Momentum conservation implies anomalous energy transport in 1D classical lattices

Tomáš Prosen and David K. Campbell

CNLS, MS B258, Los Alamos National Laboratory, Los Alamos, NM 87545
(March 21, 2022)

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, \( \kappa \). 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.

PACS number: 44.10.+i, 05.45.+b, 05.60.+w, 05.70.Ln

Since the pioneering work of Fermi, Pasta, and Ulam (FPU) revealed the “remarkable little discovery” \([6]\) 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 non-equilibrium steady state in which heat flows across the system, but the situation 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 \( \kappa \), \( \kappa \equiv \kappa_L \equiv J/\Delta T \), where \( \Delta T \) 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 the system-bath contact, one should define and study a local \( \kappa \), \( \kappa \equiv \kappa_L \equiv J/\Delta T \), where \( \Delta T \) is the local thermal gradient. A very wide range of results have been produced by previous studies of different systems:

- in acoustic harmonic chains, rigorous results \([8]\), establish that no thermal gradient can be formed in the system, with the result that formally \( \kappa_L \sim L^1 \), which can be understood heuristically by the stability of the linear Fourier modes and the absence of mode-mode coupling;
- in the “Toda lattice,” an integrable lattice model \([9,10]\), in which the result \( \kappa_L \sim L^1 \) \([11]\) can be understood in terms of stable, uncoupled nonlinear modes, the solitons, which are a consequence of the system’s complete integrability \([5]\);
- in non-integrable models with smooth potentials, including (i) the FPU system, leading eventually to claim that chaos was necessary and sufficient for normal conductivity (\( \kappa_G = \kappa_L \sim L^0 \)) \([3]\), a claim that has been countered by convincing numerical evidence for anomalous conductivity in FPU chains (\( \kappa_L \sim L^{0.4} \)) \([2,3]\); (ii) the diatomic (and hence non-integrable) Toda lattice, where initial numerical results claiming \( \kappa_L \sim L^0 \) \([4]\) have recently been refuted by a more systematic study showing \( \kappa_L \sim L^{0.4} \) \([5]\); and (iii) the “Frenkel-Kontorova model,” where recent studies have shown that (at least for low temperatures) \( \kappa_L \sim L^0 \) \([4]\):
- in non-integrable models with hard-core potentials, including (i) the “ding-a-ling” model \([7]\); (ii) the “ding-dong” model \([8]\), and (iii) even simpler single particle chaotic billiard model \([9]\), 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 et al. [10] and of Hatano [12] show that overall momentum conservation appears to a key factor in anomalous transport in 1D lattices. Lepri et al. [23] and Hatano [13] 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 [24,25] 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 non-vanishing in thermodynamic limit.

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

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

where $V_{n+1/2}(q)$ is an arbitrary (generally non-linear) 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, $U_{OS}(q_n)$, 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 $U_{OS}(q_n) = 0$ [10]. Note that we may write the Hamiltonian in Eq. (2) as

$$H = \sum_{n=0}^{N-1} h_n + 1/2, \text{ where } h_{n+1/2} \text{ is the Hamiltonian density}$$

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

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

$$\kappa = \lim_{T \to \infty} \lim_{L \to \infty} \frac{1}{L} \int_{-T}^{T} dt \langle J(t)J \rangle_{\beta}.\quad (4)$$

Here we have written the canonical average of an observable $A$ at inverse temperature $\beta$ as $\langle A \rangle_{\beta} = \int \Pi dp_n dq_n A \exp(-\beta H) / \int \Pi dp_n dq_n \exp(-\beta H)$. The order of limits in Eq. (4) is crucial to the precise definition of $\kappa$ [3]. In Eq. (4), $J = \sum_{n=0}^{N-1} J_n$ is the total heat current, and $J_n$ is the heat current density [10], given by

$$j_n = \{h_{n+1/2}, h_{n-1/2} \} = \frac{p_n}{2m_n} \left( V'_{n+1/2}(q_{n+1} - q_n) + V'_{n-1/2}(q_{n} - q_{n-1}) \right),$$

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

Using Eqs. (3,4), we find that current density given by satisfies the continuity equation

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

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 $X(t) = X((q_n, p_n(t)))$, we have

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

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

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

$$\int d\omega \bar{g}_T(\omega) \langle S_X(\omega) \rangle_{\beta} \geq 0\quad (8)$$

where $S_X(\omega) = \lim_{T \to \infty} \frac{1}{T} \int_{-T}^{T} dt e^{i\omega t} X(t)$ is the power spectrum of the signal $X(t)$. Obviously, $S_X(\omega) > 0$, and given (iii), the inequality (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 $\alpha$, we arrive at the Schwartz-like inequality

$$\left( \int dt g_T(t) \langle A(t)A \rangle_{\beta} \right) \left( \int dt g_T(t) \langle B(t)B \rangle_{\beta} \right) \geq$$

$$\geq \left( \int dt g_T(t) \langle B(t)A \rangle_{\beta} \right)^2.\quad (9)$$

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 $\dot{P} = \{H, P \} = 0$ due to translational symmetry. Since $P(t) = P$, the inequality (9) reads

$$\int dt g_T(t) \langle J(t)J \rangle_{\beta} \geq T \left( \frac{JP^2}{P^2} \right)_\beta.\quad (10)$$

The RHS of Eq. (10) can be easily evaluated: $\langle P^2 \rangle_{\beta} = N/\beta$, 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 \( \langle A(\{q_n\})B(\{p_n\}) \rangle_\beta = \langle A(\{q_n\}) \rangle_\beta \langle B(\{q_n\}) \rangle_\beta \). \( \langle V'_{n+1/2}(q_{n+1} - q_n) \rangle_\beta \) 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 \( \langle V_{n+1/2}(q_{n+1} - q_n) \rangle = \langle V'_{n+1/2}(q_{n+1} - q_n) \rangle_\beta \).) The pressure can be rewritten through the usual thermodynamic definition

\[
\phi = \frac{\partial F}{\partial L} = \frac{1}{N} \frac{\partial F}{\partial a} = \frac{1}{L} \sum_{n=0}^{N-1} \left( V'_{n+1/2}(x_{n+1} - x_n + a) \right)_\beta,
\]

where \( \exp(-\beta F) = \int \Pi_n dp_n dq_n \exp(-\beta H) \). Inserting the above and multiplying with \( \beta/L \), we find that inequality (3) reads

\[
\frac{\beta}{L} \int dt g_T(t) \langle J(t)J \rangle_\beta \geq T \phi^2. \tag{11}
\]

Since the Kubo formula can be equivalently written in terms of the window function as \( \kappa = 2^{-1/2} \lim_{T \to \infty} \int dt g_T(t) C(t) \), 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 non-vanishing 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 \( \langle V'_{n+1/2}(0) \rangle = 0 \) and the interparticle potentials are all even functions \( \langle V_{n+1/2}(q) \rangle = \langle V_{n+1/2}(-q) \rangle \) so that the forces are also expected (and found numerically for \( \beta \) FPU problem) to average to zero for arbitrary canonical thermal fluctuations. This is indeed the case for the \( \beta \) FPU problem, where \( \langle V_{n+1/2}(q) \rangle = \frac{1}{2} q^2 + \frac{1}{2} \beta q^4 \) \( \langle \rangle \), 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 \( \langle V'_{n+1/2}(0) \rangle = 0 \), we still have non-vanishing 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 \( \alpha \) FPU model, \( \langle V_{n+1/2}(q) \rangle = \frac{1}{2} q^2 + \frac{1}{2} \alpha q^3 \), for the modified diatomic Toda lattice \( \langle \rangle \), \( \langle V_{n+1/2}(q) \rangle = \exp(-q) + q \), and for the diatomic hard-point 1D gas \( \langle \rangle \), \( \langle V_{n+1/2}(q) \rangle = \{ 0 \text{ if } q > -a; \infty \text{ if } q \leq -a \} \). For the usual diatomic Toda lattice \( \langle \rangle \), \( \langle V_{n+1/2} = \exp(-q) \rangle \) the pressure is non-vanishing even at zero temperature, since \( \langle V'_{n+1/2}(0) \rangle \neq 0 \).

To augment and illustrate our analytic discussion, we have simulated numerically the current-current autocorrelation function \( \langle J(t)J \rangle / L \) in a generic anharmonic chain, namely in the “\( \alpha \beta \)” FPU model with \( \langle V_{n+1/2}(q) \rangle = \frac{1}{2} q^2 + \frac{1}{2} \alpha q^3 + \frac{1}{2} \beta q^4 \) where we take \( \alpha = 2, \beta = 4 \) and energy per particle \( E/N = 1 \). In Fig. 1 we compare 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. [24,21]).

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 \( \sim \) \( \langle q_{n+1} - q_n \rangle^2 \) and \( U_{OS} \sim q^2 \)–one can show \( \langle \rangle \) by a straightforward extension of the arguments of Ref. (4) that this momentun non-conserving model nonetheless has anomalous transport. Similarly, there is a momentum non-conserving integrable model due to Izergin and Korepin \( \langle \rangle \) that also shows anomalous conductivity \( \langle \rangle \). Finally, let us to 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 \( \langle \rangle \).

The authors gratefully acknowledge the hospitality of Center for Nonlinear Studies (CNLS), Los Alamos National Laboratory, where the work was performed. TP acknowledges financial support by the Ministry of Science and Technology of the Republic of Slovenia, and DKC thanks the CNLS supporting him as the 1998-99 Ulam Scholar. This research was supported in part by the Department of Energy under contract W-7405-ENG-36 and by the National Science Foundation under grant DMR-97-12765.

\[ a \] Permanent address: Physics Department, Faculty of Mathematics and Physics, University of Ljubljana, Jadranska 19, 1111 Ljubljana, Slovenia. e-mail: prosen@fiz.uni-lj.si

\[ b \] Permanent address: Department of Physics, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801. e-mail: dkc@uiuc.edu

[1] E. Fermi, J. Pasta, S. Ulam, Los Alamos report LA-1940
(1955); reprinted in E. Fermi. Collected Papers, Vol II (Univ. of Chicago Press. Chicago, 1965), p. 978.

[2] R. Kubo, J. Phys. Soc. Japan 12, 570 (1957); R. Kubo, p. 120 in Lectures in Theoretical Physics Vol. 1 (W. Brittin, ed) (Intercience, New York, 1959).

[3] M. Toda, Phys. Rep. 18, 1 (1975).

[4] W. M. Visscher, Meth. Comput. Phys. 15, 371 (1976).

[5] R. A. MacDonald and D. H. Tsai, Phys. Rep. 46, 1 (1978).

[6] E. A. Jackson, Rocky Mountain J. of Math. 8 127 (1978).

[7] M. Toda, Phys. Scr. 20, 424 (1979).

[8] J. Ford, Phys. Rep. 213, 271 (1992).

[9] Z. Rieder, J. L. Lebowitz, and E. Lieb, J. Math. Phys. 8 1073 (1967).

[10] M. Toda, J. Phys. Soc. Jpn. 22, 431 (1967).

[Note that in linear/integrable systems the temperature profile inside the system is nearly flat and almost the entire drop in temperature occurs near the edges. In such cases, one would find for the local thermal conductivity $\kappa L \sim \exp(\text{const} \times L)$.

[12] H. Kaburaki and M. Machida, Phys. Lett. A 181, 85 (1993).

[13] S. Lepri, R. Livi, and A. Politi, Phys. Rev. Lett. 78, 1896 (1997).

[14] E. A. Jackson and A. D. Mistriotis, J. Phys. C: Cond. Matt. 1, 1223 (1989).

[15] T. Hatano, Phys. Rev. E 59, R1 (1999).

[16] B. Hu, B.-W. Li, and H. Zhao, Phys. Rev. E 57 2992 (1998).

[17] G. Casati, J. Ford, F. Vivaldi, and W. H. Visscher, Phys. Rev. Lett. 52, 1861 (1984).

[18] T. Prosen and M. Robnik, J. Phys A: Math. Gen. 25, 3449 (1992).

[19] D. Alonso, R. Artuso, G. Casati, and I. Guarneri “Heat Conductivity and Dynamical Instability” to appear in Phys. Rev. Lett.

[20] S. Lepri, R. Livi, and A. Politi, Physica D 119, 140 (1998).

[21] S. Lepri, R. Livi, and A. Politi, cond-mat/9806133.

[22] The validity of the linear response theory that underlies the Kubo formula is not an issue here, since we will be making analytic estimates that are valid for arbitrarily small temperature differences and since we take care to isolate the pathological cases of zero internal thermal gradients.

[23] P. Mazur, Physica 43, 533 (1969).

[24] G. Casati, Foundations of Physics 16, 51 (1986).

[25] T. Prosen and D. K. Campbell, in preparation.

[26] A. G. Izergin and V. E. Korepin, Vestn. Leningr. Gos. Univ., Fiz. Khim. 22, 88 (1981).