Momentum Conservation Implies Anomalous Energy Transport in 1D Classical Lattices

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Under quite general conditions, we prove that for classical many-body lattice Hamiltonians in one dimension (1D) total momentum conservation implies anomalous conductivity in the sense of the divergence of the Kubo expression for the coefficient of thermal conductivity, κ. Our results provide rigorous confirmation and explanation of many of the existing "surprising" numerical studies of anomalous conductivity in 1D classical lattices, including the celebrated Fermi-Pasta-Ulam problem.

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Since the pioneering work of Fermi, Pasta, and Ulam (FPU) revealed the "remarkable little discovery" [1] that even in strongly nonlinear one-dimensional (1D) classical lattices recurrences of the initial state prevented the equipartition of energy and consequent thermalization, the related issues of thermalization, transport, and heat conduction in 1D lattices have been sources of continuing interest (and frustration) for several generations of physicists. The complex of questions following from the FPU study involves the interrelations among equipartition of energy (is there equipartition? in which modes?), local thermal equilibrium (does the system reach a well-defined temperature locally? if so, what is it?), and transport of energy/heat (does the system obey Fourier's heat law? if not, what is the nature of the abnormal transport?). In sorting through these questions, it is important to recall that the study of heat conduction (Fourier's heat law) is the search for a nonequilibrium steady state in which heat flows across the system, but the situation is usually analyzed, using the Green-Kubo formalism of linear response [2], in terms of the correlation functions in the thermal equilibrium (grand canonical) state. A series of reviews spread over nearly two decades has provided snapshots of the understanding (and confusion) at different stages of this odyssey [3–8].

Much of the past effort has been devoted to attempts to verify Fourier's law of heat conduction

$$\langle \vec{J} \rangle = -\kappa \nabla T\,, \tag{1}$$

where in 1D the gradient is replaced by the derivative with respect to x. Here, κ is the transport coefficient of thermal conductivity. Strictly speaking, κ is well defined only for a system that obeys Fourier's law and where a *linear* temperature gradient is established (for small energy gradients such that relative temperature variation across the chain is small; in general κ is a function of temperature, of course). In the literature the dependence of $\kappa(L)$ on the size L of the system/chain has also been used to characterize the (degree of) anomalous transport. However, the definition of κ for an anomalous conductor, where no internal temperature gradient may be established, is ambiguous. Typically, one defines it in the "global" sense, as $\kappa(L) \equiv \kappa_G \equiv JL/\Delta T$, where ΔT is the total temperature difference between the two thermal baths. However, if the temperature gradient is *not* constant across the system, and/or if there are finite temperature gaps between the thermal baths and the edges of the system due to system-bath contact, one should define and study a local κ, $\kappa \equiv \kappa_L \equiv \frac{J}{\nabla T}$, where ∇T is the *local* thermal gradient. A very wide range of results has been produced by previous studies of different systems: (1) In acoustic harmonic chains, rigorous results [9] establish that no thermal gradient can be formed in the system, with the result that formally $\kappa_G \sim L^1$, which can be understood heuristically by the stability of the linear Fourier modes and the absence of mode-mode coupling. (2) In the "Toda lattice," an integrable lattice model [3,10], in which the result $\kappa_G \sim L^1$ [11], can be understood in terms of stable, uncoupled *nonlinear* modes, the solitons, which are a consequence of the system's complete integrability [7]. (3) In nonintegrable models with smooth potentials, including (i) the FPU system, leading eventually to claim that chaos was necessary and sufficient for normal conductivity ($\kappa_G = \kappa_L \sim L^0$) [8], a claim that has been countered by convincing numerical evidence for anomalous conductivity in FPU chains ($\kappa_L \sim L^{0.4}$) [12,13]; (ii) the diatomic (and hence nonintegrable) Toda lattice, where initial numerical results claiming $\kappa_L \sim L^0$ [14] have recently been refuted by a more systematic study showing $\kappa_L \sim L^{0.4}$ [15]; and (iii) the "Frenkel-Kontorova model," where recent studies have shown that (at least for low temperatures) $\kappa_L \sim L^0$ [16]. (4) In nonintegrable models with hard-core potentials, including (i) the "ding-a-ling" model [17], (ii) the "ding-dong" model [18], and (iii) even simpler single particle chaotic billiard model [19], where numerics show convincingly that $\kappa_L = \kappa_G \sim L^0$.

This bewildering array of results has recently been partially clarified in a series of independent but overlapping studies. The numerical studies of Hu, Li, and Zhao [16] and of Hatano [15] show that *overall momentum conservation* appears to a key factor in anomalous transport in 1D lattices. Lepri, Livi, and Politi [20,21] and Hatano [15] have argued that the anomalous transport in momentum conserving systems can be understood in terms of low frequency, long-wavelength "hydrodynamic modes" that exist in typical momentum conserving systems and that hydrodynamic arguments may explain the exponents observed in FPU [20,21] and diatomic Toda lattice [15].

In the present Letter, we extend and formalize these recent results and resolve finally at least one important aspect of conductivity in 1D lattices: namely, we present a rigorous proof that in 1D *conservation of total momentum implies anomalous conductivity* provided only that the average pressure is nonvanishing in thermodynamic limit.

We consider the general class of classical 1D many-body Hamiltonians,

$$H = \sum_{n=0}^{N-1}\left(\frac{1}{2m_n}\, p_n^2 + V_{n+1/2}(q_{n+1} - q_n)\right), \quad (2)$$

where $V_{n+1/2}(q)$ is an arbitrary (generally nonlinear) interparticle interaction. Note that the potential, $V_{n+1/2}$, depends only on the *differences* between two adjacent sites; in particular, there is *no* "on-site" potential, $U_{\rm OS}(q_n)$, depending on the individual coordinates. The (finite) system is considered to be defined on a system of length $L = Na$ with periodic boundary conditions $(q_N, p_N) \equiv (q_0, p_0)$, where the actual particle positions are $x_n = na + q_n$. In our analysis the masses m_n, as well as interparticle potentials $V_{n+1/2}(q)$, can have *arbitrary dependence on the sites* n, though the examples studied in literature to date have mostly had uniform potentials $V_{n+1/2}(q) = V(q)$ and uniform, $m_n = m$, or dimerized $m_{2n} = m_1, m_{2n+1} = m_2$, masses. We require only that the Hamiltonian (2) be invariant under translations $q_n \to q_n + b$ for *arbitrary* b. This requires $U_{\rm OS}(q_n) = 0$ [16]. Note that we may write the Hamiltonian in Eq. (2) as $H = \sum_{n=0}^{N-1} h_{n+1/2}$, where $h_{n+1/2}$ is the Hamiltonian density,

$$h_{n+1/2} = \frac{p_{n+1}^2}{4m_{n+1}} + \frac{p_n^2}{4m_n} + V_{n+1/2}(q_{n+1} - q_n). \quad (3)$$

Our aim is to estimate κ, the coefficient of thermal conductivity, which is given by the Kubo formula [22]

$$\kappa = \lim_{T\to\infty}\lim_{L\to\infty}\frac{\beta}{L}\int_{-T}^{T} dt\, \langle J(t)J\rangle_\beta\,. \quad (4)$$

Here we have written the canonical average of an observable A at inverse temperature β as $\langle A\rangle_\beta = \int \prod_n dp_n\, dq_n \times A\exp(-\beta H)/\int \prod_n dp_n\, dq_n \exp(-\beta H)$. The order of limits in Eq. (4) is crucial to the precise definition of κ [2]. In Eq. (4), $J = \sum_{n=0}^{N-1} j_n$ is the total heat current, and j_n is the heat current density [16], given by

$$\begin{aligned} j_n &= \{h_{n+1/2}, h_{n-1/2}\} \\ &= \frac{p_n}{2m_n}[V'_{n+1/2}(q_{n+1} - q_n) + V'_{n-1/2}(q_n - q_{n-1})], \end{aligned} \quad (5)$$

where $\{,\}$ is the usual canonical Poisson bracket.

Using Eqs. (3) and (5), we find that current density given by (5) satisfies the continuity equation

$$\dot{h}_{n+1/2} = \{H, h_{n+1/2}\} = j_{n+1} - j_n\,. \quad (6)$$

In some references, e.g., Ref. [16], inessentially different (nonsymmetric) definition of the local heat current j_n has been used which satisfies a continuity equation (6) with a slightly different (nonsymmetric) form of the Hamiltonian density (3). However, the two definitions of the local heat current sum up to *identical* total current J.

Our ensuing analysis is similar to that used by Mazur [23], with a crucial difference: we will average correlation functions over a *finite* rather than *infinite* time domain, T. We start with an elementary inequality. For an arbitrary observable $X(t) = X[\{q_n(t), p_n(t)\}]$, we have

$$\int_{-\infty}^{\infty} dt\, g_T(t)\langle X(t)X\rangle_\beta \ge 0\,, \quad (7)$$

where $g_T(t)$ is a suitable $L^2(\mathbb{R})$ *window* function of effective width T, which has the following properties:

(i) $\int_{-\infty}^{\infty} dt\, g_T(t) = T$;

(ii) $\int_{-\infty}^{\infty} dt\, g_T^2(t) = T$;

(iii) $\tilde g(\omega) := \int_{-\infty}^{\infty} dt\, g_T(t)e^{i\omega t} > 0$ for all ω.

The natural choice satisfying these conditions is a Gaussian, $g_T(t) = \sqrt{2}\exp[-2\pi(t/T)^2]$. Using elementary Fourier analysis, the above inequality (7) is easily proved by rewriting it as

$$\int d\omega\, \tilde g_T(\omega)\langle S_X(\omega)\rangle_\beta \ge 0\,, \quad (8)$$

where $S_X(\omega) = \lim_{T\to\infty}\frac{1}{T}|\int_0^T dt\, e^{i\omega t}X(t)|^2$ is the power spectrum of the signal $X(t)$. Obviously, $S_X(\omega) > 0$, and, given (iii), the inequality of (7) and (8) is clearly fulfilled. We now write the observable X as $X = A + \alpha B$, $\alpha \in \mathbb{R}$. Optimizing with respect to the parameter α, we arrive at the Schwartz-like inequality

$$\left(\int dt\, g_T(t)\langle A(t)A\rangle_\beta\right)\times \left(\int dt\, g_T(t)\langle B(t)B\rangle_\beta\right) \ge \left(\int dt\, g_T(t)\langle B(t)A\rangle_\beta\right). \quad (9)$$

The above inequality is of quite general use. We implement it by taking $A \equiv J$ and $B \equiv P$, where $P = \sum_{n=0}^{N-1} p_n$ is the total momentum. For Hamiltonians of the form (2), P is an integral of motion $\dot P = \{H, P\} \equiv 0$ due to translational symmetry. Since $P(t) = P$, the inequality (9) reads

$$\int dt\, g_T(t)\langle J(t)J\rangle_\beta \ge T\frac{\langle JP\rangle_\beta^2}{\langle P^2\rangle_\beta}\,. \quad (10)$$

The right-hand side of Eq. (10) can be easily evaluated: $\langle P^2\rangle_\beta = \bar m N/\beta$, where $\bar m = (1/N)\sum_{n=0}^{N-1} m_n$, and $\langle JP\rangle_\beta = \beta^{-1}\sum_{n=0}^{N-1}\langle V'(q_{n+1} - q_n)\rangle_\beta$, since we have in general that $\langle A(\{q_n\})B(\{p_n\})\rangle_\beta = \langle A(\{q_n\})\rangle_\beta\langle B(\{p_n\})\rangle_\beta$. $\langle V'_{n+1/2}(q_{n+1} - q_n)\rangle_\beta$ is an average *force* between particles n and $n + 1$, i.e., *the thermodynamic pressure,* and does not depend on n. [In thermal equilibrium the average net force on particle n vanishes and hence $\langle V'_{n-1/2}(q_n - q_{n-1})\rangle_\beta = \langle V'_{n+1/2}(q_{n+1} - q_n)\rangle_\beta$.] The pressure can be rewritten through the usual thermodynamic definition

$$\phi \equiv \frac{\partial F}{\partial L} = \frac{1}{N}\frac{\partial F}{\partial a} = \frac{1}{N}\sum_{n=0}^{N-1}\langle V'_{n+1/2}(x_{n+1} - x_n + a)\rangle_\beta ,$$

where $\exp(-\beta F) = \int \Pi_n\, dp_n\, dq_n \exp(-\beta H)$. Inserting the above and multiplying with β/L, we find that inequality (9) reads

$$\frac{\beta}{L}\int dt\, g_T(t)\langle J(t)J\rangle_\beta \geq \frac{T}{a\bar{m}}\,\phi^2. \tag{11}$$

Since the Kubo formula can be equivalently written in terms of the window function as $\kappa = 2^{-1/2} \times \lim_{T\to\infty}\int dt\, g_T(t)C(t)$, where $C(t) = \lim_{L\to\infty}\langle J(t)J\rangle_\beta/L$, since $\lim_{T\to\infty} g_T(t) = \sqrt{2}$, and implementing in the above result (11) the two limits as indicated in (4), we have proved our main result.

Theorem.—In momentum conserving systems of type (2), if the pressure is nonvanishing in the thermodynamic limit, $\lim_{L\to\infty}\phi > 0$, then the thermal conductivity diverges and $\kappa \to \infty$.

Therefore, we find anomalous energy transport as a simple consequence of the total momentum conservation. The only case in which the pressure is expected to vanish at *any temperature* is when the forces between particles at zero temperature equilibrium are zero [$V'_{n+1/2}(0) = 0$] *and* the interparticle potentials are all even functions [$V_{n+1/2}(q) = V_{n+1/2}(-q)$] so that the forces are also expected (and found numerically for β FPU problem) to average to zero for arbitrary canonical thermal fluctuations. This is, indeed, the case for the β FPU problem, where $V_{n+1/2}(q) = \frac{1}{2}q^2 + \frac{1}{4}\beta q^4$ [13,21], and there the integrated correlation function diverges for more subtle (dynamical) reasons (the slow asymptotic power-law decay of current-current correlation function $\sim t^{-0.6}$).

Even if the zero temperature equilibrium forces vanish $V'_{n+1/2}(0) = 0$, we still have nonvanishing finite temperature pressure (due to "thermal expansion" of a system confined to a fixed volume $L = aN$) whenever interparticle potentials are not even. This is the case for the α FPU model, $V_{n+1/2}(q) = \frac{1}{2}q^2 + \frac{1}{3}\alpha q^3$, for the modified diatomic Toda lattice [15], $V_{n+1/2}(q) = \exp(-q) + q$, and for the diatomic hard-point 1D gas [15,24] $V_{n+1/2}(q) = \{0 \text{ if } q > -a; \infty \text{ if } q \leq -a\}$. For the usual diatomic Toda lattice [15], $V_{n+1/2} = \exp(-q)$, the pressure is nonvanishing even at zero temperature, since $V'_{n+1/2}(0) \neq 0$.

To augment and illustrate our analytic discussion, we have simulated numerically the current-current autocorrelation function $\langle J(t)J\rangle_\beta/L$ in a generic anharmonic chain, namely, in the "$\alpha\beta$" FPU model with $V_{n+1/2}(q) = \frac{1}{2}q^2 + \frac{1}{3}\alpha q^3 + \frac{1}{4}\beta q^4$ where we take $\alpha = 2$, $\beta = 4$, $m_n = a = 1$, and microcanonical ensemble of initial conditions with the energy per particle $E/N = 1$. In Fig. 1 we compare

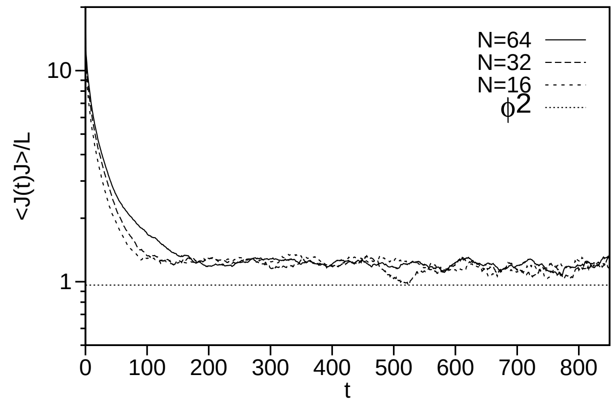

FIG. 1. Current-current autocorrelation function in the "$\alpha\beta$" FPU model with $\alpha = 2$, $\beta = 4$, and $E/N = 1$. We show numerical data microcanonically averaged over 500 pseudorandom initial conditions for three different sizes $N = 16, 32, 64$ and compare it to the squared pressure ϕ^2 (dotted line).

the results for $N = 16, 32, 64$ with the equilibrium value of the squared pressure $\phi^2 = 0.964\ldots$. We have also checked numerically that for the symmetric interparticle potential (same as above except with $\alpha = 0$) the pressure indeed vanishes and the current-current correlation functions decay asymptotically as $\sim t^{-0.6}$ (in agreement with results of Refs. [20,21]).

Given that momentum conservation implies anomalous conductivity, it is natural to ask whether the converse is true: namely, does anomalous conductivity imply that the model conserves momentum? Two counterexamples show that this result is *not* true. First, if one considers a *linear* chain of *optical* phonons—so $V_{n+1/2} \sim (q_{n+1} - q_n)^2$ and $U_{\rm OS} \sim q_n^2$—one can show [25] by a straightforward extension of the arguments of Ref. [9] that this momentum nonconserving model nonetheless has anomalous transport. Similarly, there is a momentum *nonconserving* integrable model due to Izergin and Korepin [26] that also shows anomalous conductivity [25]. Finally, let us stress that in 1D lattices the nature of dynamics, whether it be completely integrable, completely chaotic, or mixed, does not affect our result: if total momentum is conserved and the canonical average of the pressure does not vanish, the transport is anomalous. We shall address the central issue of the necessary and sufficient conditions for normal transport in a forthcoming paper [25].

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