

Ballistic transport in the classical Toda chain with harmonic pinning

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We investigate, via numerical simulation, heat transport in the nonequilibrium stationary state (NESS) of the 1D classical Toda chain with an additional pinning potential, which destroys momentum conservation. The NESS is produced by coupling the system, via Langevin dynamics, to two reservoirs at different temperatures. To our surprise, we find that when the pinning is harmonic, the transport is ballistic. We also find that on a periodic ring with nonequilibrium initial conditions and no reservoirs, the energy current oscillates without decay. Lastly, Poincaré sections of the 3-body case indicate that for all tested initial conditions, the dynamics occur on a 3-dimensional manifold. These observations suggest that the N -body Toda chain with harmonic pinning may be integrable. Alternatively, and more likely, this would be an example of a nonintegrable system without momentum conservation for which the heat flux is ballistic - contrary to all current expectations.

I. INTRODUCTION

The transport of thermal energy in Hamiltonian systems is a problem of great theoretical and practical interest [1,2]. In its simplest form, one considers heat flow in the nonequilibrium stationary state (NESS) of a system in contact with two thermal reservoirs at different temperatures. Very little is known rigorously about this problem except in the case of harmonic crystals [3] or hard rods in 1D [4]. These models are special cases of the larger class of integrable models, whose extensive numbers of conserved quantities are expected in general to lead to ballistic heat transport [5–8]. This means that if a system of length N (and cross-section A) is put in contact with heat reservoirs at temperatures T_L and T_R , $T_L > T_R$, at its left and right ends, then the heat flow in the stationary state J would be (except for boundary effects) independent of N . This is what is observed for the Toda lattice and it stands in contrast to the case where we have dissipative transport satisfying Fourier’s law, where J would be proportional to N^{-1} .

In the absence of exact results, one has to rely on heuristics and simulations. A large number of these have focused on 1D systems. These have led to the following commonly accepted truths (CAT): Integrable systems such as the Toda chain [5,9,10], the Calogero-Moser system, the harmonic chain, and hard rods have ballistic transport, i.e., $J \sim N^0$. Nonlinear non-integrable systems such as the Fermi-Pasta-Ulam (FPU) chain or the diatomic Toda chain [11] have $J \sim N^{-\alpha}$ with $\alpha < 1$, for the momentum conserving case: the actual value of α depends on the system – see [12] and references therein. When a nonintegrable system does not conserve momentum due to pinning by a one body potential, the transport is diffusive, also called “normal”, with $\alpha = 1$.

We find, via numerical simulations, that the Toda chain with harmonic pinning has ballistic transport of heat. Because this system is generally believed to be nonintegrable, either the prevailing wisdom about 1D transport needs modification or this system is in fact integrable. In either case, the result is rather surprising and requires further investigation. We note that the Poincaré sections of the 3-body case indicate that the dynamics take place on a 3-dimensional manifold for all tested initial conditions, indicating that there are 3 conserved quantities

in this case (the first two being the Hamiltonian itself and a quantity corresponding to the harmonic motion of the center of mass). We also note that when the pinning is done by a quartic potential, then the heat transport is clearly not ballistic, although we cannot give clear evidence that $\alpha = 1$. We suspect the transport is indeed diffusive, as quartic pinning is sufficient to induce diffusive scaling in the harmonic chain [13].

II. THE MODEL

Consider a 1-dimensional chain of $N + 2$ labeled particles, i.e., located on the lattice $L = \{0, 1, \dots, N, N + 1\}$, with the following classical Hamiltonian H

$$H = \sum_{i=0}^{N+1} \left[\frac{p_i^2}{2} + \frac{\nu^2}{z} q_i^z + V(r_i) \right], \quad r_i \equiv q_{i+1} - q_i, \quad z \text{ even.} \quad (1)$$

Here $\{q_i\}$ are the displacements of the particles, $\{p_i\}$ are their momenta, ν is the strength of the one-body pinning potential and $V_i \equiv V(r_i)$ is the interaction potential. For periodic boundary conditions $V_{N+1} = V(q_0 - q_{N+1})$ while for fixed boundary conditions $V_{N+1} = 0$ and $q_0 = q_{N+1} = p_0 = p_{N+1} = 0$. When $\nu = 0$ and

$$V_i = \frac{a}{b} \exp[-br_i], \quad a, b > 0, \quad (2)$$

the system is the Toda chain [14], which is a well-known integrable model for both periodic and fixed boundary conditions [15,16]. Unless otherwise specified, V_i will refer to the Toda interaction for the remainder of this work.

In this note, we numerically investigate the heat transport properties of the fixed boundary Toda chain with the addition of an on-site harmonic potential, i.e., $\nu \neq 0$ and $z = 2$. In general, such a modification is expected to break the integrability of the $\nu = 0$ system when the number of particles is greater than 2. Indeed, the only obvious conserved quantities when $\nu \neq 0$ are H itself and the center of mass term h_c

$$h_c = \frac{1}{2} \left(\sum_{i=0}^{N+1} p_i \right)^2 + \frac{\nu^2}{2} \left(\sum_{i=0}^{N+1} q_i \right)^2. \quad (3)$$

We couple particles 1 and N of the chain to Langevin baths with a coupling constant μ , which act as thermal reservoirs at temperatures T_L and T_R and induce a nonequilibrium steady state (NESS). The infinitesimal generator of motion \mathcal{L} is therefore

$$\begin{aligned} \mathcal{L}(\cdot) &= \mu B_{1,T_L}(\cdot) + \mu B_{N,T_R}(\cdot) + \mathcal{A}(\cdot), \\ \mathcal{A}(\cdot) &= \sum_{j=1}^N (p_{j+1} - p_j) \partial_{r_j} + \sum_{j=1}^N (V'_j - V'_{j-1} - \nu^2 q_j^{z-1}) \partial_{p_j}, \\ B_{j,T_{L/R}}(\cdot) &= -p_j \partial_{p_j} + T \partial_{p_j}^2, \quad j = 1, N; \quad \mu = \text{bath coupling} \end{aligned} \quad (4)$$

where $V'_j \equiv \frac{dV(r_j)}{dr_j}$. For systems like Eq. (4), the integrability of the bulk dynamics plays a central role in determining the transport properties [5], although in the quantum mechanical case this statement requires qualification [17]. The central quantity of interest is the average heat current J , which in the NESS is given by

$$J = \langle J_j \rangle = - \left\langle \frac{1}{2} (p_j + p_{j+1}) V'_j \right\rangle, \quad j \in [2, N - 1], \quad (5)$$

where $\langle \cdot \rangle$ refers to the NESS average, which in simulations is computed by first allowing the system sufficient time to relax to the NESS before time averaging. Also of interest is the NESS temperature profile T_j

$$T_j = \langle p_j^2 \rangle, \quad j \in [1, N]. \quad (6)$$

In the following, we will give evidence that when $z = 2$, $J \sim N^0$ and that T_j is independent of j in the bulk, with a jump in T_j at the reservoirs. These two properties are only expected to hold when the bulk dynamics are integrable. Indeed, because these bulk dynamics are expected to be nonintegrable and break translational invariance, one would expect $J \sim N^{-1}$ and T_j to be a continuous curve interpolating between T_L and T_R . We then show that when the pinning is anharmonic, e.g., $z = 4$, then the system satisfies the ordinary expectations. Spurred by the unexpected harmonic pinning result, we then give further evidence of nondissipative behavior in this model.

III. NONDISSIPATIVE BEHAVIOR

A. Ballistic transport

Consider the dynamics Eq. (4) for the Toda interaction Eq. (2) and $z = 2$ (harmonic pinning). We integrate Eq. (4) using a velocity Verlet algorithm adapted to include the Langevin reservoirs [18]. In Fig. 1, we show the steady state temperature profiles for several N and in Fig. 2 we show the values of the corresponding steady state currents, which we measure in three ways. J_{Bulk} is obtained by averaging J from Eq. (5) over the entire bulk of the chain, while J_L and J_R follow from the steady-state average of the energy flux from a Langevin bath

$$\begin{aligned} J_{\text{Bulk}} &= \frac{1}{N-2} \sum_{j=2}^{N-1} \langle J_j \rangle, \\ J_L &= \mu(T_L - \langle p_1^2 \rangle), \\ J_R &= \mu(\langle p_N^2 \rangle - T_R). \end{aligned} \quad (7)$$

The agreement of the three numerically obtained currents from Eq. (7) indicates that we have indeed reached the steady state. The flat temperature profile and non-scaling current illustrated in Fig. 1 and Fig. 2 is expected for the $\nu = 0$ (integrable) case, but it is entirely surprising for $\nu \neq 0$. In Fig. 3, we vary ν and show that J is a decreasing function of ν , as expected for pinned chains [19].

We show a marked change in behavior in Fig. 4 for the Toda chain with quartic pinning ($z = 4$). There, as N increases, the temperature profiles approach a smooth curve interpolating between T_L and T_R , and the current J approximately satisfies $J \sim N^{-\alpha}$, with $\alpha = 0.88$.

B. Persistent heat currents in the periodic chain

Consider now the dynamics of the system with Hamiltonian 1, $z = 2$, and interaction 2 with periodic boundary conditions and no external driving. Given the observed ballistic heat transport in the corresponding driven system, one expects any initial heat current to propagate without dissipation in the periodic system. In Fig. 6, we observe such behavior in a 200 particle system for times long enough for the current to propagate many times

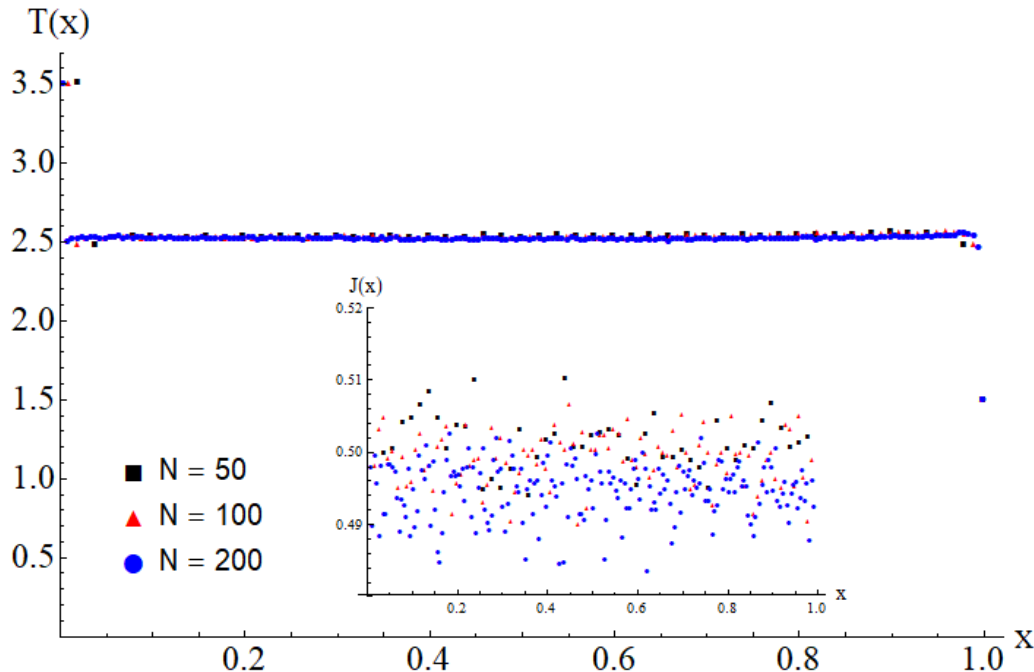


FIG. 1: Temperature profiles ($T_L = 4$, $T_R = 1$) for the Toda chain with harmonic pinning ($a = b = \mu = \nu = 1$, $z = 2$). The j -th particle occupies position $x_j = j/N$. Each profile is an average over 6 runs. The dynamics were integrated with a timestep $dt = 0.005$. We allow 2×10^9 timesteps to reach the NESS and then average the currents and temperature profiles over the same amount of time, with 2×10^4 timesteps in between each measurement. Insert: Averaged site-by-site current profile. The fact these profiles are flat indicates that we averaged in the NESS.

around the chain. Similar nondissipative behavior in the harmonically pinned Toda chain with open boundary was numerically observed in [20]. In that context, the Toda potential Eq. (2) arises as an effective interaction between well-separated solitons of certain solutions of the Gross-Pitaevskii PDE, which models solitons in Bose-Einstein condensates [21,22]. When the Toda chain was placed in a harmonic trap (which is mathematically identical to pinning each particle in the chain), a Toda soliton was observed to oscillate persistently like the spheres of a Newton’s cradle. In diffusive systems, any initial current decays to thermal noise as exemplified in Fig. 7 when the Toda chain is subject to quartic pinning ($z = 4$).

C. Poincaré sections

The observations of Sec. III A and Sec. III B for $z = 2$ sharply contradict the CAT about the behavior for nonintegrable chains that break momentum conservation. On the other hand, it is possible that the Toda chain with harmonic pinning is in fact integrable. Indeed, the Calogero-Moser Hamiltonian remains integrable when harmonic pinning is added [23]. While it is highly unlikely that such a simple generalization of a well-known integrable model would have escaped notice for decades, we present dynamical evidence that a higher conservation law exists for 3 particle Toda chains with harmonic pinning. To do so, we construct Poincaré sections of the open chain dynamics, where the end particles are free to move. Each time the particle labeled “0” returns to its initial

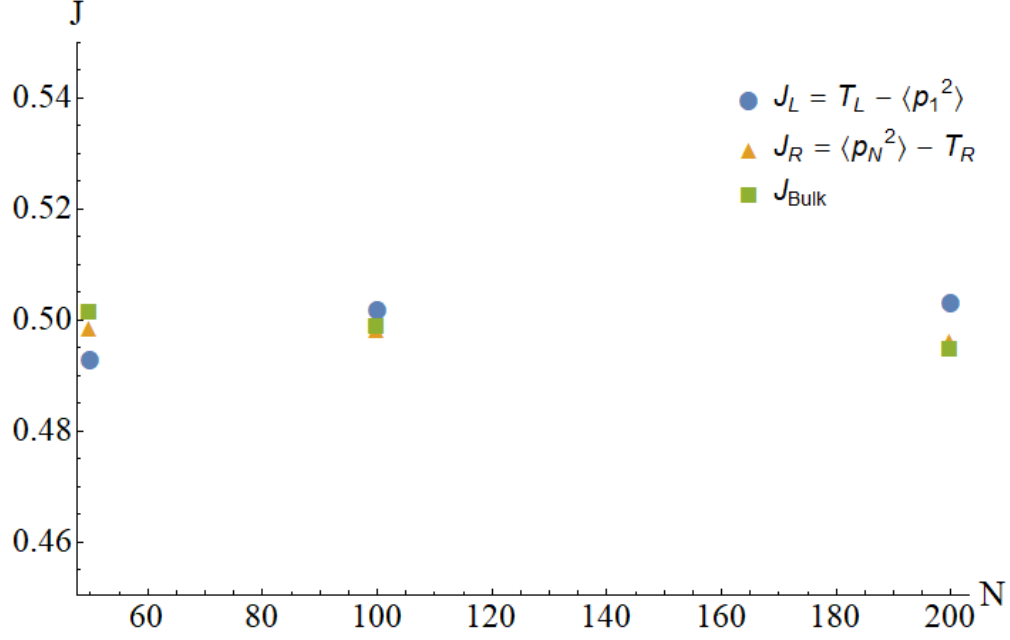


FIG. 2: The currents of the temperature profiles from Fig. 1 as a function of N . There is no appreciable decay of the currents as N increases, i.e., the transport is ballistic. The ratios of the bulk currents are $J_{100}/J_{50} = 0.995$ and $J_{200}/J_{100} = 0.992$.

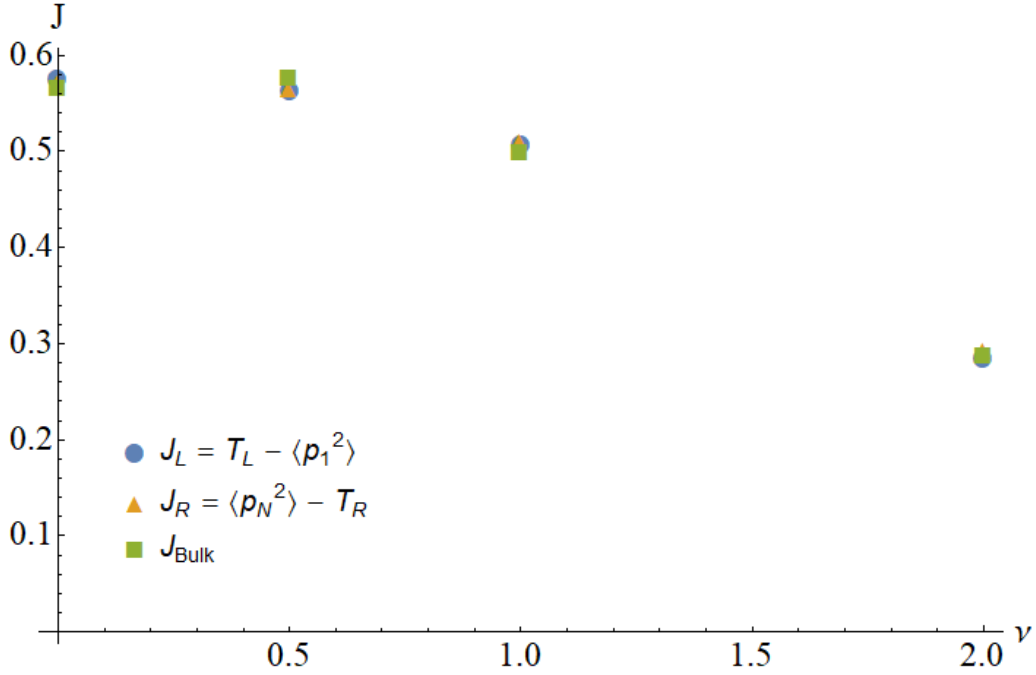


FIG. 3: Observed decrease in current as the pinning strength ν is increased for the driven Toda chain with harmonic pinning. Here $N = 100$ and all parameters are the same as in Fig. 1, save for the varying ν and a shorter relaxation and observation time, both 2×10^8 time steps. The three methods of measuring the current from Eq. (7) significantly overlap.

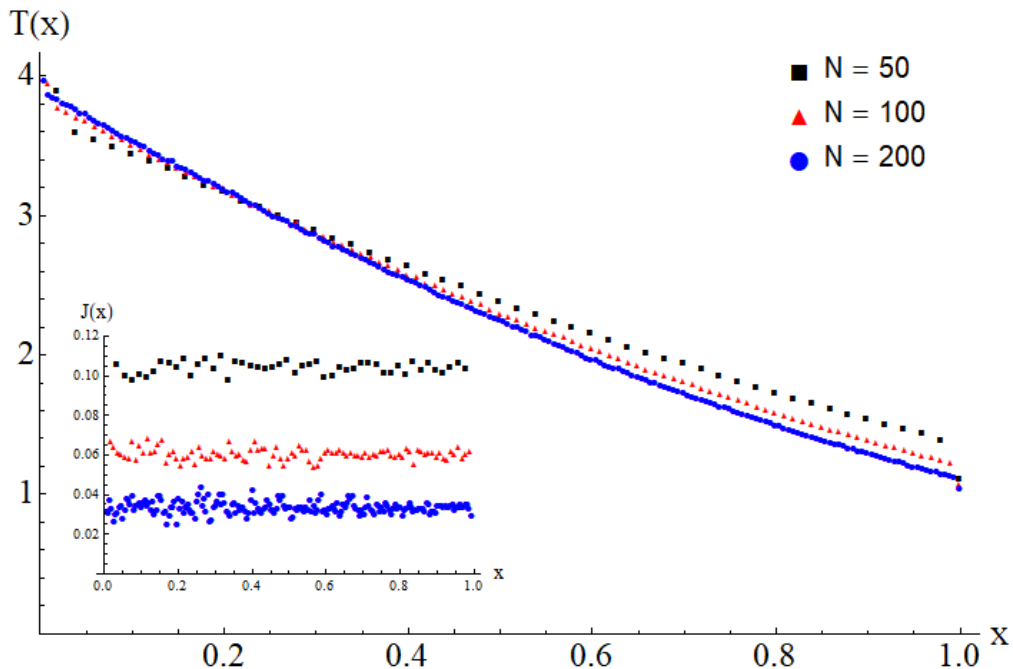


FIG. 4: Temperature profiles and currents for the Toda chain with quartic pinning ($z = 4$), with all parameters the same as in Fig. 1. Note that with increasing N the profile approaches a smooth curve between $T_L = 4$ and $T_R = 1$. Insert: Averaged site-by-site current profile. The fact these profiles are flat indicates that we averaged in the NESS.

position, we record the momenta of all three particles.

If the system were nonintegrable, the dynamics of the 3-body case would take place of a 4-dimensional manifold, for there are 6 degrees of freedom corresponding to the positions and momenta, and the conserved Hamiltonian and the conserved term h_c from Eq. (3) reduce this number to $6 - 2 = 4$. By recording sections when $q_0 = q_0(0)$ and $p_j = p$ for either $j = 0, 1$ or 2 , we therefore expect to obtain a $4 - 2 = 2$ dimensional cross section of the dynamics. For all initial conditions we tested, however, such cross sections are 1-dimensional curves, indicating the presence of an additional conserved quantity. We illustrate this point in Fig. 8. If there exists a third conserved quantity that Poisson commutes with h_c , the 3-body case is integrable.

We emphasize that the mere existence of initial conditions that constrain the dynamics to lower dimensional manifolds is generic to nonintegrable models. If, however, *all* initial conditions lead to such constrained dynamics, as is the case for Liouville integrability, then it is quite likely that more conserved quantities exist. We tested several random initial conditions for the 3-body case.

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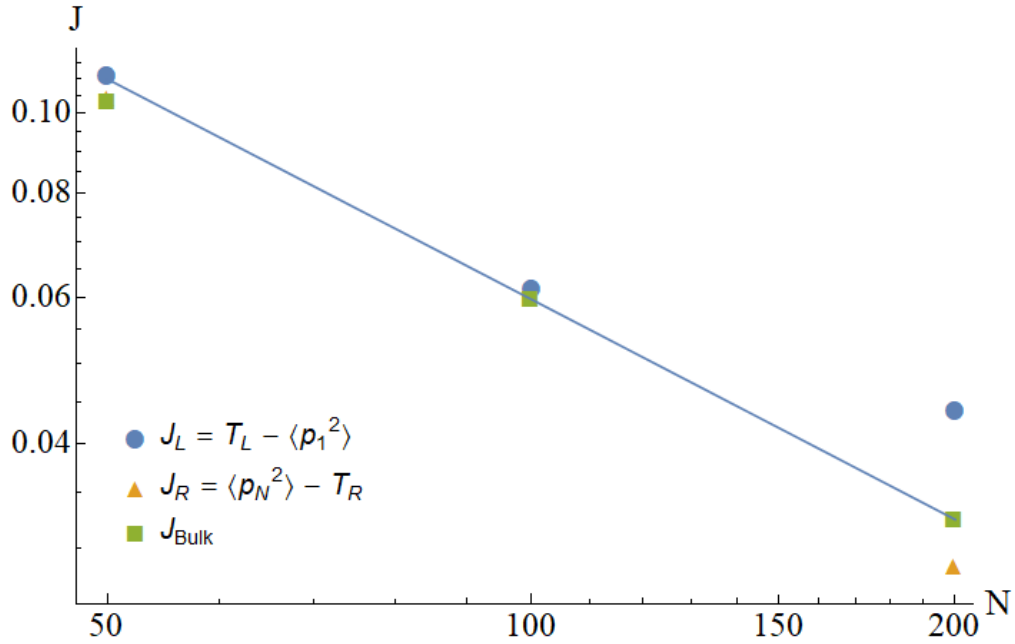


FIG. 5: Log-log plot of the scaling of J with respect to N for the temperature profiles of Fig. 4. The straight line was selected to interpolate between J_{Bulk} for $N = 100$ and $N = 200$ with $J_{\text{Bulk}} \sim N^{-\alpha}$, $\alpha = 0.88$. We use the bulk current because its variance is reduced by averaging over the chain. Note that $\alpha = 0.88$ differs appreciably from the diffusive scaling exponent of 1, but typically to truly see diffusive behavior one needs to go to larger N .

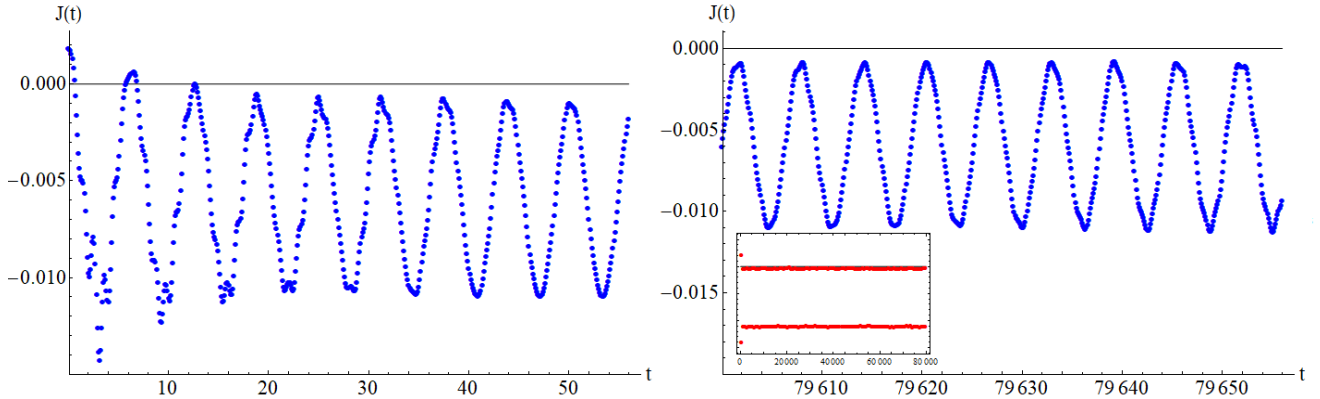


FIG. 6: Initial and long time behavior of the persistent total current in the Toda chain from Eq. (1) and Eq. (2) ($a = b = 1$) with harmonic pinning ($z = 2$, $\nu = 1$) and periodic boundary conditions, $N = 198$. The dominant frequency of the long time current is very close to the value of the pinning frequency. The dynamics were integrated with a timestep of $dt = 10^{-4}$, and initial condition $q_0(0) = -1$, $p_1(0) = 1$, $q_2(0) = 1$, with all other initial coordinates and momenta zero. The same dynamics with $dt = 10^{-3}$ are nearly identical. Insert: locally averaged maxima and minima of the current for times $t \in [0, 8 \times 10^4]$. Note in Fig. 7 the decay of the current in the quartic pinning case.

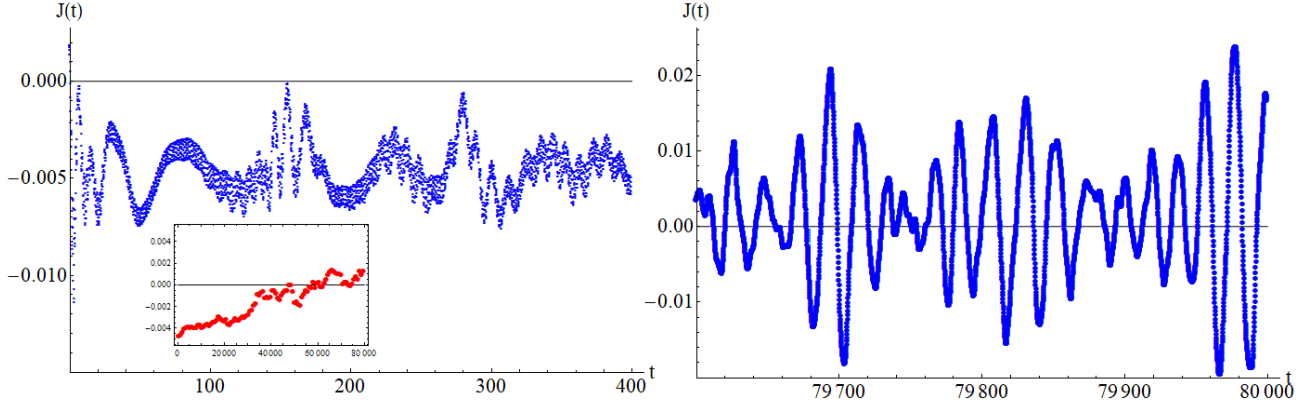


FIG. 7: Current in the Toda chain with quartic pinning ($z = 4$) for the same parameters and initial conditions as Fig. 6. The current dissipates into noise fluctuating about zero. Insert: Local average of the current for $t \in [0, 8 \times 10^4]$.

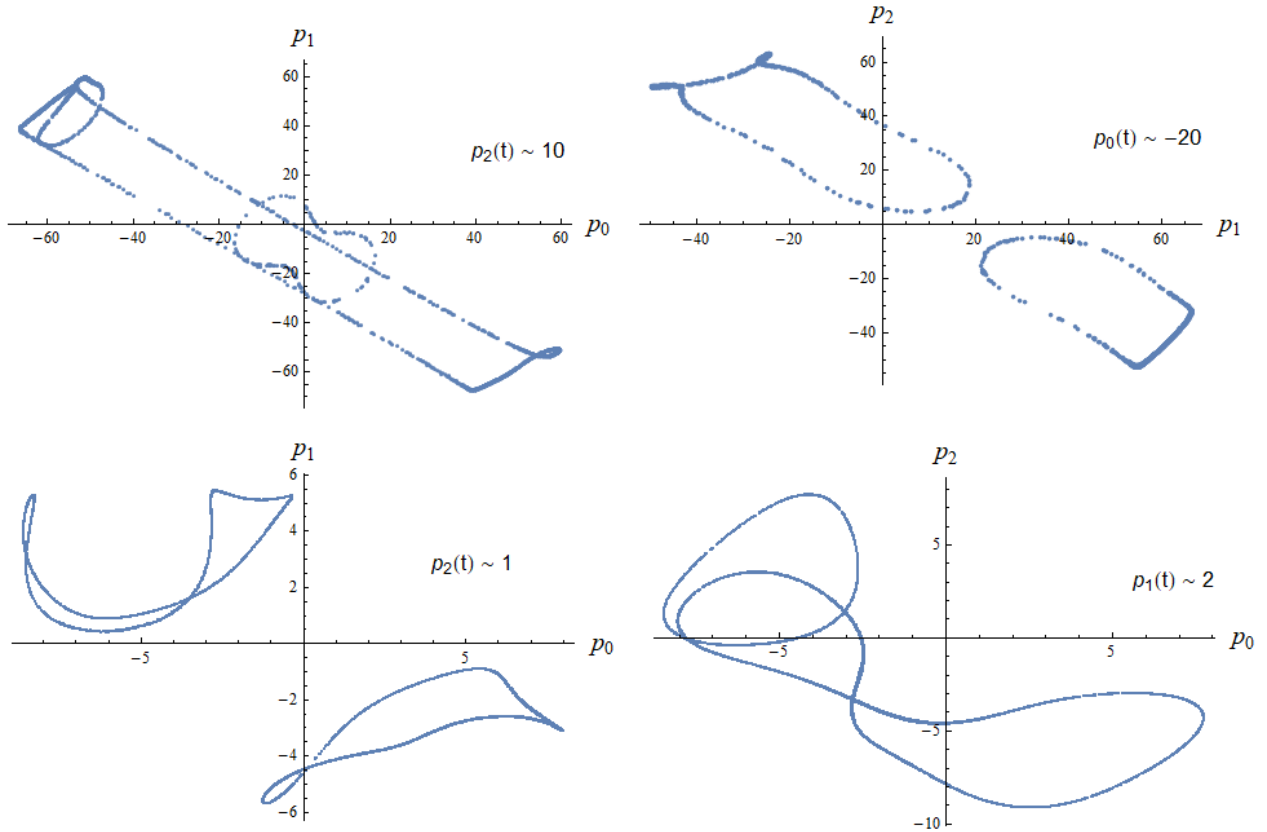


FIG. 8: Poincaré sections for the 3-body open Toda chain ($a = b = 1$) with harmonic pinning ($z = 2, \nu = 1$). The four images correspond to two different runs (top, bottom) where the momenta p_j were recorded each time $q_0(t) \sim q_0(0)$ (within a tolerance of $\delta = 0.001$). Within each cross section is indicated which momentum is kept fixed and the corresponding value. The tolerance of the fixed momentum is adjusted to allow enough points to make the shape of the curves clear.

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