

Transport Processes in Macroscopic Systems

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I will describe old and recent attempts to derive, heuristically or rigorously, the experimentally observed diffusive behavior of energy transport, i.e. Fourier's law, from microscopic models. The score to date is: no success of rigorous derivations for realistic deterministic, Hamiltonian systems, much success for stochastic models. I will focus on deterministic models and leave out topics which (I expect) will be covered by other speakers.

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Fourier's law gives the energy flux $\mathbf{J}(\mathbf{r})$ at position \mathbf{r} inside a region Λ occupied by a system with a non-uniform temperature $\mathbf{T}(\mathbf{r})$, or energy density $e(\mathbf{r})$, profile as

$$\mathbf{J}(\mathbf{r}) = -\kappa(T)\nabla T(r) = -D(e)\nabla e(\mathbf{r}), \quad \mathbf{r} \in \Lambda \subset \mathbf{R}^3$$

There are two cases where Fourier's law (FL) appears to hold for systems in \mathbf{R}^3 . (I will discuss lower dimensional systems later.)

I. Isolated systems with a nonuniform temperature profiles evolving in time according to the equation

$$\frac{\partial e(\mathbf{r},t)}{\partial t} = -\nabla \cdot \mathbf{J}, \quad \mathbf{J} = -\kappa \nabla T = -D \nabla e$$

e.g a metal bar with an initially nonuniform temperature profile.

II. Open systems with time independent nonuniform temperature profiles maintained by external heat baths, e.g a metal bar with one end held in boiling water and the other in melting ice. The stationary heat flux is then given by $\mathbf{J} = -\kappa \nabla T$ with T determined by the solution of the equation $\nabla \cdot (\kappa(T) \nabla T) = 0$, with appropriate boundary conditions.

As far as physicists are concerned, case I is the same as case II. In particular they have no doubt that one has the same κ (given by the Green-Kubo formula).

Problem for physicists: Find κ for a given material from its microscopic structure.

Problem for mathematical physicist: Prove validity of FL for systems with realistic microscopic dynamics.

Heuristic Derivation

A derivation of Fourier's law was given by Clausius and Maxwell using the concept of "mean free path" $\lambda \sim (\rho\pi\sigma^2)^{-1}$: the average distance traveled by an atom, in a gas with density ρ and collision cross-section $\pi\sigma^2$, between collisions.

They considered a gas with a temperature profile varying along the x-axis, $T(x)$. Between collisions a particle moves from x to $x + \lambda/\sqrt{3}$ carrying with it its kinetic energy, $\frac{1}{2}mv^2$ proportional to $T(x)$. In the opposite direction the amount carried is proportional to $T(x + \lambda/\sqrt{3})$.

The amount of energy transported per unit area and time across a plane perpendicular to the x -axis is then, for a “slowly” varying temperature profile, proportional to the flux of particles, given by $\rho\sqrt{T}$, times the net transport of energy per particle

$$\begin{aligned} J &\sim \rho\sqrt{T}[T(x) - T(x + \lambda/\sqrt{3})] \\ &\sim -\rho\sqrt{T}\lambda dT/dx \\ &\simeq -\sigma^{-2}\sqrt{T}\frac{dT}{dx}, \end{aligned}$$

and so $\kappa \sim \sqrt{T}$ independent of ρ , in agreement with (improved) experiment: a triumph for the kinetic (molecular) theory of matter.

Implicit assumption: well defined local temperature $T(\mathbf{q}, t)$, i.e.

“local thermal equilibrium” (LTE). This should be a reasonable approximation when $(\lambda/T)\frac{dT}{dx} \ll 1$ (but \mathbf{J} is also proportional to dT/dx .)

LTE in this case refers to a Maxwell-Boltzmann distribution,

$$f_{loc.eq.}(\mathbf{q}, \mathbf{v}) = (2\pi\beta)^{-d/2} \rho(\mathbf{q}) \exp[-\beta(\mathbf{q})(\mathbf{v} - \mathbf{u}(\mathbf{q}))^2/2].$$

where ρ , \mathbf{u} and β can also depend on t .

(One could make a version of the "Kac model" where this behavior could be proven rigorously but this would involve bringing in stochasticity.)

The theory was refined by Boltzmann, Hilbert, Chapman and Enskog, using the Boltzmann Equation to describe the time evolution of the six dimensional smoothed (coarse grained) density profile $f(\mathbf{q}, \mathbf{v}, t)$ of a gas. This yields accurate transport coefficients for hard spheres at very low density (as compared to MD simulations).

We can also consider nonequilibrium stationary solutions (NESS) of the BE for a gas in a box with Maxwell boundary conditions on the sides perpendicular to x : after a collision with the left (right) wall, the particle emerges with a velocity distribution

$$f_{\alpha}(\mathbf{v}) \sim \beta_{\alpha} |v_x| \exp[-\beta_{\alpha} v^2/2], \quad \alpha = L, R,$$

$$v_x > 0, \text{ for } x = 0, \quad v_x < 0, \text{ for } x = 1$$

With these b.c one can prove the existence of a stationary solution of the BE which will be for small gradients close to LTE with a $\bar{T}(x)$ satisfying

$$\frac{d}{dx}[\sqrt{\bar{T}(x)} \frac{d\bar{T}}{dx}] = 0, \bar{T}(0) = T_L, \bar{T}(1) = T_R, (\bar{\rho}(x) = (\text{pressure})/\bar{T}(x))$$

N.B: I do not hesitate to use stochastic b.c, as long as the bulk dynamics comes from a Hamiltonian.

From the mathematical point of view there are serious problems even on the level of the BE. The existence (but not uniqueness) of hydrodynamic (close to LTE) solutions can only be proven rigorously under very restrictive assumptions of small mean free path and types of initial conditions. For NESS one also requires that $(T_L - T_R)/(T_L + T_R)$ be quite small (Esposito, Lebowitz, Marra). For inhomogeneous initial conditions even existence of classical solutions of BE is not proven. There is also no derivation of the BE for NESS. Lanford's derivation assumes an initial state without too much correlations. Of course we expect the BE to have a much larger domain of validity but there is no proof.

Let us return to more general systems.

Microscopic to Macroscopic The derivation of autonomous macroscopic equations for "macrovariables" M such as the heat equation $\frac{\partial e}{\partial t} = \nabla \cdot (\mathbf{D} \nabla e)$ from microscopic dynamics is one of the basic unsolved problems of nonequilibrium statistical mechanics.

Difficulties arise already at the conceptual level : Are such time asymmetric equations compatible with the time symmetric (classical or quantum) dynamics?

In classical mechanics the microstate of a system is specified by a point $X = (\mathbf{r}, \mathbf{v}_1, \dots, \mathbf{r}_N, \mathbf{v}_N) \in \Gamma$, the phase space of the system. The time evolution is given by the solution of the Hamiltonian equations of motion $X(t) = \phi_t X(0)$ which are time symmetric, i.e. letting $RX = (\mathbf{r}_1, -\mathbf{v}_1, \dots, -\mathbf{r}_N, -\mathbf{v}_N)$ we have $\phi_t R \phi_t X = RX$. for all $t \in (-\infty, \infty)$, as long as the system is isolated (A similar time reversibility holds for quantum systems with $R\Psi = \bar{\Psi}$).

Macrostates:

Let $\Gamma_M \subset \Gamma$ be the set of phase points X such that $M(X) = M$. The existence of an autonomous equation for M_t whose solution gives $M_1 \rightarrow M_2$ when $t_2 \rightarrow t_1$, implies that “almost all” points in a phase space region Γ_{M_1} at time t_1 , go into Γ_{M_2} at time t_2 . Now by Liouville’s theorem, the Liouville volume of M_2 , $|\Gamma_{M_2}| \geq |\Gamma_{M_1}|$. Thus the entropy of M_2 , $S_B(M_2) \equiv \log|\Gamma_{M_2}| \geq S_B(M_1) \equiv \log|\Gamma_{M_1}|$. If the evolution is in fact given by a dissipative equation like the diffusion equation, the Navier Stokes equations or the BE then $|\Gamma_{M_2}| \gg |\Gamma_{M_1}|$ since the entropy scales with N . This means that $S_B(M)$ which can be computed from equilibrium considerations, when the system is in LTE, must be a Lyapunov function for such macroscopic equations. This is indeed the case of the heat equation and BE (but that is another talk).

The existence of a macroscopic autonomous evolution equation implies not only that $|(\phi_{t_2-t_1}\Gamma_{M_1}) \cap \Gamma_{M_2}| \sim |\Gamma_{M_1}| \ll |\Gamma_{M_2}|$, but also that the “future” time evolution (but not the past time evolution) of almost all the phase points in $(\phi_{t_2-t_1}\Gamma_{M_1}) \cap \Gamma_{M_2}$ behave as if they were typical of Γ_{M_2} .

Clearly the derivation of such macroscopic equations from Hamiltonian or quantum dynamics is a very difficult task which will require much work and ingenuity.(Poincare 1893 quote)

A necessary (but far from sufficient input) ingredient in such a derivation is the large difference in the microscopic and macroscopic time scales.

Hydrodynamical Scaling Limit

To make precise the scale separation necessary to obtain *exact* macroscopic laws, in analogy to the Law of Large Numbers, it is necessary to consider a limit in which the ratio of macro to micro spatial scale $\epsilon^{-1} \rightarrow \infty$; ϵ^{-1} could be the size of a macroscopic box in microscopic units. The kind of hydrodynamical equations we *might* get then depends on the macroscopic time scale $\epsilon^{-\alpha}$;

$\alpha = 1$ Euler

$\alpha = 2$ Diffusive

$\alpha = \text{other?}$

$$\mathbf{q} = \epsilon^{-1} \mathbf{r}, \tau = \epsilon^{-\alpha} t$$

\mathbf{r}, t *macro*; \mathbf{q}, τ *micro*

The hydrodynamic equations obtained this way will then of necessity inherit this scale invariance:

Diffusion eq.: $\alpha = 2$,

Euler Equations: $\alpha = 1$

Derivation of macroscopic equations requires showing that the microscopic system behaves, on the macroscopic scale, as if it was close to state of local equilibrium (LTE). That is, it is *locally* close to a homogeneous equilibrium state specified by local values of the conserved quantities - which then change only on the much slower macroscopic time scale according to the macroscopic equations.

This is analogous to what we saw in the heuristic derivation of Fourier's law for a dilute gas.

To describe the state of LTE consider an isolated macroscopic system with Hamiltonian

$$H(P, Q) = \sum_{i=1}^N \left[\frac{p_i^2}{2m} + \sum_{j \neq i} \phi(q_j - q_i) + u(q_i) \right]$$

A LTE state is then described by an ensemble density

$$\begin{aligned} & \mu_{\text{loc.eq.}}(P, Q : \beta_0(\mathbf{x})) \\ & \sim \exp \left\{ - \sum_{i=1}^N \beta_0(\epsilon q_i) \left[\frac{p_i^2}{2m} + \sum_{j \neq i} \phi(q_j - q_i) + u(q_i) \right] \right\} \end{aligned}$$

Want to prove that for $\epsilon \ll 1$

$$\mu_t(P, Q) \simeq \mu_{\text{loc.eq.}}(P, Q; \beta(\mathbf{x}, t))$$

where \mathbf{x} and t are in macroscopic units and $\beta(\mathbf{x}, t)$ is the solution of a suitable macroscopic equation. More generally one would also have a velocity field $\mathbf{u}(\mathbf{x}, t)$ and density field $\rho(\mathbf{x}, t)$ - imposed via a chemical potential $\lambda(\mathbf{x}, t)$.

As already noted a mathematical derivation of such behavior from Hamiltonian dynamics is exceedingly difficult and has not been achieved so far for any realistic classical system. (The same is true for quantum systems)

On the other hand Olla, Varadhan and Yau did (almost) succeed in deriving the Euler equations from the microscopic dynamics ("almost" because they needed to add a little stochasticity to the dynamics.)

The only Hamiltonian system for which such a macroscopic equation has been derived just by scaling of space and time is a system of non interacting point particles moving among a fixed periodic array of convex scatterers with finite horizon (Sinai Billiard).

Let $\mathbf{y}(t)$ and $\mathbf{v}(t)$ be the position and velocity of a particle at time t . Suppose that the position $\mathbf{y}(0)$ and the angle of the velocity $\mathbf{v}(0)$, ($|\mathbf{v}(t)| = |\mathbf{v}(0)|$), are chosen from some smooth distribution, then $Y_\epsilon(t) = \epsilon \mathbf{y}(t/\epsilon^2)$ converges weakly to Brownian motion with positive diffusion tensor \mathbf{D} . (Bunimovich, Sinai, Chernov)

It follows from this that the density profile of a macroscopic system of independent point particles all with the same speed v , moving in such a periodic array satisfies, under appropriate hydrodynamic scaling, the diffusion equation (Fick's law)

$$\frac{\partial n(\mathbf{x}, t)}{\partial t} = \nabla \cdot (\mathbf{D} \cdot \nabla n(\mathbf{x}, t))$$

N.B. There is no proof of such a result for the case when the scatterers have random positions (Lorentz model)

The tensor \mathbf{D} is obtained from the Einstein-Green-Kubo relation

$$\mathbf{D} = \int_0^\infty dt \langle \mathbf{v}(t) \mathbf{v}(0) \rangle$$

where $\langle \quad \rangle$ is wrt the “equilibrium” isotropic distribution of velocities.

Similar formulas are expected hold for all transport coefficients, i.e. thermal conductivity, viscosity, etc., in general interacting systems with \mathbf{J} , the corresponding flux, taking the place of \mathbf{v} .

The existence of such integrals is a central question in deriving Fourier’s law.

There are also other important cases where autonomous macroscopic (or mesoscopic) equations were derived from Hamiltonian or quantum dynamics in certain “kinetic” limits. These include:

i) Boltzmann eq. for short times(Lanford): derived for hard spheres with diameter σ in the limit $\sigma \rightarrow 0$, particle density $\rho \rightarrow \infty$, $\rho\sigma^2 \sim \lambda^{-1}$ fixed.

ii) Vlasov equation (Braun and Hepp)

iii) Laser equation (Hepp and Lieb)

iv) Linear Boltzmann eqn. for random hard scatterers (Gallavotti, classical; Spohn, Yau, Erdos, quantum)

v) Fokker-Planck type,or Landau eqn.
for weak scatterers (Dürr, Goldstein, Lebowitz)

NESS of Crystals

Let me come now to attempts, still very much ongoing, of deriving Fourier's law directly from considerations of nonequilibrium stationary states of microscopic systems. I will focus mostly on insulator crystals. In such systems the microscopic dynamics concern the vibrations of the atoms about their equilibrium positions which form a regular lattice.

We consider now the NESS of such a crystal in contact with thermal reservoirs at different temperatures. These reservoirs act at the boundaries of the systems. Let us consider for simplicity one dimension. The internal Hamiltonian is given by :

$$H = \sum_{i=1}^N \left[\frac{p_i^2}{2m_i} + \phi(q_i - q_{i+1}) + u(q_i) \right] = K + V$$

with q_i the displacement (say in vertical direction) from the equilibrium position i and $q_0 = q_{N+1} = 0$.

The time evolution is then given by:

$$m_i \ddot{q}_i = \dot{p}_i = -\frac{\partial V}{\partial q_i} + \{-\lambda_i p_i + \sqrt{2m_i T_i \lambda_i} \mathcal{F}_i\}$$

where V is the potential energy and the terms in the bracket represent the effect of the reservoirs at specified temperature T_i modeled by Langevin forces (Ornstein-Uhlenbeck process). We shall assume that

$$\lambda_i = 0 \text{ for } i \neq 1, N; \quad \langle \mathcal{F}_i(t) \mathcal{F}_i(t') \rangle = \delta(t - t') \text{ for } i = 1, N$$

The above time evolution equations lead, as is well known, to a Fokker-Planck type equation for the probability density $\mu(X, t)$, $X = (q_1, q_2, \dots, q_N, p_1, \dots, p_N)$.

$$\frac{\partial \mu_t(X)}{\partial t} + (\mu_t, H) = \sum_{\alpha=1, N} \lambda_{\alpha} \frac{\partial}{\partial p_{\alpha}} [p_{\alpha} \mu_t + \beta_{\alpha} m_{\alpha} \frac{\partial}{\partial p_{\alpha}} \mu_t]$$

The stationary state of this system is described by μ_{st} which satisfies the above equation with the time derivative set equal to zero. When the temperature of the left reservoir $T_1 \equiv T_L$ is not equal to the temperature of the right reservoir $T_N = T_R$, μ_{st} will be a NESS.

Consider first general anharmonic interactions ϕ and u :

Questions

1. Do there exist NESS described by measures $\mu_s(X)$?
2. Are they unique?
3. Starting from some arbitrary initial distribution $\mu_0(X)$ will $\mu_t(X) \rightarrow \mu_s(X)$ as $t \rightarrow \infty$.

4. What is the nature of the stationary measure? In particular how does the energy flux in the NESS $J_N = \langle j(X) \rangle_s$ depend on N .

Write

$$J_N = \mathcal{K}_N(T_L - T_R)/N, \quad T_L > T_R$$

Then, if Fourier's law held for $\mathcal{K}_N \rightarrow \mathcal{K} > 0, N \rightarrow \infty$.

Some exact results

1. Eckmann, Pillet, and Rey-Bellet (1999) considered a 1d chain in contact with infinite phonon baths at temperatures T_L and T_R . They were able to prove existence, uniqueness and exponential approach to μ_s under suitable conditions on ϕ and u . This turned out to be nontrivial since the phase space is not compact. Later Ray-Bellet and Thomas proved the Gallavatti-Cohen theorem for these NESS. Their results also hold for the model considered here.

What about $d > 1$?

2. The existence of NESS of fluids in a domain Λ with Maxwell b.c. on different parts of $(\partial\Lambda)_\alpha$ were proven by Goldstein, Lebowitz, Presutti (1979), and Goldstein, Ianiro and Kipnis, under the assumption that the pair interactions $v(r)$ is smooth and repulsive, i.e $v'(r) < 0$ for all $r > 0$. When these hold, there is an exponential approach to a unique stationary measure which is absolutely continuous wrt Lebesgue measure. Possible extension of this result to include hard cores is currently under investigation.
3. There have also been various works by Ruelle, by Jaksic and Pillet and others proving the existence of NESS for quantum systems with various kinds of reservoirs; phonon baths, spin systems, Ideal Fermi or Boson gases, etc.

Unfortunately none of these prove Fourier's law or its violation. A serious attempt to derive Fourier's law for weakly anharmonic crystals in $d = 3$ was made by Bricmont and Kupiainen in (2007). Unfortunately they had to resort in the end to an uncontrolled approximation involving truncation(in a sophisticated way) of the BBGKY hierarchy. Thier work is related to that of Spohn *et al* in deriving a phonon Boltzmann equation.

What do we know about the heat flux in the general case:

The average energy flux from the reservoirs into the system is readily shown to be

$$-J_\alpha = \lambda_\alpha [T_\alpha - \langle p_\alpha^2 \rangle], \quad \alpha = 1, N(L, R)$$

with $\frac{d\langle H \rangle}{dt} = -(J_L + J_R)$

The average energy flux between sites i and $i + 1$ is

$$J_{i,i+1} = \frac{1}{2} \left\langle \frac{\partial \phi(q_{i+1} - q_i)}{\partial q_i} (p_i + p_{i+1}) \right\rangle_\mu$$

Furthermore, the total “ Gibbs entropy production”

$$\sigma = J_L/T_L + J_R/T_R + \frac{d}{dt} \left[- \int \mu_t(X) \log \mu_t(X) dX \right] \geq 0$$

can be proven to be non-negative (by easy calculation).

In the stationary state (assuming it exists)

$$-J_L = +J_R = J_{i,i+1} = J \quad \text{independent of } i$$

$$\sigma = J\left(\frac{1}{T_R} - \frac{1}{T_L}\right) \geq 0, \quad \text{so } J \geq 0 \text{ if } T_L > T_R$$

i.e. we can prove that heat does not flow from cold to hot in the steady state. This is actually something that holds for general systems with a large class of stochastic reservoirs, e.g for particles in a box with Maxwell boundary conditions.

Computer Simulations Of Anharmonic Case As already noted very little is known about the nature of the NESS for the anharmonic case. Results from computer simulations strongly suggest that : In $d=3$, Fourier's law always holds. In $d=1$, Fourier's law holds if there is pinning, i.e $u(\mathbf{q}_i) \neq 0$ and momentum is not conserved. Without pinning the heat conduction is anomalous with $\kappa_N \sim N^\alpha$, $\alpha > 0$. In $d=2$ with $u(\mathbf{q}_i) = 0$, $\kappa_N \sim \log N$.

Harmonic Crystal: Consider now the case when

$$\phi(q) = \frac{1}{2}\omega^2 q^2, \quad u(q) = \frac{1}{2}\nu^2 q^2$$

For this system we can answer all questions for all d . In particular

$$\mu_t(X) \rightarrow \mu_s(X) \sim \exp\left[-\frac{1}{2}\mathbf{X} \cdot \mathbf{C}^{-1} \cdot \mathbf{X}\right]$$

Here \mathbf{C} is $2N$ by $2N$ covariance matrix. Unlike equilibrium, this Gaussian NESS mixes position and momentum. In particular the heat flux $J_{i,i+1} \simeq \langle q_i p_{i+1} \rangle \neq 0$, when $T_L \neq T_R$

Setting $T(i) \equiv \langle p_i^2 \rangle / m$ the profile is very flat, $T(i) \simeq \frac{1}{2}(T_L + T_R)$ and the heat flux is given by : $J_N \sim N[(T_L - T_R)/N] =$ independent of N , as $N \rightarrow \infty$, so $\mathcal{K}(N) = \lim_{T_L \rightarrow T_R} J/[T_L - T_R/N] \sim N$

(NO FOURIER LAW)

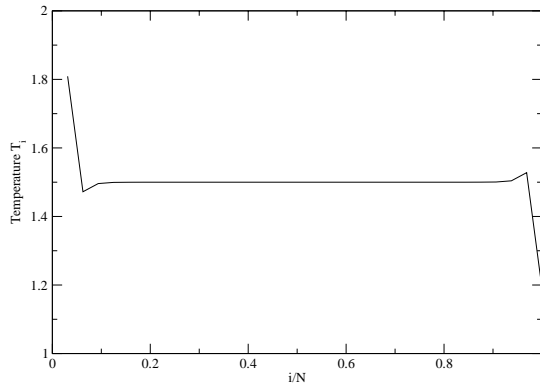
Expressions for \mathbf{C} in $d = 1$ were given in RLL and for $d > 1$ by Nakazawa (1970). We have generally

$$\mathbf{C} = \frac{1}{2}(T_L + T_R)C_{eq}(T = 1) + \frac{1}{2}(T_L - T_R)\hat{\mathbf{C}}$$

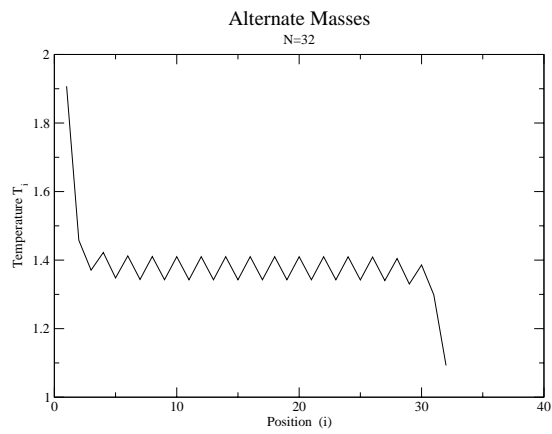
where $\hat{\mathbf{C}}$ satisfies linear equations and is independent of T_L and T_R

Fig 1 shows $T(i)$ for $m_i = m$

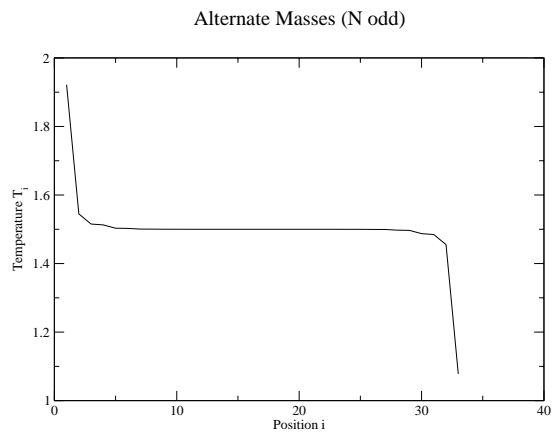
Fig 2 shows $T(i)$ when the masses alternate



Temperature Profile for equal mass harmonic chain (N=32)



Temperature Profile for alternating mass harmonic chain ($N=32, m_1 = 0.6, m_2 = 1.4 \dots$)

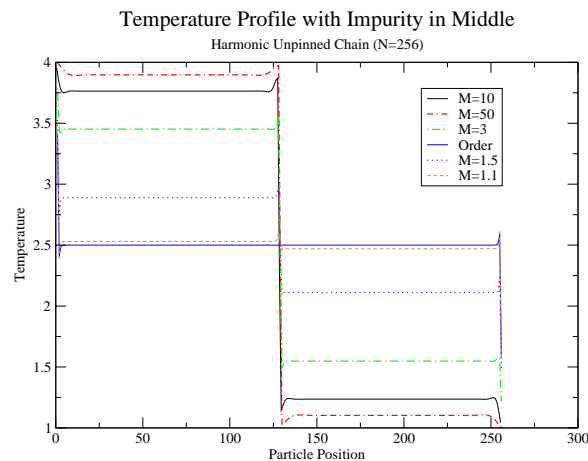


Temperature Profile for alternating mass harmonic chain ($N=33, m_1 = 0.6, m_2 = 1.4 \dots$)

I should also mention here the work of Rubin and Greer and of Spohn and L who considered the case of an infinite harmonic crystal (chain) in which the left (right) end is initially described by a Gibbs measure with temperature $T_L(T_R)$.

They proved that as $t \rightarrow \infty$ the system approaches a stationary translation invariant Gaussian NESS with a constant heat flux. The exact relation between the covariance of that measure and that obtained from the RLL model when $N \rightarrow \infty$ has not been fully clarified. It seems possible that the mean energy $\langle p_i^2 \rangle$ and the heat flux $\langle q_i p_{i+1} \rangle$ are sufficient to determine the NESS. But this is not clear at the moment.

A related question is what happens when there is an inhomogeneity in the system, such as a different mass. The NESS is then no longer translation invariant (when looked at from the vicinity of the impurity). So what does it look like (an explicit calculation by Venkateshan for the RLL model is shown in Fig 3). This problem is similar to that of a quantum system where a quantum dot is placed between leads acting as ideal Fermi gases at different chemical potentials (considered by Mehta and Andrei and also by Jaksic and Pillet).



Harmonic crystals with random masses

The heat flux J_N is very different if one considers harmonic crystals with random masses (a reasonable representation of isotropically disordered crystals at low temperatures).

It is then possible to prove (Casher-L, others), using Fürstenberg's theorem about products of random matrices, that for the pinned harmonic chain (1D) the heat flux J_N in the NESS decays exponentially with N . This is due to the localization of the phonon modes.

For the case where the pinning occurs only at the boundaries (C-L, Dhar,...)

$$J_N \sim N^{-3/2}$$

When there is no pinning at all, which corresponds in a way to considering a segment of an infinite chain then (Verheggen, Dhar)

$$J_N \sim N^{-1/2}$$

In the unpinned cases the energy is carried across the system by low frequency long wavelength phonons which barely see the disorder.

Nothing rigorous is known about heat transport in random mass harmonic crystals in dimensions greater than one. Computer simulations and non-rigorous arguments suggest that Fourier's law holds in three dimensions with pinning, but not in two (Dhar *et al*). Connection to localization in quantum systems?

Other models with Hamiltonian bulk dynamics: Mexican, Rotor, Casatti *et al*, Eckmann and Young, Chernov-L, Gaspard and Gilbert
Models with deterministic non-Hamiltonian bulk dynamics: (Gaussian Thermostats) Gallavotti-Cohen, Ruelle
Other: Gershenfeld, Derrida, L

I will now discuss briefly the C-L, Ruelle, and GDL examples.

Deterministic non-Hamiltonian Bulk Dynamics

A. Gershenfeld, B. Derrida, J.L. Lebowitz

Ianiro - L model: N -Point particles on a line of length L are in contact with heat reservoir walls at temperatures T_a and T_b via Maxwell boundary conditions, i.e. particles leaving the wall after a collision have a velocity distribution,

$$f_\alpha = \beta_\alpha |v| \exp\left[-\frac{1}{2}\beta_\alpha v^2\right], \quad \alpha = a, b$$

with $v > 0$ at $x = 0$ and $v < 0$ at $x = L$.

We can also have more general, even deterministic boundary reservoirs, e.g. all particles hitting the left wall come out with velocity v_a and all those hitting the right wall come out with velocity $-v_b$.

If the system followed Hamiltonian dynamics particles would just exchange velocities when they collide, which is the same as saying that they pass through each other without colliding, i.e. it would be just like an ideal gas. The current would then be, for a given density, $n = N/L$, independent of N , just as for the ordered harmonic crystal(Frisch-L).

To remedy this I-L introduced the following collision rules: if two particles going in opposite directions meet they each reverse their velocities, i.e.

$$v, v' \rightarrow -v, -v' \text{ when } vv' < 0$$

while if they meet with both going in the same direction they just exchange velocities (the same as passing each other). Note that the speed of any particle, say $|v_i|$, is not changed by the collisions.

Interestingly enough I-L could solve exactly the Boltzmann equation for this model. This means that we assume that the joint density of having a particle with velocity v meet a particle with velocity v' at its right, with $v > v'$, at position x , is just equal to the product $f(x, v)f(x, v')$ (Boltzmann's "stosszahl" ansatz).

The stationary solution of this BE gave a linear density and temperature profile and a heat flux J_N which goes as N^{-1} , i.e. Fourier's law holds according to the BE.

Alas: this result is not consistent with the simulations which gave $J_N \sim N^{-.7}$. Clearly the ansatz leading to the BE is not valid. What is going on in low dimensions?

Stochastic Bulk Dynamics: When one adds to the Hamiltonian dynamics a non momentum conserving stochasticity, e.g. random reversal of the velocities of each oscillator, then Fourier's law is valid in all dimensions, both for the regular (Olla, et al) and random harmonic system (Bernardin). Also true for regular anharmonic (Bernardin, Olla) What about momentum conserving noise? O.K. in $d = 3$, for harmonic case (BBO) but not in $d = 1, 2$

Dhar, Venkateshan, L have carried out simulations on a harmonic chain with velocity flips both for regular and random masses. The NESS has correlations which satisfy autonomous equations which for the covariances are identical to those obtained from **self-consistent reservoirs**. The non-Gaussian NESS corresponds to a state of local equilibrium with a linear temperature profile.