# On the open Toda chain with external forcing

Percy Deift, Luen-Chau Li, Herbert Spohn,
Carlos Tomei, Thomas Trogdon

To the memory of V.S. Buslaev

Euler Institute, St. Petersburg, June 20-22, 2021

The theme:

"If it looks like a duck, walks like a duck

and quacks like a duck... it´s a duck !"

In 1967, M. Toda introduced the eponymous Toda system with Hamiltonian

$$H(q,p) = \frac{1}{2m}\sum_{n\in\mathbb{Z}} p_n^2 + \frac{a}{b}\sum_{n\in\mathbb{Z}} e^{-b(q_{n+1}-q_n)} + a\sum_{n\in\mathbb{Z}} (q_{n+1}-q_n), \text{ with } a,b>0 \tag{1}$$

for particles of equal mass $m > 0$ with positions $q = \{q_n\}$ on the line, and momenta $p = \{p_n\}$. The corresponding Hamiltonian equations have the form

$$\begin{aligned} \dot{q}_n &= \tfrac{\partial H}{\partial p_n} = \tfrac{1}{m} p_n, \\ \dot{p}_n &= -\tfrac{\partial H}{\partial q_n} = -a\left(e^{-b(q_{n+1}-q_n)} - e^{-b(q_n-q_{n-1})}\right), \end{aligned} \tag{2}$$

for $-\infty < n < \infty$, and so

$$\ddot{q}_n = -\frac{a}{m}\left(e^{-b(q_{n+1}-q_n)} - e^{-b(q_n-q_{n-1})}\right). \tag{3}$$

Scaling $q_n \to b\,q_n\,, \quad t \to t\sqrt{\frac{m}{ab}},$ the equations turn into

$$\dot{q}_n = p_n\,, \quad \dot{p}_n = e^{(q_{n+1}-q_n)} - e^{(q_n-q_{n-1})} \tag{4}$$

which are generated by the Hamiltonian

$$H = \frac{1}{2}\sum_{n\in\mathbb{Z}} p_n^2 \; + \; \sum_{n\in\mathbb{Z}} e^{q_n - q_{n+1}} \; + \; c\sum_{n\in\mathbb{Z}} (q_n - q_{n+1}) \; , \tag{5}$$

for any constant $c \in \mathbb{R}$. The restriction to periodic boundary conditions

$$q_{n+N} = q_n + s \; , \quad p_{n+N} = p_n$$

with $s = -\sum_{n=1}^{N-1}(q_n - q_{n+1})$ was investigated, first numerically and then analytically, culminating in the proof by Hénon, and shortly thereafter by Flaschka and independently Manakov, that the (periodic) system was integrable.

The so called *open Toda chain* (also called ‘Toda with fixed ends´) is the finite $N$-dimensional system that remains after setting

$$q_0 = -\infty \; , \quad q_{N+1} = \infty$$

in (5), resulting in the system

$$
\begin{aligned}
\dot{q}_n &= p_n, \quad 1 \le n \le N, \\
\dot{p}_1 &= -e^{q_1 - q_2} \\
\dot{p}_n &= e^{q_{n-1} - q_n} - e^{q_n - q_{n+1}}, \quad 2 \le n \le N-1, \\
\dot{p}_N &= e^{q_{N-1} - q_N}.
\end{aligned}
\tag{6}
$$

generated by the Hamiltonian

$$
H_F(q,p) = \frac{1}{2} \sum_{n=1}^{N} p_n^2 + \sum_{n=1}^{N-1} e^{(q_n - q_{n+1})} .
$$

Motivated by their approach to the periodic case, Flaschka and Manakov showed that (6) could be written in Lax-pair form by setting

$$
\begin{aligned}
a_n &= -p_n/2, \; 1 \le n \le N, \\
b_n &= \tfrac{1}{2} e^{(q_n - q_{n+1})/2}, \; 1 \le n \le N-1,
\end{aligned}
\tag{7}
$$

and defining the symmetric and skew-symmetric matrices

$$
L_F = \begin{pmatrix} a_1 & b_1 & \dots & 0 \\ b_1 & a_2 & \ddots & 0 \\ \vdots & \ddots & \ddots & b_{N-1} \\ 0 & 0 & b_{N-1} & a_N \end{pmatrix} = L_F^T \, , B_F = \begin{pmatrix} 0 & -b_1 & \dots & 0 \\ b_1 & 0 & \ddots & 0 \\ \vdots & \ddots & \ddots & -b_{N-1} \\ 0 & 0 & b_{N-1} & 0 \end{pmatrix} = -B_F^T \, .
$$

Then if $q_n(t), p_n(t)$ solve (6), $L_F(t)$ solves the Lax-pair equation

$$\dot{L}_F = [L_F, B_F] \, , L_{F,0} = L_F(t=0) \text{ given by } q_n(0), p_n(0) \tag{8}$$

from which it follows that

$$\text{eigenvalues of } L_F(t) = \text{ eigenvalues of } L_F(0) = \{\lambda_1 > \lambda_2 > \ldots > \lambda_N\} \, ,$$

so providing $N$ constants of the motion for the open Toda lattice

$$\Rightarrow \text{Liouville integrability.}$$

Subsequently J.Moser showed how to use (8) to solve (6) explicitly in terms of rational functions of exponentials. Furthermore, Moser showed that the system has the following remarkable long-term scattering behavior:

$$q_n(t) = \alpha_n^{\pm} t + \beta_n^{\pm} + O(e^{-\delta|t|}), \; t \to \pm\infty, \; \delta > 0, 1 \le n \le N \tag{9}$$

$$p_n(t) = \alpha_n^{\pm} t + O(e^{-\delta|t|})$$

with

$$\alpha_n^+ = -2\lambda_n, \quad \alpha_n^- = -2\lambda_{N-n+1}, \quad 1 \le n \le N \tag{10}$$

and scattering shift as $t$ goes from $-\infty$ to $\infty$, given by

$$\beta_n^+ - \beta_{N-n+1}^- = \sum_{\ell \neq n} \phi_{\ell n}, \; 1 \le n \le N, \tag{11}$$

where

$$\phi_{\ell n} = \begin{cases} \ln(2\lambda_\ell - 2\lambda_n)^2, & \ell > n \\ -\ln(2\lambda_\ell - 2\lambda_n)^2, & \ell < n. \end{cases}$$

And so the velocity of the particle $q_{N-n+1}$ at $t \to -\infty$ is transferred to the particle $q_n$ at $t \to \infty$, with a phase shift $\beta_n^+ - \beta_{N-n+1}^-$.

When I came across formula (11), I was astounded that one could compute the scattering shifts (equivalently, the scattering matrix) for an $N$-particle system explicitly, and I asked Moser how this was possible. Moser´s reply was somewhat mysterious: he said

‘Every scattering system is integrable´ .

What Moser meant was the following.

Suppose one has the solution of a Hamiltonian system

$$(q(t), p(t)) = (q_1(t), \ldots, q_N(t), p_1(t), \ldots, p_N(t)) \in \mathbb{R}^{2N}$$

with Hamiltonian $H$ and with the property that, as $t \to \infty$,

$$p(t) = p_\infty + o(1/t),$$
$$q(t) = q_\infty + tp_\infty + o(1),$$

for some constants $(q_\infty, p_\infty)$. Let $U_t(q(0), p(0)) = (q(t), p(t))$ be the solution of the system with initial data $(q(0), p(0))$ and let

$$U_t^0(q^0(0), p^0(0)) = (q^0(t), p^0(t)) \ ,$$

where $(q^0(t), p^0(t))$ solves the free particle motion with Hamiltonian $H^0(q, p) = p^2/2$, so

$$p^0(t) = p^0(0)$$
$$q^0(t) = q^0(0) + p^0(0)t \ .$$

Then as $t \to \infty$

$$\begin{aligned} U^0_{-t} \circ U_t(q_0, p_0) &= U^0_{-t}(q_\infty + p_\infty t + o(1), p_\infty + o(1/t)) \\ &= (q_\infty + p_\infty t + o(1) - (p_\infty + o(1/t))t, p_\infty + o(1/t)) \\ &= (q_\infty + o(1), p_\infty + o(1/t)) \to (q_\infty, p_\infty) \quad \text{as} \ \ t \to \infty \ . \end{aligned}$$

Thus the wave operator

$$W(q_0, p_0) \equiv \lim_{t \to \infty} \ U^0_{-t} \circ U_t(q_0, p_0) = (q_\infty, p_\infty)$$

exists.

But then

$$U^0_{-t} \circ U_t \circ U_s = U^0_s \circ U^0_{-(t+s)} \circ U_{t+s}$$

implies

$$W \circ U_s = U^0_s \circ W$$

or, if $W^{-1}$ exists,

$$U_s = W^{-1} \circ U^0_s \circ W \ . \qquad (12)$$

Now $U^0_{-t} \circ U_t$ is symplectic for all $t$ and so $W$, and hence $W^{-1}$, are symplectic. Thus (12) shows us that $U_s$ is symplectically equivalent to $U^0_s$, and hence is completely integrable. Indeed, if $\alpha_1, \ldots, \alpha_N$, are commuting integrals for $H^0$, then $\beta_i = \alpha_i \circ W$, $i = 1, \ldots, N$ are commuting integrals for $H$:

$$\beta_i \circ U_t(q(0), p(0)) = \alpha_i \circ W \circ U_t(q(0), p(0)) = \alpha_i \circ U^0_t(W(q(0), p(0)) = \text{constant}$$

and as $W$ is symplectic,

$$\{\beta_i, \beta_j\} = \{\alpha_i \circ W, \alpha_j \circ W\} = \{\alpha_i, \alpha_j\} \circ W = 0 \ . \qquad (13)$$

Said differently, the above calculation shows more generally that ‘if a system behaves like an integrable system, then it is an integrable system!’ or, as in the famous ‘Duck Test’, ‘if it looks like a duck, walks like a duck and quacks like a duck... it’s a duck!’

Referring back to Moser´s long-time estimate (9), we now understand why the open Toda lattice is integrable.

Remarks:
1. From the 'duck´, we learn that there is an interesting Catch 22 in the problem: we could not have derived, by any means, utilizing any and all dynamical tools, the asymptotic behavior of the system, unless it was integrable in the first place!
2. Moser´s argument can be used to prove the integrability of a variety of dynamical systems, for example, Moser´s proof of the integrability of a charged particle in a dipole field (the so called Störmer Problem). In another direction, P.D. and X. Zhou showed, contrary to expectation, that the perturbed defocusing NLS equation in the line

$$iq_t + q_{xx} - 2|q|^2 q - \epsilon K(|q|^2) q = 0 \tag{14}$$

$$q(x, t = 0) = q_0(x) \to 0 \,, \qquad \text{as } |x| \to \infty$$

is integrable for $0 < \epsilon < \epsilon_0$ for some $\epsilon_0 > 0$. Here $K(|q|^2) = O(|q|^\ell)$ as $|q| \to 0$, for suitably large $\ell > 2$.

In this talk we consider Toda's original system (5) in the finite fixed-end case, with $c \neq 0$. The Hamiltonian for the system has the form

$$H_c(q,p) = \frac{1}{2}\sum_{n=1}^{N} p_n^2 + \sum_{n=1}^{N-1} e^{q_n - q_{n+1}} + c\sum_{n=1}^{N-1}(q_n - q_{n+1}),$$

giving rise to the associated Hamiltonian equations

$$\begin{aligned} \dot{q}_n &= p_n\,, \quad 1 \le n \le N, \\ \dot{p}_1 &= -\,e^{q_1 - q_2} - c, \\ \dot{p}_n &= e^{q_{n-1} - q_n} - e^{q_n - q_{n+1}}\,, \quad 2 \le n \le N-1, \\ \dot{p}_N &= e^{q_{N-1} - q_N} + c. \end{aligned} \tag{15}$$

Note that

$$c\sum_{n=1}^{N-1}(q_n - q_{n+1}) = c(q_1 - q_N),$$

and we think of $H_c$ as the Hamiltonian of a lattice of particles $q_1, \ldots, q_N$ with external forces acting on the endpoints via the potential $cq_1 - cq_N$.
When $c > 0$, the forces

$$-\frac{\partial}{\partial q_1} c(q_1 - q_N) = -\,c \qquad -\frac{\partial}{\partial q_N} c(q_1 - q_N) = c$$

stretch the lattice , and when $c < 0$, they compress the lattice.

The system $H_c$ arose naturally in the study (H.S.) of the statistical mechanics of the Toda lattice.

The numerical calculations below suggest strongly that in the case $c > 0$, $H_c$ is integrable. And indeed, our main result is to show, using Moser's integrability argument, that this is the case. In the case $c < 0$, we will argue below that the numerical calculations suggest that also in this case there is integrable structure, or near integrable structure, but the problem remains open.

As a benchmark, Figure 1 displays the solution of open Toda lattice $H_F$ with $N = 20$ particles and randomply chosen initial data.

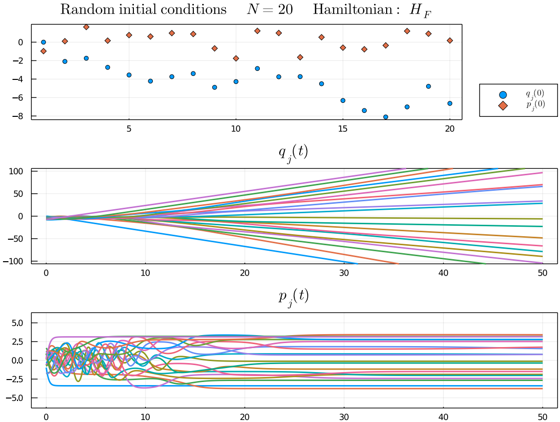
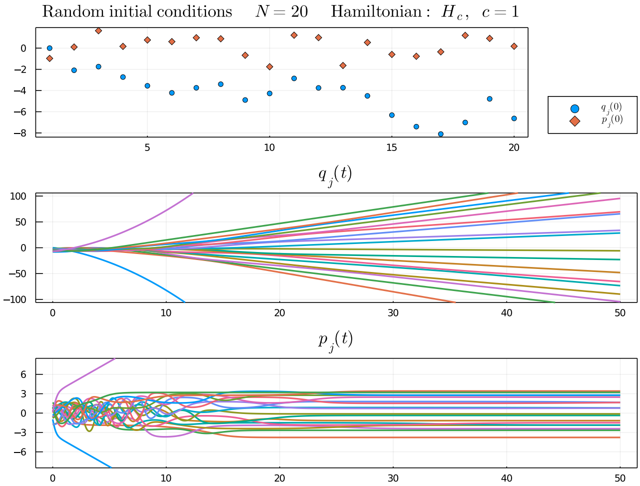


Figure 2 display the solution of the perturbed Toda lattice $H_c$ with $c = 1, N = 20$ particles and randomly chosen data.



As $t \to \infty$,

$$p_i(t) = p_{i,\infty} + o(1)\,, \quad q_i(t) = q_{i,\infty} + tp_{i,\infty} + o(1)\,, \quad 2 \le i \le N-1$$

for suitable constants $p_{i,\infty}, q_{i,\infty}$. But

$$\begin{aligned} p_1(t) &= -ct + O(1)\,, \quad q_1(t) = -ct^2/2 + O(t)\,, \\ p_N(t) &= ct + O(1)\,, \quad q_N(t) = ct^2/2 + O(t)\,. \end{aligned}$$

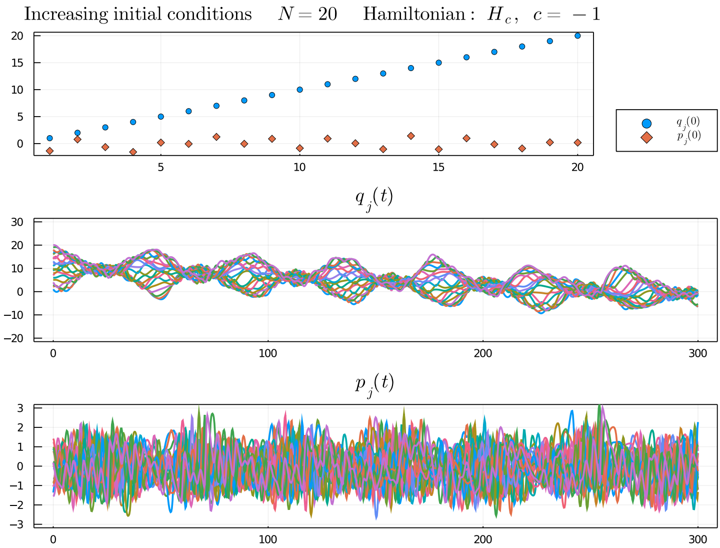
This suggests that the solutions of the $H_c$ equations behave like solutions of a system of $N$ particles $q_1, \ldots, q_N, p_1, \ldots, p_N$ consisting of a Toda lattice $q_2, \cdots, q_{N-1}, p_2, \cdots, p_{N-1}$ decoupled from a pair of (decoupled) particles $q_1, p_1, q_N, p_N$ solving

$$\begin{aligned} \dot{p}_1 &= -c\,, \quad \dot{q}_1 = p_1 \\ \dot{p}_N &= c\,, \quad \dot{q}_N = p_N\,. \end{aligned}$$

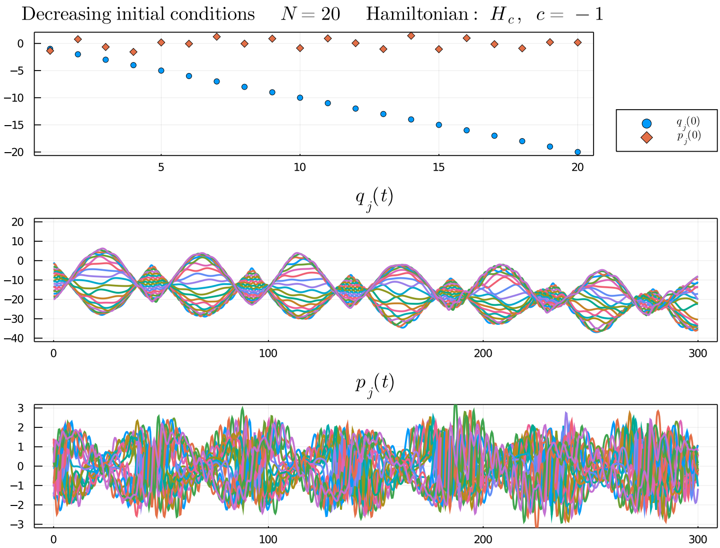
Such a system of $N$ particles is clearly completely integrable. What we will show is that solutions of the perturbed Toda system with Hamiltonian $H_c, c > 0$, indeed behave asymptotically like solutions of the decoupled system, and hence in view of Moser's observation, the perturbed system is integrable.

Figures 3, 4 and 5 display the solutions of the perturbed lattice $H_c$ with $c = -1$ and different initial data. In all three cases, the solution $q_n(t)$ appears to evolve almost periodically in time, modulo a slight gradient (the gradient arises from the fact that the total momentum $p_1 + \ldots + p_N$ is conserved and so $q_1(t) + \ldots + q_N(t)$ moves linearly: however, for some unexplained reason, all the particles come together at essentially periodic intervals, $t_1 < t_2 < \ldots < t_k < \ldots$ and so $q_n(t_k) \simeq (1/N)(q_1(t_k) + \ldots q_N(t_k))$ lie on a line for $n = 1, \ldots, N$ and $t = t_k$).

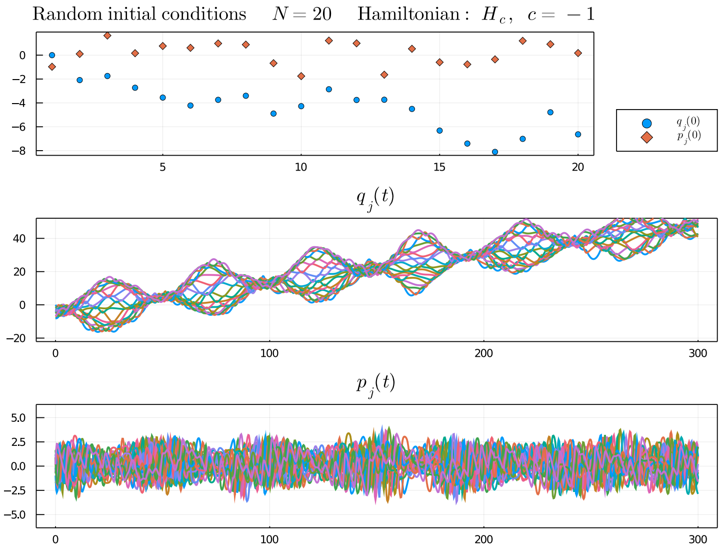
In the first two cases, this behavior persists at least up to times $t \sim 300$, but in the third case, the almost periodicity begins to unravel after $t \sim 200$.



Increasing initial conditions $N = 20$ Hamiltonian : $H_c$, $c = -1$
$q_j(0)$
$p_j(0)$
$q_j(t)$
$p_j(t)$



Decreasing initial conditions $N = 20$ Hamiltonian : $H_c$, $c = -1$
$q_j(0)$
$p_j(0)$
$q_j(t)$
$p_j(t)$



Random initial conditions $N = 20$ Hamiltonian : $H_c$, $c = -1$
$q_j(0)$
$p_j(0)$
$q_j(t)$
$p_j(t)$

These calculations bring to mind the celebrated computations of E. Fermi, J. Pasta, S. Ulam and M. Tsingou, in which the authors, anticipating ergodicity, found, unexpectedly, almost periodic behavior in the solutions of a particular nonlinear lattice system. This meant that in some sense the system was 'remembering' its past, and the only way a mechanical system can 'remember' its past is if it has many integrals of the motion. In this way, the discovery was viewed as strong evidence for integrability and led eventually, and famously, to the discovery by Kruskal-Zabusky and Gardner- Greene-Kruskal- Miura that the Korteweg de Vries equation is completely integrable.

Over the years, as the power of computers grew, it became clear that Fermi et al. had just not run their equations long enough: With longer computations, they would have found that the almost periodicity unravelled and ergodicity emerged. A very interesting understanding of Fermi et al. was given recently by Gallone, Ponno and Rink in arXiv:2010.03520 as follows:

The lattice equations for unidirectional lattice waves can be written schematically in the form

$$\dot{x} = V(x) + O(h^2)$$

where $h^2$ is a continuum limit parameter, $h^2 \to 0$, and

$$\dot{y} = V(y)$$

is KdV. It follows that the solution of the lattice equation $x(t)$ behaves like the (integrable) KdV equation for times $T$ of order $h^{-2}$, i.e., $Th^2 = O(1)$, when $x(t)$ begins to diverge from $y(t)$. Thus, the lattice has many $h^2$-accurate integrals up to times of order $h^{-2}$. It turns out, however, that the near-integrability persists for much longer times $T$ of order $h^{-4}$, and this they are elegantly able to explain by showing that in fact $x(t)$ solves a system of the form

$$\dot{x} = W(x) + O(h^4)$$

and now

$$\dot{y} = W(y)$$

is a solution of the KdV hierarchy, and hence, also, integrable.

We are led to the following speculation: Is the Fermi et al. problem a guide to what we see for $c < 0$? Fermi et al. raises the issue of whether there is some integrable system associated with the lattice, which describes the solutions of the lattice equations to high accuracy for large, but not infinite, times. In this way, for large times, the system would have excellent, but not perfect, 'memory'. The problem is intriguing and open!

Remark: The Fermi-Pasta-Ulam-Tsingou paradox, as it is called, is a modern illustration of the interesting phenomenon that sometimes science makes progress, not because of the accuracy of its instruments, but rather because of their inaccuracy. If computers in the 1950's could have made longer calculations, would KdV have been discovered as an integrable system? If Copernicus had more accurate instruments, sensitive to the fluctuations in the planetary orbits, would Kepler have been able to come up with his perfect laws?

The integrability of $H_c$ with $c > 0$ is proved in steps.

Step 1: We prove that solutions of (15) generated by $H_c$ with initial data $q_n(0), p_n(0), 1 \leq n \leq N$, are unique and exist globally (the same is true for $c < 0$, but we are only interested in $c > 0$.

Step 2: We show that as $t \to \infty$ the particle system (15) splits up into two parts: a core Toda lattice $q_2, \ldots, q_{N-1}, p_2, \ldots, p_{N-1}$ obeying

$$\begin{aligned} \dot{q}_n &= p_n, \quad 2 \leq n \leq N-1, \\ \dot{p}_2 &= -e^{q_2 - q_3} + O_2(t) \\ \dot{p}_n &= e^{q_{n-1} - q_n} - e^{q_n - q_{n+1}}, \quad 3 \leq n \leq N-2, \\ \dot{p}_{N-1} &= e^{q_{N-2} - q_{N-1}} - O_{N-1}(t) \end{aligned} \tag{16}$$

where

$$O_2(t) = e^{q_1 - q_2} = O(e^{-\gamma t^2}) \,, \quad O_{N-1}(t) = e^{q_{N-1} - q_N} = O(e^{-\gamma t^2}), \gamma > 0 \tag{17}$$

and two decoupled particles $q_1, q_N, p_1, p_N$ separated from the core lattice,

$$q_1(t) \to -\infty \,, \quad q_N(t) \to \infty \ \text{ as } \ t \to \infty.$$

Step 3: Here for solutions $q_1(t), q_2(t), \ldots, q_N(t), p_1(t), p_2(t), \ldots, p_N(t)$ we obtain precise asymptotics for the inner core

$$q_2(t), \ldots, q_{N-1}(t), p_2(t), \ldots, p_{N-1}(t) \ .$$

Let $U_t(q(0), p(0)) = (q(t), p(t))$ be the solution of (15). Let $\hat{U}_t(\hat{q}(0), \hat{p}(0)) = (\hat{q}(t), \hat{p}(t))$ denote the solution of the Hamiltonian

$$H_c^d(q,p) = \frac{1}{2}\sum_{n=1}^{N} p_n^2 + \sum_{n=2}^{N-2} e^{q_n - q_{n+1}} + c(q_1 - q_N) \ . \tag{18}$$

in which the inner Toda core $q_2(t), \ldots, q_{N-1}(t), p_2(t), \ldots, p_{N-1}(t)$ is decoupled from the particles $q_1$ and $q_N$. Finally consider the solution

$$U_t^{\#}(q^{\#}(0), p^{\#}(0)) = (q^{\#}(t), p^{\#}(t))$$

of the equations generated by the ‘free´ decoupled Hamiltonian

$$H_c^{\#}(q,p) = \frac{1}{2}\sum_{n=1}^{N} p_n^2 + c(q_1 - q_n) \ .$$

Step 4: From the asymptotics in Step 3, as $t \to \infty$ solutions of (15) behave like ‘free´ particles, and the convergence is sufficiently rapid so that Moser’s argument applies and the wave operator

$$W^{\#}(q(0), p(0)) = \lim_{t\to\infty} U^{\#}_{-t} \circ U_t(q(0), p(0)) \tag{19}$$

exists.

On the other hand, standard Toda estimates as in (9) also show that as $t \to \infty$, the solutions $(\hat{q}(t), \hat{p}(t))$ of the equations generated by $\hat{H}_c$ also behave like 'free´ particles, and the convergence is sufficiently rapid so that Moser´s argument again applies and the wave operator

$$\hat{W}^{\#}(\hat{q}(0), \hat{p}(0)) = \lim_{t\to\infty} U^{\#}_{-t} \circ \hat{U}_t(\hat{q}(0), \hat{p}(0)) \tag{20}$$

exists. A separate argument then shows that $(\hat{W}^{\#})^{-1}$ exists and a short calculation then shows that

$$W = (\hat{W}^{\#})^{-1} \circ W^{\#} \tag{21}$$

is an intertwining operator for $\hat{U}_t$ and $U_t$,

$$\hat{U}_t \circ W = W \circ U_t \tag{22}$$

and the integrability of $H_c$ then follows from the integrability of $\hat{H}_c$.

Step 5: Here we show how to use $W$ to construct action-angle variables for $H_c$ and also how to write the equations (15) generated by $H_c$ in Lax-pair form.

Finally a technical comment. What makes the proof work is the super-exponential decay of the terms $O_2(t)$ and $O_{n-1}(t)$ in (16), (17). All the other terms in (16) decay only at an exponential rate and the particles $q_1$ and $q_N$ run away from the inner core $q_2, \ldots, q_{N-1}$. This super-exponential decay is obtained by a multi-layer bootstrap, the first step of which follows from the following elementary calculation. Let

$$H_c(q,p) = \frac{1}{2}\sum_{n=1}^{N} p_n^2 + \sum_{n=1}^{N-1} e^{q_n - q_{n+1}} + c \sum_{n=1}^{N-1}(q_n - q_{n+1}) = h_0 = constant.$$

Then

$$(p_1 - p_n)^2 \leq 2(P_1^2 + p_N^2) \leq \frac{1}{2}\sum_{n=1}^{N} p_n^2 \leq 4(h_0 - c\Delta) \quad \text{where} \quad \Delta = q_1 - q_N \,.$$

Hence $(\dot{\Delta})^2 \leq 4(h_0 - c\Delta)$ and so by integrating we find

$$h_0 \geq c(q_1 - q_N) \geq h_0 - (ct + c')^2 \,, \qquad \text{where} \;\; c' = (h_0 - c(q_1(0) - q_n(0))^{1/2} \,.$$

This a priori bound, that the particles $q_1$ and $q_n$ can move apart, but not too far apart, provides the key control for the system.