Role of conserved quantities in normal heat transport in one-dimension

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Although one-dimensional systems that exhibit translational symmetry are generally believed to exhibit anomalous heat transport, previous work has shown that the model of coupled rotators on a one-dimensional lattice constitute a possible exception. We investigate the equilibrium spatiotemporal correlations of energy and momentum of the rotor model, and find that both these fields diffuse normally. The normal diffusion is explained within the framework of stochastic hydrodynamics by observing that the angle variables do not constitute a conserved field, which leads to the absence of long-wavelength currents in the system. As an outcome of our analysis, we propose some general criteria for normal transport based on the existence of conservation laws.

The nature of heat transport in one-dimensional systems has been in debate over the last few decades. Most numerical as well as analytical studies of momentum-conserving systems show an anomalous behaviour of the heat conductivity \( \kappa \) [1–17]. In the limit of large system size \( N \), one generally finds that

\[
\kappa \sim N^\alpha
\]

with \( 0 < \alpha < 1 \), which means that the thermodynamic limit for the conductivity does not exist and Fourier’s law is not valid. However, there are certain contradicting claims in the literature regarding the generality of this scenario. It has been claimed that the value of \( \alpha \) may depend on the properties of the inter-particle potential and that one can get normal transport, i.e. \( \alpha = 0 \), in certain kinds of potentials and parameter regimes. For example, normal transport has been reported in the so-called rotor model at sufficiently high temperatures [18, 19]. On the other hand there are other studies on several systems including the \( \alpha - \beta \) Fermi-Pasta-Ulam system, which find normal transport at low temperatures and anomalous transport at high temperatures [20–21]. Extensive numerical studies of some cases suggest the possibility that some of these may be arising from finite-size effects [22]. The recent approach to transport theory, based on fluctuating hydrodynamics [15–17], offers the possibility of a unifying perspective. The main aim of this Letter is to provide an understanding of the numerical observations on the rotor model within the framework of fluctuating hydrodynamics, which helps illustrate the role of conservation laws in heat transport.

We consider one-dimensional systems on a ring, each particle described by a coordinate \( q(x) \) and momentum \( p(x) \), with \( x = 1, \ldots, N \). Defining \( r(x) = q(x + 1) - q(x) \), the Hamiltonian is written as \( H = \sum_{x=1}^{N} e(x) \), where \( e(x) = \frac{p^2(x)}{2} + V[r(x)] \). The key ingredient in hydrodynamics is to identify the locally conserved fields in the system, with their fluctuations around the equilibrium value represented by the vector \( \bar{u}(x,t) = \{ u_1, \ldots, u_n \} \) for \( n \) conserved variables. The corresponding currents are denoted by \( \bar{j}(x,t) \). In stochastic hydrodynamics, one adds noise and dissipation terms to the currents, and takes the continuum limit to obtain

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

(1)

The noise terms \( \xi \) are stationary Gaussian processes satisfying \( \langle \xi_\alpha(x,t) \rangle = 0 \) and \( \langle \xi_\alpha(x,t) \xi_\beta(x',t') \rangle = \delta_{\alpha\beta} \delta(x-x') \delta(t-t') \). The noise and dissipation matrices \( B, D \) satisfy the fluctuation-dissipation relation \( DC^0 + C^0 D = BB^T \), where \( C^0_{\alpha\beta}(x) = \langle u_\alpha(x,0) u_\beta(0,0) \rangle \), angular brackets denoting equilibrium averages. The introduction of the stochastic and dissipative terms rules out integrability indirectly, and also allows one to derive and solve the corresponding Fokker-Planck equations with a plausible ansatz [17]. But quite apart from the mathematical convenience, it is important to understand what they physically represent. In deriving the continuum hydrodynamic equations, one necessarily loses information about the short-wavelength behavior, with the continuum equations containing only the modes that relax on the longest length and time scales. Although a rigorous derivation is lacking, the fluctuation and dissipation terms may be taken to represent the effects of the faster modes on the long-wavelength behavior of the system. The fluctuation-dissipation relation asserts that these modes are thermalized, whereas the lack of correlation of the noise terms in space and time in indicate their fast relaxation in equilibrium.

In the general one-dimensional non-integrable system, one has three conserved fields and corresponding currents given respectively by \( \bar{u} = (r, p, e) \) and \( \bar{j} = (-p, P, pP) \), where the field now represents the local fluctuations of stretch, momentum and energy about their respective equilibrium values. The local pressure field is \( P(x,t) \equiv -\partial_r V(r(x,t)) \). The thermodynamic pressure is given by \( P = -\langle \partial_r V(r) \rangle \). This is the case addressed in [17], where the hydrodynamics is treated by expanding the currents up to second order in the fields:

\[
\bar{j}_\alpha = A_{\alpha\beta} u_\beta + H_{\alpha\beta\gamma} u_\beta u_\gamma.
\]

(2)

The tensors \( A \) and \( H \) are expressed in terms of the derivatives of the pressure \( P \) with respect to the energy and volume of the corresponding microcanonical ensemble, using Maxwell-type
relations in standard thermodynamics. When the expansion is truncated to first order (i.e., set \( H_{\alpha}^0 \beta = 0 \)), the resulting linear hydrodynamics can be diagonalized to obtain the three normal modes \( \phi_\alpha \), one of which is a stationary heat mode and the other two are sound-modes travelling at speeds \( \pm c \). The second-order terms in the expansion can then be expressed as a coupling between these normal modes \( \phi_\alpha \), and the dynamical correlators \( \langle \phi_\alpha(x,t) \phi_\beta(0,0) \rangle \) of the resulting theory are calculated within a mode coupling approximation. In particular one finds that the heat mode correlators exhibit superdiffusive (Lévy) scaling, which implies super-diffusive transport of heat and universal non-zero values for \( \gamma \). The predicted exponents are well-verified numerically \[23, 24\].

Thus to explore the possibility of normal diffusion of heat, one has to look for cases in which there are less than three conserved fields. Since energy is necessarily a constant of motion, the only possibilities are where either the stretch \( s(x) \) or the momentum \( p(x) \) (or both) are not conserved. We claim that any of these cases lead to normal transport of energy. The case of non-conservation of momentum has been treated quite extensively through several models in the literature, and thus we focus primarily on the case where stretch is not conserved. However, as we shall show later, the hydrodynamics is practically identical for the two cases.

To explore the case of non-conserved stretch, consider a Hamiltonian \( H \) with \( V(r) = \cos(r) \), commonly known as the coupled rotator (CR) model. Convincing numerical evidence \[18, 19\] exists for a finite thermodynamic conductivity in this model, based on direct molecular dynamics simulations of the steady state as well as equilibrium current autocorrelations. Note that since the potential is periodic, the angle variables \( r(x) \) should be taken to lie within an appropriate finite range to ensure that the partition function is finite and therefore the canonical ensemble is well-defined. For our analysis we restrict it within the interval \((0, 2\pi)\), although any range that is an integer multiple of \( 2\pi \) should be expected to have identical macroscopic properties. The equation of motion of \( r(x) \) within the range \((0, 2\pi)\) is \( \dot{r}(x) = p(x + 1) - p(x) \), but since \( r \) is restricted within the cell, one should add boundary terms at \( 0 \) and \( 2\pi \) such that the \( r(x) \) are reset whenever the prescribed range is exceeded. This discontinuity in \( r(x) \) is not in general compensated by a simultaneous change in the nearest neighbours, which means that \( r(x) \) is not a locally (or globally) conserved field.

What is relevant for us is that the thermodynamic conjugate of stretch, the pressure \( P \), must thus be identically zero. In the case of stretch-conserving models, a non-zero pressure is incorporated into the equilibrium description by modifying the Gibbs weight of each microstate such that \( \text{Prob}\{r(x)\} \sim \Pi_x e^{-\beta[V(r(x)) + Pr(x)]} \). This measure remains invariant under the dynamics since \( \sum_x r(x) \) is conserved. However, when the stretch is not conserved, as in the case of the CR model, the measure is invariant only for \( \dot{P} = 0 \). It is important to emphasise that the equilibrium pressure of the rotator model is identically zero, unlike the special case of zero pressure in stretch conserving systems, where the derivatives of pressure with respect to energy and volume are finite even at zero pressure and thus the normal modes remain coupled. For the CR model, the non-conserved field \( r \) drops out from the hydrodynamic description. Since \( \dot{P} \) is identically zero, the coupling tensors \( A \) and \( H \) in Eq. \[2\] (and any higher-order terms that may be included) vanish, and the hydrodynamic currents \( J \) are zero. The local pressure continues to fluctuate on a mesoscopic scale, but these fluctuations are effectively incorporated into the stochastic and dissipative terms in the net current. Thus the conserved field in this model is \( \vec{u} = (p, e) \), and the corresponding hydrodynamic equations are

\[
\partial_t u_\alpha = -\partial_x [\partial x D_{\alpha\beta} u_\beta + B_{\alpha\beta} \xi_\beta].
\]

As in the case of stretch-conserving systems, we find numerically that the cross-correlations decay rapidly, and then the auto-correlations \( C_{\alpha\alpha}(x,t) \equiv \langle u_\alpha(0,0) u_\alpha(x,t) \rangle \) can be shown to be

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

implying diffusive transport of both momentum and energy. Sound modes are absent in the hydrodynamic limit.

We check these predictions with numerical simulations. We have performed molecular dynamics simulations of the CR model in equilibrium, choosing the initial conditions from the Gibbs distribution, and integrating the system using the fourth order Runge-Kutta as well as the velocity Verlet algorithm. The normalized correlation functions of momentum, \( C_p(x,t)/C_p(0,0) \) and energy, \( C_e(x,t)/C_e(0,0) \) are shown in Fig. \[1\], for temperature \( T = 1 \) and a system of size \( N = 400 \). The momentum and energy modes have been scaled diffusively and show excellent collapse. In fact, the scaled correlation functions are fitted very well by Gaussian functions (dashed curves), showing that the correlation functions are as predicted in Eq. \[4\]. Similar diffusive nature of momentum correlations in the rotator model have recently been reported in \[25\].

Using Fourier’s law it can be shown that \( \kappa = D s \), where \( D \) is the energy diffusivity and \( s \) is the specific heat density. For the present system it is calculated that the partition function

\[
Z = \int_{-\infty}^{\infty} dp e^{-\frac{1}{2} \beta p^2} \int_0^{2\pi} dr e^{-\beta \cos(r)} = \sqrt{\frac{2\pi}{\beta}} I_0(\beta),
\]

where \( I_n(\beta) \) is the \( n \)-th modified Bessel function of the first kind. From this one finds that

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

For our parameters, \( s = 0.9168 \), and using \( D \) as determined from the numerical fitting in Fig. (1b), we get \( \kappa = 0.5749 \).

We compare this value of the thermal conductivity with two other independent ways of numerically determined \( \kappa \). If the conductivity is finite, then from the Green-Kubo formula, it is given by

\[
\kappa = \lim_{\tau \to \infty} \frac{\langle Q^2 \rangle}{2NT^2 \tau},
\]
obtained from the standard definition. In both these cases, steady-state heat current is calculated and the conductivity is determined from Langevin baths at temperatures of the heat current. Two ends of the rotor chain are connected with 

$$\sum \langle u(0,0)u(x,t) \rangle = \sum \langle u(0,0)u(x,0) \rangle = \langle u^2(0,0) \rangle,$$

where the last equality is for initial product measure. Since \( r(x) \) is not conserved in the CR model, we expect \( S(t) = \sum \langle r(0,0)r(x,t) \rangle \) to decay with time and go to zero at long times. Since the non-conservation is a consequence of periodicity, the time-scale associated with the decay of \( S(t) \) must be the time-scale required for the variables \( r_i \) to reach the boundary of the interval \([0, 2\pi]\), or equivalently for the time required for the particle to escape the potential well represented by one wavelength of the potential. In the limit of low temperature, this time-scale approaches the Kramers escape time \( \tau \sim \exp(\Delta E/T) \). In other words, at low temperatures and long times, we expect \( S(t) \sim \exp(-t/\tau) \), with \( \tau \) proportional to \( \exp(2/T) \). Fig. (3) shows the exponential behavior of \( S(t) \), and the inset shows that the decay time indeed scales with \( T \) approximately as predicted (see caption for details). It was reported in [19] that there exists a transition from anomalous to normal diffusion in the CR model between \( T = 0.2 \) and \( T = 0.3 \). However, as seen in Fig. [3] the \( S(t) \) correlation continues to decay at temperature 0.2 and below, but the very slow rate of decay means that it is hard to numerically observe the asymptotically normal diffusion on numerically accessible time scales. So the apparent normal diffusion reported in [19] is possibly a finite-size effect. A similar objection to the claim was made in [18], though not from the viewpoint of conservation laws.

At low temperatures, each angle variable spends most of its time fluctuating near the potential minimum. At short times, the hydrodynamics must be well-approximated by an anharmonic expansion of the CR potential around the minimum (\( r = \pi \) in our case), while the crossover to normal diffusive behavior occurring at the time-scales indicated in Fig. (3). To check this, we simulated the corresponding models after truncating the interparticle potential at the harmonic term (obtaining \( V(r) = r^2/2 \) as well as at the first stable anharmonic term (obtaining \( V(r) = r^2/2 - r^4/24 + r^6/720 \)), and compared it with the CR model. The results for \( C_{rr}(x,t) = \langle r(0,0)r(x,t) \rangle \) are shown in Fig. (4). We see that at very short times (left figure), the three different models collapse, whereas at slightly larger times (right figure) the harmonic approximation diverges but the anharmonic approximation still holds good.

At much larger times, however, we see a remarkably different behavior in the CR model. The sound peak is found to decay exponentially with time (Fig. 5), unlike the long-range power-law scaling observed for anharmonic chains [17]. This clearly indicates the short-time sound modes are transient and
FIG. 3: Plot of $S(t)$ at various temperatures for the CR model with $k = 1$. Note that the decay is exponential, and even at the lowest temperature a slow decay is evident. The inset shows the logarithm of the correlation time against $1/T$, which appears linear. The straight line fit is $y = 1.82x - 2.6$, so that $\Delta E = 1.82$, which is in reasonable agreement with the expected value 2 at this level of approximation.

FIG. 4: Plot of $C_{rr}(x)$ for the CR model and the corresponding harmonic and anharmonic expansions, at $T = 0.1$. The left graph is at $t = 5$, and the right one at $t = 25$.

disappear on a thermodynamic scale, unlike in anharmonic chains.

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 the hydrodynamic currents for stretch and energy fields would be absent, thus leading to normal diffusion of these fields. Indeed for the harmonic model with random velocity flips (which conserves energy and density but not momentum), a rigorous derivation of the hydrodynamic limit (see Sec. (3) of [26]) finds macroscopic diffusion equations similar to Eq. (3), with the field index running over stretch and energy fields. Thus in conclusion, we claim that whenever stretch

(momentum) is not conserved in a one-dimensional model, the momentum (stretch) and energy fields exhibit normal diffusion. The possibility of normal transport in one-dimension has been a matter of long-standing debate, and in this work we identify sufficient hydrodynamic criteria for normal transport of energy in one-dimensional systems.

Note: During preparation of this manuscript we came to know of a related work on this problem [27] with similar conclusions as ours.

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