Normal Transport in One Dimension: The Coupled Rotator Model

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Fourier's Law

- Let us consider heat transport phenomena in one-dimensional systems:

$$H = \sum_{l=1}^{N} \frac{p_l^2}{2m} + \sum_{l=1}^{N+1} V(q_l - q_{l-1}) \tag{1}$$

- In steady state, one naively expects:

$$j = -\kappa \frac{\partial T}{\partial x} \tag{2}$$

Combined with continuity equation (and ignoring nonlinear powers of temperature gradients)

$$\frac{\partial T}{\partial t} = D \frac{\partial^2 T}{\partial x^2} \tag{3}$$

where $D = \kappa / c_v$. "Normal Diffusion".

Fourier's Law is empirical.

If Fourier's Law holds,

- Temperature profile is linear: T(x)$=T+\Delta T(1-\frac{x}{L})$.
- The size-dependent heat conductivity is calculated as

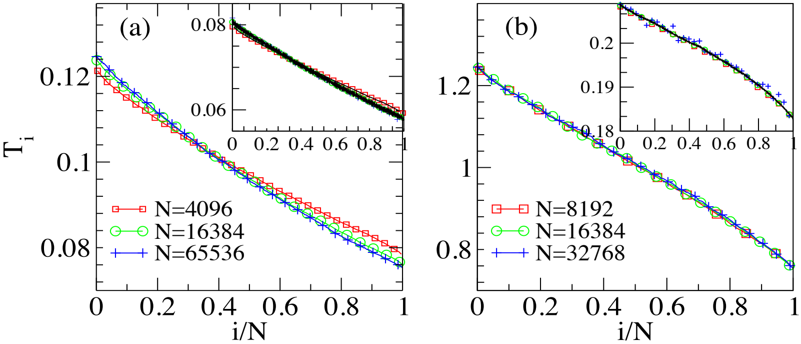
$$\kappa(N) = -J(N)\frac{N}{\Delta T} \tag{4}$$

If Fourier's Law holds,

$$\lim_{N\to\infty} \kappa(N) = \kappa \tag{5}$$

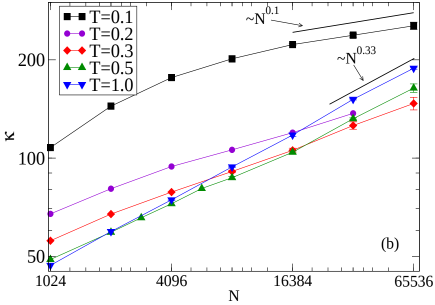
κ depends on the inter-particle potential $V(x)$ and the thermodynamic state variables.

Temperature Profiles of the Fermi-Pasta-Ulam Chain



Plot of temperature profiles for different system sizes for free boundary conditions at temperatures $T = 0.1$ and $T = 1.0$.

Free Boundary Conditions



Plot of the conductivity κ versus system size in the FPU $\alpha - \beta$ model for free BCs.

Hydrodynamic Theory for Equilibrium

Defining the "stretch" variables $r(x) = q(x+1) - q(x)$, the Hamiltonian reads:

$$H = \sum_{x=1}^{N} \epsilon(x), \qquad \epsilon(x) = \frac{p^2(x)}{2} + V[r(x)] \ ,$$

The locally conserved quantities - stretch, momentum and energy - satisfy

$$\begin{aligned} \frac{\partial r(x,t)}{\partial t} &= \frac{\partial p(x,t)}{\partial x}, \\ \frac{\partial p(x,t)}{\partial t} &= -\frac{\partial P(x,t)}{\partial x}, \\ \frac{\partial e(x,t)}{\partial t} &= -\frac{\partial [p(x,t)P(x,t))]}{\partial x} \ , \end{aligned} \tag{6}$$

where $P(x) = -V'(x)$ is the local pressure.

We switch to normal modes $\vec{\phi}$ of the linearized equations, and up to the first nonlinear term, the hydrodynamic equations read:

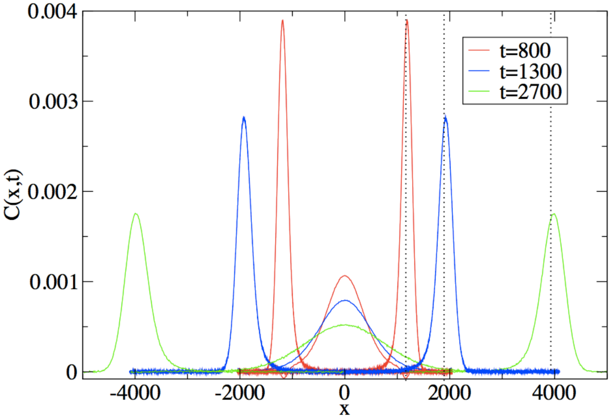
$$\boxed{\partial_t \phi_\alpha = -\partial_x \left[c_\alpha \phi_\alpha + G^\alpha_{\beta\gamma} \phi_\beta \phi_\gamma - \partial_x D_{\alpha\beta} u_\beta + B_{\alpha\beta} \xi_\beta \right] \ .}$$

The quantities of interest are the equilibrium correlations

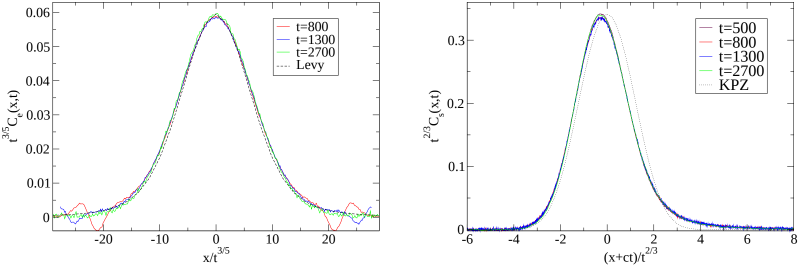
$$C_{\alpha\beta}(x,t) = \langle \phi_\alpha(x,t) \phi_\beta(0,0) \rangle.$$

Equilibrium Correlations of the FPU Chain

Das et al, Phys. Rev. E, 2014



Parameters: $k_2 = 1,\ k_3 = 2,\ k_4 = 1,\ T = 0.5,\ P = 1$, system size $N = 8192$. Correlation functions for the heat mode and the two sound modes.



Scaled plots of heat mode and left moving sound mode correlations.

The hydrodynamic theory does not depend on the details of the inter-atomic potential, and should be valid for any system which has three conserved fields – stretch (i.e the bond vector), momentum and energy.

Does this leave any room for normal heat transport in one-dimensional translationally invariant systems? Assuming that the fluctuating hydrodynamic theory is correct, a third universality class could exist only for systems which have less than three conserved quantities.

The Coupled Rotator Model

The Hamiltonian of the coupled rotator model is $H = \sum_{l=1}^{N} e(l)$, where $e(l) = \frac{{p_l}^2}{2} + V_0 cos(r_l)$. where $r_l = q_{l+1} - q_l$.

Previous simulations have shown finite conductivity convincingly, at least at high temperatures. It was even claimed that there is a transition from anomalous to normal conductivity between $T = 0.2$ and 0.3, for $V_0 = 1$.

This is surprising since the model is translationally invariant.

The stretch $r(x)$ is restricted within the cell $[0, 2\pi]$ with periodic boundary conditions, so $r(x)$ is not a conserved field.

For stretch-conserving models, the Gibbs weight $Prob(\{r(x)\}) \sim \Pi_x \; e^{-\beta[V(r(x))+\bar{P}r(x)]}$. This measure is invariant since $\sum_x r(x)$ is conserved.

When the stretch is not conserved, the measure is invariant only for $\bar{P} = 0$.
For $\bar{P} \neq 0$, the system is inherently in a non-equilibrium state.

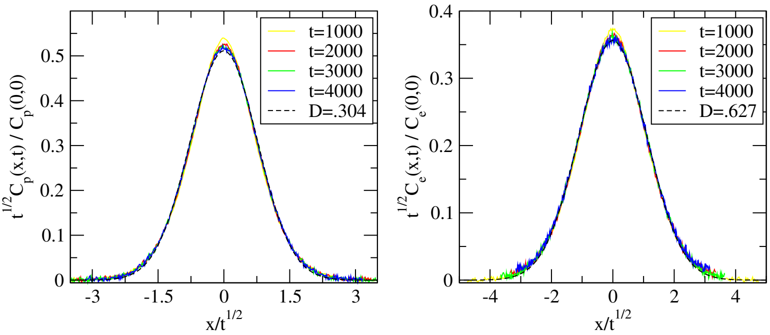
Pressure in the rotator model in equilibrium is *identically* zero.

Therefore coupling tensors of nonlinear hydrodyanmics vanish. The conserved field in this model is $\vec{u} = (p, e)$.

$$\partial_t u_\alpha = -\partial_x \left[-\partial_x D_{\alpha\beta} u_\beta + B_{\alpha\beta} \xi_\beta \right] \ . \tag{7}$$

Solution:

$$C_{\alpha\alpha}(x,t) = \frac{1}{\sqrt{4\pi D_{\alpha\alpha} t}} \exp \ \left[-\frac{x^2}{4 D_{\alpha\alpha} t} \right] \ . \tag{8}$$



Autocorrelation of momentum (left) and energy (right), normalized with $C(0,0)$. The dashed black lines correspond to Gaussians with the respective diffusion constants mentioned in the figures.

Using Fourier's law it can be shown that $\kappa = Ds$. where D is the energy diffusivity and s is the specific heat density.

$$s \equiv \frac{1}{T^2}\frac{\partial^2}{\partial\beta^2}lnZ = \frac{1}{2}\left[1+\beta^2(1+\frac{I_2(\beta)I_0(\beta)-2I_1(\beta)^2}{I_0(\beta)^2})\right].$$

For our parameters, $s = 0.9168$, and using D as determined from the numerical fitting, we get $\kappa = 0.5749$.

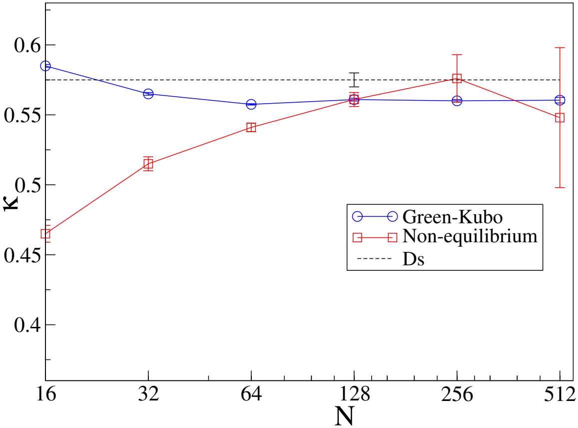
We compare this value with the conductivity obtained directly through two other independent ways.

1. When the conductivity is finite, then from the Green-Kubo formula it is given by

$$\kappa = \lim_{\tau \to \infty} \frac{\langle Q_\tau^2 \rangle}{2NT^2\tau},$$

where $Q_\tau = \int_0^\tau J(t)dt$, and the total heat current $J = \sum_{x=1}^{N} p(x)\partial V/\partial r(x)$.

2. A second way of determining κ is through direct non-equilibrium simulation of the heat current.



Plot of conductivity through three different methods.

Characterizing the non-conservation of stretch

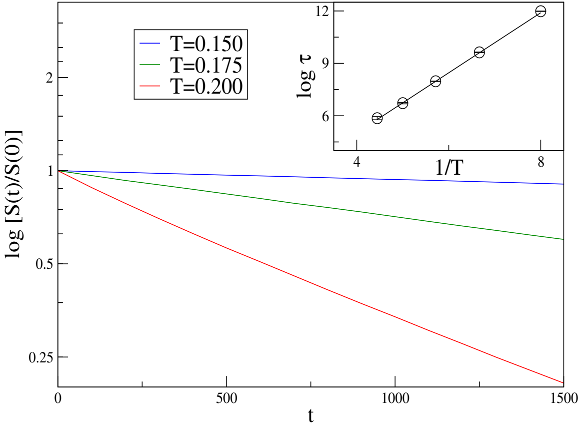
For any conserved field u with zero mean, the following exact sum rule holds:

$$\sum_x \langle u(0,0)u(x,t)\rangle = \sum_x \langle u(0,0)u(x,0)\rangle$$

Since $r(x)$ is not conserved in the CR model, we expect $S(t) \equiv \sum_x \langle r(0,0)r(x,t)\rangle$ to decay with time and go to zero at long times.

The decay time-scale, in the limit of low temperature, approaches the Kramers escape time $\tau \sim \exp(\Delta E/T)$.

So we expect $S(t) \sim \exp(-t/\tau)$, with τ proportional to $\exp(2V_0/T)$.

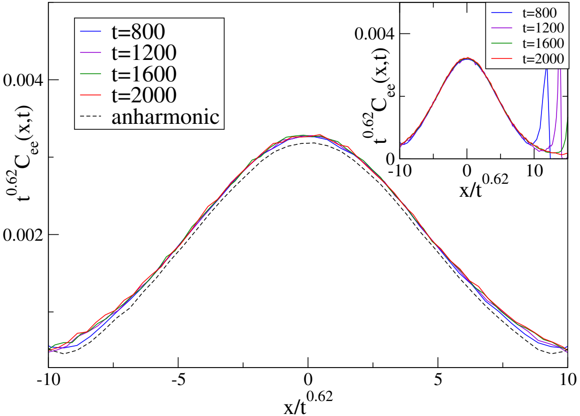


Plot of $S(t)$ at various temperatures for the CR model with $V_0 = 1$. The straight line fit is $y = 1.82x - 2.6$, so that $\Delta E = 1.82$

The coupled rotator model at low T: Anomalous scaling at intermediate times

At low temperatures, each angle variable spends most of its time fluctuating near the potential minimum, and the hydrodynamics must be well-approximated by an anharmonic expansion of the CR potential around the minimum: $V(r) = r^2/2 - r^4/24 + r^6/720$.

This system has three conserved modes – like the FPU chain. It should satisfy the usual scaling for even potential at zero pressure, i.e Levy-2/3 for heat mode, diffusive for sound modes.



Scaled plots of $C_{ee}(x)$ for the CR model, for $T = 0.2$. The dashed line is for the corresponding anharmonic model, at $t = 800$. Including higher order terms in the anharmonic potential should produce an even better approximation. The inset shows the correspodning plots for the anharmonic model with the same scaling.

Conclusions

For momentum non-conserving models, one expects the roles of the stretch and momentum fields to become interchanged. The momentum correlations would be short-ranged, and consequently the hydrodynamic currents for stretch and energy fields would vanish, leading to normal diffusion of these fields.

It has so far been believed that breaking translational symmetry is crucial to normal heat conduction, but the CR model had remained a puzzle. We show that it is not translational invariance but the absence of conserved fields that decides whether heat transport is normal.

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