Nekhoroshev theorem for the Dirichlet Toda chain

A case study in perturbation theory using symmetry principles

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Abstract

In this work, we prove a Nekhoroshev theorem for the Toda chain with Dirichlet boundary conditions, i.e., fixed ends. The Toda chain is a special case of a Fermi-Pasta-Ulam (FPU) chain, and in view of the unexpected recurrence phenomena observed numerically in these chains, it has been conjectured that theory of perturbed integrable systems could be applied to these chains, especially since the Toda chain has been shown to be a completely integrable system. Whereas various results have already been obtained for the periodic lattice, the Dirichlet chain is more important from the point of view of applications, since the famous numerical experiments have been performed for this type of system. Mathematically, the Dirichlet chain can be treated by exploiting symmetries of the periodic chain. Precisely, by considering the phase space of the Dirichlet chain as an invariant submanifold of the periodic chain, namely the fixed point set of a certain symmetry of the periodic chain, the results obtained for the periodic chain can be used to obtain similar results for the Dirichlet chain. The Nekhoroshev theorem is a perturbation theory result which does not have the probabilistic character of other results such as those of the KAM theorem.

Introduction

Perturbation theory of integrable systems can be a powerful tool to explain the behaviour of certain Hamiltonian systems, which themselves are not integrable systems, but which can be thought of as approximations of integrable systems. Starting in the 1950's, Fermi-Pasta-Ulam chains have become an important example of such systems, especially since the unexpected regularity properties observed by Fermi et al. are still not fully understood. The Toda chain is a special case of such systems, since it has especially strong integrability properties and can be therefore be analyzed to a much greater extent.

Symmetry enters the discussion when one examines various kinds of boundary conditions: The model with periodic boundary conditions is structurally more fundamental, whereas the model with Dirichlet (fixed ends) boundary conditions is more important for applications. The two models can be connected with each other by a transformation which maps the chain with fixed ends to an invariant submanifold of the periodic chain. This invariant submanifold is the fixed point set of a certain symmetry of the periodic chain. By investigating the properties of this symmetry transformation of the periodic chain, one can thus obtain conclusions about the Dirichlet chain, and thus maybe make some contribution to an explanantion of the surprising results of Fermi's simulations.

Overview

1. The Toda chain
2. Historical background: Fermi, Pasta, Ulam, Toda
3. Theoretical background: Perturbed Hamiltonian systems
4. Symmetries of the periodic Toda chain
5. Using symmetries for treating the Dirichlet Toda chain as a special case of the periodic Toda chain
6. Convexity for the periodic and Dirichlet chains
7. Mathematical tools used for proving the convexity results

The Toda chain

Mathematical model

Hamiltonian of the 1D Toda chain

$$H_{Toda} = \frac{1}{2}\sum_{n=1}^{N} p_n^2 + \alpha^2 \sum_{n=1}^{N} e^{q_n - q_{n+1}}$$

Periodic boundary conditions:

$$(q_{n+N}, p_{n+N}) = (q_n, p_n) \qquad \forall\, n \in \mathbb{Z}.$$

Dirichlet boundary conditions (fixed ends):

$$q_0 = q_{N+1} = p_0 = p_{N+1} \equiv 0.$$

Comparison of boundary conditions

- The case with *periodic* boundary conditions is theoretically more important.
- The case with *Dirichlet* boundary conditions is practically more important.
- We use symmetries to transfer results from the periodic case to the Dirichlet case.

Historical background: Fermi, Pasta, Ulam, Toda

- New MANIAC-I computer in Los Alamos in the 1950s
- *Fermi's idea*: Simulation of a 1D chain of harmonic oscillators, weakly perturbed by nonlinear forces
- simple example of irreversible statistical mechanics
- *Goal*: Numerical test of the phenomenon of "thermalization", i.e. equipartition of energy, ergodicity
- *Result of the simulation:* After a certain time, almost all energy is back to the lowest frequency mode!
- *FPU paradox*: Nonlinearity is not enough to guarantee equipartition of energy.
- Violation of Fermi's "theorem" on ergodicity in nonlinear systems
- *Toda chain*: Special case of FPU chains with high integrability properties
- The high integrability properties make it possible to apply results of perturbation theory globally on the entire phase space

Theoretical background: Perturbed Hamiltonian systems

Perturbed Hamiltonian systems:

- Hamiltonian systems are a special case of dynamical systems with strong integrability properties. They are important as *well understood approximations to non-integrable systems*
- Two main results on the stability of perturbed integrable systems: KAM theorem, Nekhoroshev theorem
- KAM theorem: Consider a perturbed Hamiltonian $H = H_0(I) + \epsilon H_1(x, y)$, where $H_0(I)$ is the unperturbed Hamiltonian in the action variables $I = (I_1, \ldots, I_n)$. If the unperturbed Hamiltonian $H_0(I)$ is a *nondegenerate* function of the action variables, then the stability of the unperturbed system is preserved under the perturbation $\epsilon H_1(x, y)$ for a *majority* of initial conditions, if ϵ is small enough
- Nekhoroshev theorem: Consider a perturbed Hamiltonian $H = H_0(I) + \epsilon H_1(x, y)$, where $H_0(I)$ is the unperturbed Hamiltonian in the action variables $I = (I_1, \ldots, I_n)$. If the unperturbed Hamiltonian $H_0(I)$ is a *convex* function of the action variables, then the stability of the unperturbed system is preserved under the perturbation $\epsilon H_1(x, y)$ for *all* initial conditions, if ϵ is small enough
- Comparison of the KAM and Nekhoroshev theorems: Both theorems have conditions which are in general difficult to check for a given system; the Nekhoroshev theorem has the advantage that its stability assertion holds for all (sufficiently small) perturbations of H_0, whereas the KAM theorem only holds for most (sufficiently small) perturbations of H_0
- The KAM theorem is of *probabilistic* nature, whereas the Nekhoroshev theorem is of *deterministic* nature.
- The assumptions of the KAM theorem are weaker and easier to check, those of the Nekhoroshev theorem are stronger and more difficult to check.

Symmetries of the periodic Toda chain

- Two basic symmetries of the periodic chain:

$$T : (q_1, \ldots, q_N, p_1, \ldots, p_N) \mapsto (q_2, q_3, \ldots, q_N, q_1, p_2, p_3, \ldots, p_N, p_1),$$
$$S : (q_1, \ldots, q_N, p_1, \ldots, p_N) \mapsto -(q_{N-1}, \ldots, q_1, q_N, p_{N-1}, \ldots, p_1, p_N);$$

- Relationships between T and S:

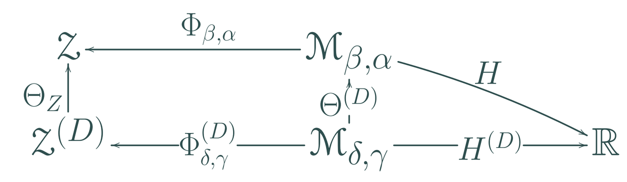
$$T^N = S^2 = \mathrm{Id}, \qquad TS = ST^{-1}$$

- It turns out that the *fixed point set* of S plays an important role in the investigation

Using symmetries for treating the Dirichlet Toda chain as a special case of the periodic Toda chain

Commutative diagram relating various spaces and transformations of the two cases (periodic and Dirichlet):

- $\mathcal{M}_{\beta,\alpha}$: phase space of the periodic chain
- $\mathcal{M}_{\delta,\gamma}$: phase space of the Dirichlet chain
- $\mathcal{Z}$: phase space of the periodic chain in normal form coordinates
- $\mathcal{Z}^{(D)}$: phase space of the Dirichlet chain in normal form coordinates
- Θ_Z, $\Theta^{(D)}$: Embeddings of the respective phase spaces



Symmetries used in this embedding:

- The image of the embedding $\Theta^{(D)} : \mathcal{M}_{\delta,\gamma} \to \mathcal{M}_{\beta,\alpha}$ is the fixed point set $\mathrm{Fix}(S)$ of the symmetry S of the periodic map.
- By making pulllbacks by the embeddings, we can use results about the behaviour of the periodic chain on the fixed point set $\mathrm{Fix}(S)$ to obtain results on the Dirichlet chain

Convexity for the periodic and Dirichlet chains

- The Hamiltonian of the periodic lattice is a *convex function* of the $N - 1$ action variables
- If we restrict ourselves to the fixed point set of the symmetry S, the action variables are no longer independent, there are only $\frac{N}{2} - 1$ independent action variables
- On the fixed point set of the symmetry S, the Hamiltonian of the periodic lattice is a *convex function* of the $\frac{N}{2} - 1$ independent action variables
- By taking the pullback Θ_Z, we can conclude that the Hamiltonian of the Dirichlet chain is also a convex function of all action variables of the Dirichlet chain.
- The convexity guarantees that the Nekhoroshev theorem can be applied to the system.

Mathematical tools used for proving the convexity results

- *Lax pair* formulation of the dynamical equations: $\dot{L} = [B, L]$ where B and L and suitable matrices. From this it follows that the eigenvalues of L are conserved quantities, which establishes the integrability property.
- *Riemann surface* associated to the matrix L, cycles and differentials on the surface: It can be shown that the oscillation frequencies of the Toda chain can be written as integrals of certain differentials on the surface.
- *Algebraic geometry*: We use a result after Krichever to prove the nondegeneracy of the frequency map; this results uses results on the geometry of the Riemann surface and its differentials.

References

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