Transport in perturbed classical integrable systems: the pinned Toda chain

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Abstract

Nonequilibrium and thermal transport properties of the Toda chain, a prototype of classically integrable system, subject to additional (nonintegrable) terms are considered. In particular, we study via equilibrium and nonequilibrium simulations, the Toda lattice with a power-law pinning potential, recently analyzed by Lebowitz and Scaramazza \textsuperscript{arXiv:1801.07153}. We show that, according to general expectations, even the case with quadratic pinning is genuinely non-integrable, as demonstrated by computing the Lyapunov exponents, and displays normal (diffusive) conductivity for very long chains. However, the model has unexpected dynamical features and displays strong finite-size effects and slow decay of correlations to be traced back to the propagation of soliton-like excitations, weakly affected by the harmonic pinning potential. Some novel results on current correlations for the standard integrable Toda model are also reported.

Keywords: Thermal transport, Integrability, Non-linearity, Lyapunov spectra

1. Introduction

Heat transport in classical low-dimensional lattices \textsuperscript{[1] 2 3} has been quite a debated problem in the last decades and only recently unconventional effects (e.g., divergence of heat conductivity, superdiffusion, the peculiar role played by nonlinearity, integrability and disorder, etc.) have come to a satisfactory explanation. General theoretical approaches like nonlinear fluctuating hydrodynamics provides us a way of predicting the basic features of anomalous heat conductivity in one-dimensional chains of nonlinearly-coupled oscillators \textsuperscript{4 5 6 7}, while rigorous predictions of the anomalous behavior in stochastic conservative evolution of similar chains have been obtained \textsuperscript{8 9 10 11}. Anyway, a good deal of numerical studies have paved the path of most of these achievements and still allow us to obtain inference about many still open problems, like the way anomalous behaviors depend on the kind of nonlinearity \textsuperscript{12 13 14}, dimension (e.g. 1 or 2D) \textsuperscript{15}, disorder and the kind of the interaction (e.g., short- or long-range; deterministic or stochastic) \textsuperscript{16 17}.

Although the general scenario for nonintegrable systems in low-dimensions seems rather well established, there is a renewed interest in integrable systems, both classical and quantum. The most famous classical example is the celebrated Toda model \textsuperscript{18}. The natural expectation would be to have ballistic heat transport mediated by solitons \textsuperscript{18}, as confirmed by the Mazur-bound type of arguments \textsuperscript{19 20}. Beyond this, there are intriguing features that make this class of systems less obvious and worth being investigated. For instance, the Hard Point Chain model (a gas of point particles colliding elastically in one dimension) turned out to display anomalous conductivity even in the integrable limit of equal masses \textsuperscript{21}. Moreover, diffusive and even anomalous spin transport was demonstrated for a classically integrable Landau-Lifshitz spin chain \textsuperscript{22}. On more general grounds, an interesting distinction between interacting and non-interacting integrable systems was recently proposed \textsuperscript{23}. It was argued that in the latter case irreversible processes may occur, yielding nonvanishing Onsager coefficients. Motion of thermally activated Toda solitons would fall in this latter class due to the phenomenon termed nondissipative soliton diffusion \textsuperscript{24}, i.e., the stochastic sequence of spatial shifts experienced by the soliton as it moves through the lattice and interacts with other excitations without momentum exchange. A more recent study \textsuperscript{25} showed that dynamical scaling is ballistic but also that correlation of hydrodynamic modes are non trivial.

The next question, which has an obvious physical relevance, concerns the role of perturbations away from integrability. It may be envisaged that strong enough changes of the Hamiltonian of integrable one-dimensional systems will generically bring them back within one of the known classes of transport behavior. For instance, the “diatomic” versions of both the Toda \textsuperscript{26} and Hard Point Chain \textsuperscript{27} models both display anomalous conduction in the Kardar-Parisi-Zhang universality class. Also, momentum-conserving
stochastic perturbation of the Toda model yield energy superdiffusion \([28]\). The situation may however be more subtle in the limit of very small perturbations: for instance, the FPU model in the region of the parameter space where it is close to the Toda chain \([29]\) displays an apparent diffusive transport \([29, 31]\). A similar feature occurs in the diatomic Hard Point gas with mass ratio close to one \([32]\).

For all the above reasons, we are motivated to study in detail the classical Toda chain and its perturbations. The present work is organized as follows. In Section 2 we present the main model, the pinned Toda chain first considered in this context in \([33]\) and discuss qualitatively its dynamics. In Section 3 we compute the Lyapunov exponents of the model to show that the pinning generically destroys integrability. Proceeding in our analysis, we consider current correlations of the Toda model in Section 4 while in Section 5 we study the effect of pinning and perturbations on these observables. Thermal transport of the pinned Toda chain is studied in Section 6 in the classical nonequilibrium setup, where the system is in contact with two boundary reservoirs at different temperatures. Finally, a discussion is given in the concluding Section.

2. The pinned Toda chain

In this paper we focus on the study of a one-dimensional Toda lattice of \(N\) particles in the presence of a pinning potential, whose Hamiltonian reads \([33]\)

\[
H = \sum_{i=1}^{N} H_i = \sum_{i=1}^{N} \left[ \frac{p_i^2}{2m} + V(q_{i+1} - q_i) + \frac{\nu^2}{z} |q_i|^2 \right],
\]

where \(q_i\) and \(p_i\) are canonically conjugated variables, \(m\) is the mass of each oscillator, \(z > 1\) is a real exponent and \(\nu\) a real frequency, and

\[
V(x) = \frac{a}{b} \left( e^{-bx} + bx - 1 \right).
\]

We will set \(a = b = 1\) and \(m = 1\) and denote the energy density (energy per particle) as \(E = H/N\) henceforth. Most of the simulations are performed with periodic boundary conditions, unless otherwise stated.

In the case of the standard Toda model (\(\nu = 0\)), transport is ballistic, meaning that the finite-size thermal conductivity diverges linearly with the systems size \(N\). In linear-response language, this correspond to the existence of a nonvanishing Drude weight, namely a finite value of the currents power spectra at zero frequency \([19]\). This is roughly related to the density of thermally-excited solitons and implies a non-zero value of the current-current correlations at large times, a generic feature of integrability \([20, 34, 23]\).

The presence of the pinning potential is expected to destroy the integrability of the Toda chain, while leaving only one conserved quantity: the total energy \([1]\). In particular, it manifestly breaks space-translation invariance and, accordingly, the conservation of total momentum, yielding an optical dispersion in the harmonic limit, with a gap at zero wavenumber proportional to the parameter \(\nu\). From the point of view of transport, we thus expect that the model will display standard diffusive behavior, as known for other similar pinned chains, like the discrete Klein-Gordon and others \([1, 2]\). Actually, the case \(z = 2\) is somehow special as for periodic boundary conditions it admits a second integral of motion, termed “center of mass” \(h_c\) in \([33]\) (see also Refs. \([35, 39, 37]\))

\[
h_c = \frac{1}{2} \left( \sum_i p_i \right)^2 + \frac{\nu^2}{2} \left( \sum_i q_i \right)^2.
\]

Note also that \(h_c\) is conserved for an arbitrary choice of the interparticle potential \(V(x)\), as it can be easily ascertained by computing its time derivative. Nonetheless, even in this case, we may expect diffusive transport, as observed in other similar models admitting two conserved quantities like the rotor (XY) chain \([35, 39]\) or the Discrete Nonlinear Schrödinger equation \([40, 41, 42]\).

The dynamics of the model is illustrated in Fig. 1. In the upper panels we report the space-time evolution of the local energy field \(H_i\) for the Toda chain, and the pinned Toda chain with \(z = 2\) and 4 and for two types of initial conditions, a locally perturbed thermal state, Figs.1a, and an unperturbed one, Figs.1b (by thermal state we mean a generic microcanonical state obtained assigning random velocities to all the particles. Lower panels (c) are the structure factors versus frequency \(\omega\) for a fixed wave-number \(k = \pi/256\).
with $z = 2$ behaves somehow more similar to the unperturbed Toda model than in the case $z = 4$. Actually, a significant ballistic propagation is observed, akin to soliton motion, drastically different from the diffusive-like spreading shown in the rightmost panels. Also in the central panel of Fig. 1 a clear dispersion of velocities is present, a feature different from what seen in generic nonintegrable chains, like the Fermi-Pasta-Ulam model. This difference is distinctly captured by the dynamical structure factors (Figs. [4]): $S(k, \omega)$ are defined as the modulus squared of the spatio-temporal Fourier transform $\hat{q}(t)$ of the particle displacements $q_i(t)$

$$S(k, \omega) = \langle |\hat{q}(k, \omega)|^2 \rangle. \quad (4)$$

Since we are working with periodic boundary conditions, the allowed values of the wave number $k$ are always integer multiples of $2\pi/N$. For $z = 2$, $S(k, \omega)$ displays a narrow peak at finite frequency, whose position is proportional to the wavenumber $k$. Clearly, this case is qualitatively more similar to the Toda case and definitely different from the chain with $z = 4$ that only show a central diffusive peak.

The heat conduction problem for a pinned Toda chain coupled to external heat baths has been studied in a recent paper by Lebowitz and Scaramazza [33]. The main surprising result there reported is that for $\nu \neq 0$ and $z = 2$ the model seems to exhibit ballistic transport of energy, as it should be expected for an integrable model, like a chain of harmonic oscillators or a pure Toda lattice. On the other hand, if $z = 4$ the ballistic transport disappears and one obtains temperature profiles that are closer to the expected Fourier linear behavior (despite they still exhibit sensible deviations from that). Such numerical analysis, prompted the Authors to argue that the Toda chain with harmonic pinning might be integrable or, more likely, an example of a nonintegrable system without momentum conservation for which the heat flux is ballistic.

Altogether, this phenomenology and the results of [33], suggest that transport in the harmonically pinned case may display some features of solitonic propagation, possibly related to its underlying integrable model, that we investigate in the following.

3. Nonintegrability of the pinned Toda chain

In this Section we first demonstrate that the pinned Toda chain is genuinely nonintegrable also in the case $z = 2$ through computation of Lyapunov spectra. The spectra $\lambda_i$, $i = 1, \ldots, 2N$ are computed with the standard method [33] for chains with periodic boundary conditions and the same parameter values adopted in [33], as well as with different combinations of the energy density, particle number and frequency $\nu$.

The equations of motion $\dot{q}_i = -\partial H/\partial p_i$ and $\dot{p}_i = \partial H/\partial q_i$ and the associated tangent-space equations used to evaluate the Lyapunov exponents have been integrated with a standard 3-rd order symplectic algorithm [44, 45].

![Figure 2: (a) Lyapunov spectra (normalized to the maximum exponent $\lambda_{\text{max}}$ and plotted versus the rescaled index $i/N$) of the Toda chain with harmonic pinning ($z = 2$) and $\mathcal{E} = 1$ for $N = 16, 32$ and $64$. For $N = 256$: (b) maximal Lyapunov exponent $\lambda_{\text{max}}$ as function of the pinning potential exponent $z$, for different values of the energy density $\mathcal{E} = 0.05, 0.1, 1, 2.5, 20$ and $250$, and fixed $\nu = 1$; (c) $\lambda_{\text{max}}$ as function of the ratio $\nu^2/z$ for $z = 1.5, 2$ and $4$ for fixed energy density $\mathcal{E} = 5$.](image)

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with fixed time step $\delta t = 0.01$, while for the simulations presented in the following Sections we used the 4-th order scheme with $\delta t = 0.05$.

In Fig. 2 (a) we show the Lyapunov spectra of model 1 with $z = 2$ for different values of $N$: they display the usual convergence to the limit form, typical of generic chaotic Hamiltonian system [46]. We also checked that in the harmonic pinning case there exist, beyond the two vanishing Lyapunov associated with energy conservation, an additional pair of zero exponents as it should in view of the existence of the additional conserved quantity $h_c$ given in Eq. (3).

In addition, we have evaluated the dependence of maximum Lyapunov exponent, $\lambda_{\text{max}} \equiv \lambda_1$, on the model parameters. In Fig. 2 (b) we show $\lambda_{\text{max}}$ as a function of $z$ for $N = 256$ and $\nu = 1$ for different values of the energy density in the range $5 \times 10^{-2} \leq \mathcal{E} \leq 2.5 \times 10^{2}$, while in Fig. 2 (c) we show $\lambda_{\text{max}}$ as a function of $\nu^2/z$ for $N = 256$ and $\mathcal{E} = 5$ for $z = 1.5, 2$ and $4$. In all cases $\lambda_{\text{max}}$ is always positive, which further excludes the possibility that model described by the Hamiltonian (1) can be integrable even for particular values of $z$. Remarkably, for low values of $\mathcal{E}$, $\lambda_{\text{max}}(z)$ has an evident non-monotonic trend with a minimum in $z = 2$, that gradually disappears for increasing values of $\mathcal{E}$. Such non-monotonicity with the energy
density $\mathcal{E}$ is independent on the system size $N$, but it is seemingly depending on the pinning strength $\nu$ for fixed values of $N$ and $\mathcal{E}$. This confirms that the harmonic pinning is somehow special from the dynamical point of view, as we will show in the following sections.

4. Currents correlation: the Toda chain

We now turn to the main observable related to transport, namely current-current correlations (or equivalently current power spectra) computed in equilibrium. Let us discuss first the case of the Toda chain. Although several studies of dynamical correlations for various observable exist in the literature [47, 48, 24] it is useful to reconsider the behavior of flux correlations in detail.

The Toda model has $N$ integrals of motion, and to each of them a local current can be associated through a continuity equation [23]. Usually one considers the total (volume-averaged) currents $J_k$ ($k = 1, \ldots, N$) that are directly related to the Onsager matrix. In principle one has to deal with a $N \times N$ matrix of correlations $\langle J_k(t) J_j(0) \rangle$. Here we limit ourselves to considering the two simplest integrals, namely total momentum and total energy, along with their respective total currents

$$J_1 = \sum_{i=1}^{N} F_i; \quad J_2 = \frac{1}{2} \sum_{i=1}^{N} (\dot{q}_{i+1} + \dot{q}_i) F_i.$$  \hspace{1cm} (5)

where $F_i = - V'(q_{i+1} - q_i)$ is the interparticle force. In Fig. 3 we report their power spectra $\langle |\dot{J}_1|^2 \rangle$ averaged over a random Gaussian distribution of velocities (this may not be fully representative of the real statistical ensemble, which for completely integrable systems should be the Generalized Gibbs Ensemble [19]). Note that the value at $\omega = 0$ (the Drude weight) is not vanishing but it is not reported in the figures. From this analysis, there is an indication that both spectra vanish for $\omega \to 0$. Actually, the typical frequency scale below which the spectra approach a small value is of order $1/N$, as demonstrated by the rescaled data in the insets of Fig. 3. It is natural to associate this time-scale to the typical time of transit of solitons across the chain. If we take the $N \to \infty$ limit before the $\omega \to 0$ limit, as we should in the calculation of transport coefficients via the Green-Kubo formula, there would be a finite Onsager coefficient, yielding some entropy production on top of the ballistic contribution. In this respect, the data are fully consistent with regarding the Toda chain as an interacting integrable model, as recently surmised in [23].

5. Currents correlation: the pinned Toda chain

Let us now turn to the effect of pinning. In this case we consider the energy current correlation only. The results are shown in the main panel of Fig. 4.

Figure 3: Power spectra of the momentum- (a) and energy- (b) currents of the Toda lattice (see Eq. 5) for different chain lengths $N$ and $\mathcal{E} = 1$. Insets: same data as a function of the rescaled frequencies $\omega N$.

For $z = 4$, $\langle |\dot{J}_2|^2 \rangle$ approach a constant for $\omega \to 0$ implying, as expected, a relatively fast decay to zero of correlations and finite thermal conductivity. For the harmonic case $z = 2$ the same conclusion holds, but the saturation occurs below a much smaller value of frequency. In addition, and somehow surprisingly, there exist a wide intermediate range of frequencies where the spectra display a power law

$$\langle |\dot{J}_2|^2 \rangle \propto \omega^{-\theta}; \quad \omega_1 < \omega < \omega_2$$  \hspace{1cm} (6)

with a nontrivial exponent $\theta \approx 5/3$. Such unusual behavior is very stable with the system size (the black dashed and the red solid curves, corresponding respectively to $N = 1024$ and $N = 2048$, almost overlap) and it should be compared with the case $z = 4$, where correlations decay much faster. We also checked that simulations at lower energy density, e.g. $\mathcal{E} = 0.1$, yield similar results (data not reported).

To ascertain whether the underlying Toda potential is relevant we compared the data with the FPU approximation of the Toda potential, namely by replacing $V$ in Eq. (1) with its power-series expansion truncated to fourth order. Remarkably, the spectra change completely, yielding a faster decay of correlations. From this we conclude that the presence of an underlying integrable model is essential to observe the power-law behavior given by Eq. (6).

The above results indicate that different classes of perturbations of the Toda model may have drastically different and unexpected effect on transport. To illustrate this further let us for instance consider the Hamiltonian

$$H_1 = \sum_{i=1}^{N} \left[ \frac{p_i^2}{2m} + V(q_{i+1} - q_i) + \frac{\mathcal{E}}{2} (q_{i+1} - q_i)^2 \right].$$  \hspace{1cm} (7)

that has the usual three conservation laws (total energy, momentum and elongation) and is thus expected to belong
energy current power (a.u.)

\[ \frac{\omega}{\epsilon} \]

\[ \omega^{-5/3} \]

Figure 4: Power spectra of the energy current for a pinned Toda lattice with \( z = 2 \) and \( \mathcal{E} = 1 \) and \( N = 1024 \) (solid lines) and \( 2048 \) (dashed line). The green dot-dashed line marks the power-law \( \omega^{-5/3} \) trend of the spectra for \( z = 2 \). For comparison, the energy spectrum for a pinned FPU lattice with the same \( \mathcal{E} \), \( z = 2 \) and \( N = 1024 \) (cyan line) is reported. Data has been shifted vertically for better readability. Inset: power spectra of the energy current for a Toda lattice perturbed by a momentum-conserving harmonic potential, Eq. 6. The frequency axis is divided by the perturbation strength \( \epsilon \) for comparison.

6. Nonequilibrium properties

In this Section, we further demonstrate that transport in the harmonically pinned Toda chain obeys Fourier’s law, but that finite-size effects are indeed very relevant. We have performed nonequilibrium numerical simulations for system sizes much larger than those studied in \([33]\), while integrating the equations of motion over definitely much longer time. We have adopted free boundary conditions for the oscillators at site 1 and \( N \), while a fraction \( N_0 = N/16 \) of oscillators at the two chain ends have been independently thermalized by Maxwellian heat reservoirs at temperature \( T_L \) and \( T_R \), respectively, as in \([16]\).

In Fig. 5 we show the stationary temperature profiles \( T_i = \rho f^2(t) \), where the bar denotes the average over time \( t \), for the case \( z = 2 \), with \( \nu = 1 \) and different chain sizes in the range \( 64 \leq N \leq 16384 \). In all cases the external temperatures were fixed to \( T_L = 4 \) and \( T_R = 1 \) and the total integration time \( t_f \) was chosen equal to \( 5 \times 10^6 \) units, which was sufficient for reaching stationary conditions for all system sizes here considered (see below). It can be seen clearly that even relatively long chains (up to \( N \approx 10^5 \)) exhibit almost flat temperature profiles. Conversely, only for \( N > 10^3 \) a linear temperature profile interpolating between \( T_L \) and \( T_R \) is definitely distinguishable, although with significant finite-size effects in the form of temperature drops close to thermalized interfaces. These jumps account for the well-known phenomenon of an effective impedance between the heat reservoirs and the chain \([50]\), because of the mismatch of response time between the reservoir time constant and the typical relaxation time scales of fluctuations, which is associated with the kind of nonlinear modes propagating through the chain.

To complement our analysis, in the inset of Fig. 5 we present as function of \( N \) the value of the left (circles) and right (triangles) heat fluxes \( J_L \) and \( J_R \), that were computed as the average energy exchanged by the system with each reservoir per unit time \([10]\). The two curves nicely overlap, thus confirming that the system has reached a nonequilibrium steady state. Consistently with the behavior of temperature profiles, the plateau initially visible for small \( N \) (reminiscent of ballistic conduction of integrable systems \([11]\)) starts to bend for \( N > 10^3 \), although with a trend quite far from the scaling expected for standard diffusion, \( J_{L,R} \propto N^{-1} \): see the black dashed line.

We also addressed the question of how the system relaxes to the nonequilibrium steady state and how the typical timescales depend on size and initial conditions. In Fig. 6 we report the slope \( s(t) \) of the temperature profile in the bulk (excluding directly thermalized particles) as a function of the rescaled integration time \( t/N \) up to \( t/N = 10 \). The two different sets of curves, dashed and
solid, correspond to different initial conditions, namely (i) a flat profile at \((T_R + T_L)/2\) and (ii) a Fourier profile, linearly interpolating between \(T_L\) and \(T_R\), respectively. For a certain time \(t\), \(s(t)\) is obtained by fitting time-dependent temperature profiles \(\bar{T}(x, t)\) with linear functions \(f(x, t) = s(t)x + c(t)\), where \(c(t)\) is an offset and \(x = (i - N_0)/(N - 2N_0)\). The function \(\bar{T}(x, t)\) is computed by averaging local square momenta over temporal windows of length 0.1\(N\) and over an ensemble of 64 independent realizations of the dynamics. For the system sizes reported in Fig. 6 \(s(t)\) converges to an asymptotic slope \(\tilde{s}\) on a timescale, which is order \(N\) for both kinds of initial condition. For small pinning frequencies \(\nu^2 = 0.1\) (panel (a)), \(\tilde{s}\) is tiny, as one can imagine that the scattering of Toda solitons induced by the pinning potential is very weak. For larger \(\nu\) (panels (b) and (c)), \(\tilde{s}\) approaches larger and larger values upon increasing the system size \(N\), although the value expected for Fourier profiles, \(\tilde{s} = (T_R - T_L)\) is never observed with these parameters.

Altogether, we can conclude that heat transport in the pinned Toda chain is affected by very important finite size effects. For relatively large chains and a rather broad range of pinning strengths, energy transport through the chain is dominated by a ballistic contribution, due to traveling Toda-like solitons, that are very weakly affected by the soft pinning potential. The propagation speed of such structures is quite larger than the speed of acoustic waves in the lattice, they are therefore allowed to travel very large distances before being “scattered” by the pinning component. Since in particularly short chains the scattering effect is practically ineffective, the Toda-like solitons provide the major contribution to a quasi ballistic hydrodynamic behavior.

7. Summary and perspectives

The first conclusion of the work is that the Toda chain with harmonic pinning is no exception to the belief that chains with on-site potential belong to the class of normal (Fourier) heat diffusion. From this point of view the additional integral of motion \([3]\) does not seem to play a crucial role. Although the model is chaotic in the usual sense (Section 5), it displays however some form of solitonic transport, yielding a relatively slow and unexpected decay of current correlations. In this respect, we should also mention the case of the Fermi-Pasta-Ulam-\(\beta\) model equipped with a substrate quadratic potential that unexpectedly exhibits landmarks of heat superdiffusion [51]. Actually, it should be noted that the presence of the underlying Toda potential seems essential here. This phenomenology calls for a deeper theoretical explanation, to understand why the quadratic pinning is so special and why coherent transport is so weakly affected by it.

Another conclusion regards the general question of the effects of perturbations on an otherwise integrable system. We have shown in Section 4 that the Toda model nicely fits into the class of interacting integrable systems but also that different types of modifications of its Hamiltonian can yield very different results and qualitatively change the decay laws of current correlations (Section 5). We admit that we have no general arguments to account for those observations, that deserve further study.

Finally, another open problem concerns the issue of finite-size effects. After long practice of the sport of numerical simulations, both at and out of equilibrium, one reaches the conclusion that finite size and finite time effects are quite difficult to be properly controlled in the problem of heat conduction and should be handled with care (see Section 6). On the other hand, when dealing with relatively small systems, like nanowires, nanotubes, single molecules, graphene layers and similar nanosystems, finite size effects become a problem of intrinsic physical interest. For both of these reasons, it would be highly desirable having at disposal a theoretical approach that accounts for sub-leading terms, beyond asymptotic predictions concerning long-time behavior of very large, i.e. truly macroscopic, systems. This said, it should be pointed out that this is quite a difficult task to be accomplished, if one considers the many difficulties already encountered for producing an asymptotic hydrodynamic approach. In order to take into account finite size effects one should be able to build up a “second-order” hydrodynamic theory out of a first-order one, that already revealed quite difficult to be properly worked out.

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