Q & J \\ -J & P \end{pmatrix}$.

Next, anticipating translation invariance in the directions orthogonal to the 1-direction we write

$$G(x,y) = \int e^{ip(x_1+y_1)+ik(x-y)} G(p,k) dp dk \tag{11}$$

where the integrals over p and k_1 are Riemann sums on a $\frac{\pi}{2N}$ lattice. The inverse of A_4 is written as

$$-A_4^{-1} = \int_0^\infty e^{tA_4} dt = \int_0^\infty R(t)^{\otimes 4} dt$$

where $R(t) = e^{tA}$. In Fourier space the latter is

$$\widehat{R}(t,q) = \frac{1}{2} \sum_{s=\pm 1} e^{(is\omega(q)-\epsilon)t} \begin{pmatrix} 1 & -is\omega(q)^{-1} \\ is\omega(q) & 1 \end{pmatrix}, \tag{12}$$

Then some algebra yields the following expression for the nonlinear term

$$N(p,k) = \sum_{\mathbf{s}} \int d\nu (\sum_1^4 s_i \omega(p_i + k_i) + i\epsilon)^{-1} \prod_{i=1}^2 W_{s_i}(p_i, k_i) \cdot \begin{pmatrix} 0 & 0 \\ 1 & is_4\omega(p_4+k_4) \end{pmatrix}$$
$$s_3\omega(p_3+k_3)\Big[\omega(p_3+k_3)^{-2}\delta(2p_3)W_{s_4}(p_4,k_4) - \omega(p_4+k_4)^{-2}\delta(2p_4)W_{s_3}(p_3,k_3)\Big] \tag{13}$$

where

$$d\nu \;=\; \delta(2p - \sum(p_i+k_i))\delta(\sum(p_i-k_i))\delta(p-k-p_4-k_4) d\mathbf{p} d\mathbf{k}, \tag{14}$$

and $\mathbf{k} = (k_i)_{i=1}^4$ and similarily for $\mathbf{p}$ and $\mathbf{s}$. W is the following combination

$$W_s(p,q) = \widehat{Q}(p,q) + is\omega(p+q)^{-1}\widehat{J}(p,q). \tag{15}$$

Eq. (9) is a nonlinear set of equations for the pair correlation functions of our model. In [4] we have proven that they have a unique solution which we now proceed to explain. The 1,2-component of (9) (coming from $\frac{d}{dt} < qp >$) gives

$$P = \omega(p,k)^2 Q + \tfrac{1}{2}((J\Gamma - \Gamma J) - \mathcal{N}_{12}(p,k) - \mathcal{N}_{12}(p,-k)) \tag{16}$$

where $\omega(p,k)^2 = \frac{1}{2}(\omega(p+k)^2 + \omega(p-k)^2)$. Since the nonlinear term $\mathcal{N}$ depends only on Q and J this expresses P in terms of them. The rest of (9) then yields two equations for the two unknown functions Q and J which become

$$\delta\omega^2(Q,J)^T + \mathcal{N}(Q,J) + (\Gamma J + J\Gamma, \Gamma P + P\Gamma)^T = (0,C)^T \tag{17}$$

where $N(Q,J) = (\mathcal{N}_{12}(p,-k) - \mathcal{N}_{12}(p,k), -\mathcal{N}_{22}(p,k))^T$ and $\delta\omega^2(p,k) = \omega(p+k)^2 - \omega(p-k)^2$. An important property of $\mathcal{N}$ is that, for all T, $\mathcal{N}(TQ_0, 0) = 0$ where $Q_0 = \omega^{-2}$. For $\gamma = 0$

these form a 1-parameter family of solutions of (17). In the equilibrium case $T_1 = T_2$ and $\gamma \neq 0$ only one of these persists, namely the one with $T = T_1$. This is the analogue in the closure equation of the true equilibrium Gibbs state which has $Q = Q_0 + \mathcal{O}(\lambda)$.

Since we are looking for a solution that is locally in x_1 close to this equilibrium we need to understand the linearization of the nonlinear term $\mathcal{N}$ at G_0. It turns out that it is given by an operator which is a multiplication operator in the slow variable p:

$$\mathcal{N}(TQ_0 + \delta Q, \delta J)(p,k) = \mathcal{L}_p(\delta J(p,\cdot), \delta Q(p,\cdot))^T(k). \tag{18}$$

$\mathcal{L}_p$ is a matrix of operators $\mathcal{L}_{ij}(p)$. Each of these acts on functions of k as a sum of a multiplication and an integral operator

$$(\mathcal{L}_{ij}(p)f)(k) = A(p,k)f(k) + \int B(p,k,k')f(k')dk'. \tag{19}$$

The integral kernel $B(p,k,k')$ is of the form

$$\begin{aligned} B(p,k,k') = = \sum_{\mathbf{s}} \int \Delta\Big(\sum_{i=1}^{2} s_i\omega(k_i) + s_3\omega(k'+p) + s_4\omega(p-k)\Big) \\ \cdot\delta(k-k_1-k_2-k')\rho_{\mathbf{s}}(k_1,k_2,k',k,p)dk_1dk_2 \end{aligned} \tag{20}$$

where $\Delta(x) = \delta(x)$ or $\mathcal{P}\left(\frac{1}{x}\right)$ and $\rho_{\mathbf{s}}$ is a smooth function. $A(p,k)$ is given by a similar expression integrated over k'.

The integrand in (20) represents *phonon scattering*. The delta functions impose momentum and energy conservation when $p = 0$ (it turns out that only terms with $\sum s_i = 0$ contribute) which is the point where our functions are peaked: the translation invariant equilibrium has support at $p = 0$ and the nonequilibrium solution will also have most of its mass in the neighborhood of this point. Thus it is important to understand $\mathcal{L}_0$. For parity reasons $\mathcal{L}_{ij}(0) = 0$ for $i \neq j$ whereas $\mathcal{L}_{11}(0)$ is invertible. Invertibility of $\mathcal{L}_0$ would then follow from invertibility of $\mathcal{L}_{22}(0)$. This, however, is not the case: $\mathcal{L}_{22}(0)$ has *two zero modes*.

One of them is easy to understand. Since $\mathcal{N}(TQ_0, 0) = 0$ for all T, taking derivative with respect to T, one finds $\mathcal{L}_{22}(0)\omega^{-2} = 0$. There is, however, also a second zero mode: $\mathcal{L}_{22}(0)\omega^{-3} = 0$.

While the first zero mode has to persist for the full Hopf equations due to the one parameter family of Gibbs states that solve them for $\gamma = 0$, the second one is an artifact of the closure approximation. The phonon scattering described by the nonlinear term conserves phonon energy, leading to the first zero mode, and also phonon number, leading to the second one. The connected six-point correlation function which was neglected in the closure approximation would produce terms that violate phonon number conservation and remove the second zero mode. However, for weak anharmonicity its eigenvalue would be close to zero and should be treated as some perturbation of the present analysis.

The second zero mode leads one to expect that our equations have in the $\gamma = 0$ limit a two parameter family of stationary solutions which indeed is the case. These are given by

$$Q_{T,A}(x,y) = T\int e^{ik(x-y)}(\omega(k)^2 - A\omega(k))^{-1}dk. \tag{21}$$

The second zero-mode is proportional to the derivative of $Q_{T,A}$ with respect to A, at $A = 0$. We are then led to look for solutions in the form

$$Q(x,y) = Q_{T(\mathrm{x}),A(\mathrm{x})}(x-y) + q(x,y), \tag{22}$$

where the first term is of *local equilibrium* form with slowly varying temperature and "chemical potential" profiles $T(\mathrm{x})$ and $A(\mathrm{x})$ and where q is a perturbation orthogonal to the zero modes in a suitable inner product.

Projecting equation (17) on the complementary subspace of the zero modes yields a nonlinear equation for J and q with an invertible linear part. It can be solved by fixed point methods in a suitable Banach space and yields J and q as functionals of T and A. The heat and phonon number currents are given in momentum space by

$$\mathcal{J}^{\alpha}(\mathrm{p}) = -i \int dk e^{-i\mathrm{p}/2} \omega(\mathrm{p}/2, k)^{\alpha} \sin k_1 J(\mathrm{p}/2, k) \tag{23}$$

for $\alpha = 1, 0$ respectively and are thus nonlinear functionals of ∇T and ∇A. This relation is the precise form of the Fourier law. In particular we get relation (1) for the heat current, up to corrections $\mathcal{O}(\frac{\lambda^2 \Delta T}{N})$ (here $\Delta T = T_2 - T_1$), with the thermal conductivity given by:

$$\kappa(T(x)) = \frac{c}{\lambda^2 T(x)^2}.$$

Projecting then equation (17) to the two left zero modes of $\mathcal{L}_{22}(0)$ yields two conservation laws for the currents which become nonlinear (and nonlocal) elliptic equations for the functions $T(\mathrm{x})$ and $A(\mathrm{x})$ whose solutions give for the *inverse temperature* $\beta(x) = T(x)^{-1}$ a linear profile: $\beta(x) = \beta_1 + \frac{|x|}{N}(\beta_2 - \beta_1)$, with corrections of order $\mathcal{O}(\Delta T \lambda^2 \frac{|x|}{N})$ or of higher order in N^{-1}.

The main technical assumptions we need to prove these claims are smallness of $\frac{1}{N}$, λ and ΔT. For convenience we take also the coupling γ to the reservoirs small, as $\gamma = N^{-1+\alpha}$ for some small $\alpha > 0$. The coupling γ is important to fix the boundary conditions for the elliptic equations determining T and A, but, for this, one only needs it to be bigger than N^{-1}. We also need for our analysis that ω^2 is sufficiently *pinning*; in fact, we will choose $\omega^2 = (-\Delta + m^2)^2$, with m large enough, i.e. in momentum space $\omega(k) = 2\sum_{i=1}^{d}(1 - \cos k_i) + m^2$. This choice simplifies several estimates.

The most crucial assumption is that the space dimension has to be at least three. This is because of the low regularity of the collision kernels in eq. (20). To prove the spectral properties of the linear operators (19) we need compactness of the integral operator B in a nice enough space. In three dimensions this holds in a space of Hölder continuous functions whereas in two dimensions this is not the case. Even in three dimensions, the resulting solutions have low regularity in momentum space which translates into long range correlations in physical space.

We finish by comparing our equations to the standard kinetic theory (see [13] for a discussion of the kinetic theory of phonon systems). In our setup, the kinetic limit is a *scaling limit*. One rescales x_1 to the unit interval and takes $N \to \infty$, $\lambda \to 0$, while keeping $R = N\lambda^2$ constant. Our equations then formally become, for $\gamma = 0$, the following equation for the function $V(x, k) = \omega Q(x, k) + iJ(x, k)$, where $x \in [0, 1]$:

$$\nabla\omega(k)\nabla_x V(x, k) = RN(V) \tag{24}$$

with

$$\begin{aligned} N(V) = \frac{9\pi^2}{2} \int & dk_1 dk_3 dk_3 (\omega(k)\omega(k_1)\omega(k_2)\omega(k_3))^{-1}. \\ & \delta(\omega(k) + \omega(k_1) - \omega(k_2) - \omega(k_3))\delta(k + k_1 - k_2 - k_3). \\ & [V(k_1)V(k_2)V(k_3) - V(k)(V(k_1)V(k_2) + V(k_1)V(k_3) - V(k_3)V(k_3))] \end{aligned} \tag{25}$$

where the integration is over $k_i \in [0, 2\pi]^d$.

Equation $N(V) = 0$ has a two parameter family of solutions corresponding to (21): $V_{T,A}(x,k) = \frac{T}{\omega(k)-A}$. Then, imposing, a posteriori, boundary conditions on equation (24), of the form $T(0) = T_1$, $T(1) = T_2$, $A(0) = A_1$, $A(1) = A_2$, one expects, for R large, the solution of (24) to be approximately of the form $V_{T(x),A(x)}$, with $T(x), A(x)$ solved from a scaling limit of our equation for them that becomes

$$\partial_x(D(T(x), A(x))(\partial_x T(x), \partial_x A(x))^T) = 0, \tag{26}$$

where D an explicit 2×2 matrix obtained by taking the scalar product of L^{-1} with suitable vectors related to $V_{T(x),A(x)}$ and orthogonal to the zero modes (see [2]). Solving (26) with the prescribed boundary conditions then gives the approximate solution $V_{T(x),A(x)}$ of (24).

From perturbation theory one expects the full Hopf equations to reduce in the kinetic limit to the equation (25). Thus our closure equations should have the same kinetic scaling limit as the full theory. It should be emphasized that they are more general than the kinetic equations. Indeed, we do not take any limit: λ, τ and N are fixed and we prove that our solution has the expected properties, with precise bounds on the remainder, for λ and τ small and N large. From a mathematical point of view, the Boltzman equation (25) has its own problems due to the continuum nature of the variable x. Since we work with N finite, some of these unphysical problems are absent in our analysis.

In conclusion, the closure equations provide an approximation to the full Hopf equations of the nonequilibrium state that allow us to rigorously show how the Fourier law emerges as the system size gets large. Moreover, this approximation should become exact in the kinetic scaling limit. It should provide a starting point for an eventual first principles proof of the Fourier law.

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