ON THE OPEN TODA CHAIN WITH EXTERNAL FORCING

PERCY DEIFT, LUEN-CHAU LI, HERBERT SPOHN,
CARLOS TOMEI, THOMAS TROGDON

In honor of Shmuel Agmon and his many contributions to mathematics

The Duck Test: 'If it looks like a duck, walks like a duck and quacks like a duck... it's a duck!'

Abstract. We consider the open Toda chain with external forcing, and in the case when the forcing stretches the system, we derive the longtime behavior of solutions of the chain. Using an observation of Jürgen Moser, we then show that the system is completely integrable, in the sense that the $2N$-dimensional system has N functionally independent Poisson commuting integrals, and also has a Lax-Pair formulation. In addition, we construct action-angle variables for the flow. In the case when the forcing compresses the system, the analysis of the flow remains open.

In 1967, Morikazu Toda introduced [27] the eponymous Toda system with Hamiltonian

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

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

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

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

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

Toda's goal in considering H was to investigate further the observation of J. Ford and J. Waters [12], found by numerical computation, that nonlinear systems have 'normal modes where a normal mode is defined as a motion in

2010 *Mathematics Subject Classification.* 37J35.
Keywords: Toda lattice, Liouville integrability, wave operator, action-angle variables

which each oscillator moves at essentially constant amplitude (energy) and at a given frequency'. As Toda notes, the existence of such normal modes implies, in particular, the non-ergodic character of the system. Toda's specific goal in [27] was to discover an exact, explicit form for such normal modes for H, and he found (in the case $m = 1$) such modes in the form of a travelling wave solution for (3),

$$q_{n+1} - q_n = -\frac{1}{b} \log \left(1 + \frac{4(K\nu)^2}{ab} \left[\mathrm{dn}^2(2K(\nu t \pm \frac{n}{\lambda})) - \frac{E}{K} \right] \right) , -\infty < n < \infty ,$$

where for given any wave length λ and modulus $0 < k < 1$, $K = K(k)$ and $E = E(k)$ are complete elliptic integrals

$$K = \int_0^{\pi/2} \frac{d\theta}{\sqrt{1 - k^2 \sin^2 \theta}} , \quad E = \int_0^{\pi/2} \sqrt{1 - k^2 \sin^2 \theta}\, d\theta,$$

and the frequency ν is given by

$$\nu = \frac{1}{2K} \sqrt{\frac{ab}{\left(\frac{1}{\mathrm{sn}^2(2K/\lambda)} - 1 + \frac{E}{K} \right)}} .$$

Here sn and dn are the standard Jacobi elliptic functions.

In the case that n runs over $\mathbb{Z}$ in (1), the linear term $a \sum_{n \in \mathbb{Z}} (q_{n+1} - q_n)$ plays no role. Scaling

$$q_n \to b q_n , \quad t \to t \sqrt{\frac{m}{ab}}$$

in (3), we see that we can restrict our attention to the case

$$H = \frac{1}{2} \sum_{n \in \mathbb{Z}} p_n^2 + \sum_{n \in \mathbb{Z}} e^{q_n - q_{n+1}} + c \sum_{n \in \mathbb{Z}} (q_n - q_{n+1}) , \tag{4}$$

where c is any constant.

In the periodic case,

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

for some $N \in \mathbb{N}$ and $s \in \mathbb{R}$, equations (2) scaled as above take the form

$$\begin{aligned} \dot{q}_n &= p_n \\ \dot{p}_n &= \left(e^{(q_{n+1} - q_n)} - e^{(q_n - q_{n-1})} \right) \end{aligned} \tag{5}$$

for $1 \le n \le N$, where $q_{N+1} = q_1 + s$ as above and $-s = \sum_{n=1}^{N} (q_n - q_{n+1})$. In an extensive numerical investigation in the cases $N = 3$ and $N = 6$, J. Ford, S. Stoddard and J. Turner [11] found strong evidence that the lattice was integrable. And indeed, inspired by [11], M. Hénon [14] and, independently, H. Flaschka

[9] showed that there are N independent integrals for (5). Also independently, S. Manakov [20][1] proved the same result, viz., there are N independent integrals for (5). The starting point of Hénon's analysis was the integrability of the hard-sphere gas, which is a limiting form of the Toda lattice. On the other hand, Flaschka and Manakov based their analysis on the observation that (5) can be written in Lax-pair form as follows: set

$$a_i = -p_i/2\ , \quad b_i = \frac{1}{2}e^{(q_i-q_{i+1})/2}\ , 1 \le i \le N\ ,$$

where $q_{N+1} = q_1 + s,\ p_{N+1} = p_1$, and in the variables a_i, b_i, equations (5) take the form

$$\dot{a}_i = 2(b_i^2 - b_{i-1}^2)\ , \quad \dot{b}_i = b_i(a_{i+1} - a_i)\ , \quad 1 \le i \le N\ , \tag{6}$$

where $b_0 = b_N$ and $a_{N+1} = a_1$. Note that the *stretch parameter* s is now part of the initial conditions.

Define the symmetric matrix

$$L = \begin{pmatrix} a_1 & b_1 & 0 & b_N \\ b_1 & a_2 & \ddots & 0 \\ 0 & \ddots & \ddots & b_{N-1} \\ b_N & 0 & b_{N-1} & a_N \end{pmatrix} = L^T$$

and the skew-symmetric matrix

$$B = \begin{pmatrix} 0 & -b_1 & 0 & b_N \\ b_1 & 0 & \ddots & 0 \\ 0 & \ddots & \ddots & -b_{N-1} \\ -b_N & 0 & b_{N-1} & 0 \end{pmatrix} = -B^T\ .$$

Then, if $q_i(t), p_i(t)$ solve (5), so that $a_i(t), b_i(t)$ solve (6), then $L = L(t)$ solves

$$\dot{L} = [L, B] = LB - BL$$

with $L_0 = L(t = 0)$ given by $q_i(0), p_i(0)$. By the general theorem of Lax [18], it follows immediately that $t \mapsto L(t)$ is an isospectral deformation, i.e.,

$$\operatorname{spec} L(t) = \operatorname{spec} L_0,\ \ t > 0.$$

In particular, the eigenvalues $\lambda_1, \dots, \lambda_N$ of L_0 are N constants of the motion for (5), and in [9], Flaschka relates the λ_i's to the integrals of the motion obtained by Hénon. Furthermore, in [20], Manakov showed that the λ_i's Poisson commute, so that the Hamiltonian system (5) is completely integrable in the sense of Liouville. In principle, this meant that the periodic Toda system could be solved up to

[1]For the record: the articles by Hénon and Flaschka were submitted on August 13, 1973 and August 22, 1973, respectively, and the article of Manakov was submitted on February 8, 1974. Also, Henon, Flaschka and Manakov only considered the case with $s = 0$, but their methods go through for general s.

quadrature, and indeed in [16] M. Kac and P. van Moerbeke showed how to use the Lax-pair formalism to partially solve (5) in terms of hyperelliptic function theory: A full solution was given shortly thereafter by E.Date and S.Tanaka [3].

The methods of Hénon, Flaschka and Manakov can also be used to prove the integrability of the Toda lattice with other boundary conditions, particularly the so-called open Toda lattice (sometimes referred to as Toda with "fixed-ends"—see below), and also scattering systems with infinitely many particles (see [14], [9], [20] and also [8]).

In this paper we are particularly interested in the *open Toda lattice* where the Hamiltonian has the form

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

giving rise to the equations

$$\begin{aligned} \dot{q}_n &= p_n, \quad 1 \le n \le N, \\ \dot{p}_1 &= -e^{q_1 - q_2} \\ \dot{p}_n &= e^{q_{n-1}-q_n} - e^{q_n - q_{n+1}}, 2 \le n \le N-1, \\ \dot{p}_N &= e^{q_{N-1}-q_N}. \end{aligned} \tag{7}$$

One can view (7) as arising from (5) with $N+2$ particles $q_0, q_1, \ldots, q_N, q_{N+1}$ by setting

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

so that the ends are "fixed" at $\pm\infty$: For this reason the open Toda lattice is sometimes referred to as Toda with "fixed-ends". Equations (7) can be written in Lax-pair form by setting

$$\begin{aligned} a_i &= -\, p_n/2,\ 1 \le n \le N, \\ b_i &= \frac{1}{2} e^{(q_n - q_{n+1})/2},\ 1 \le n \le N-1, \end{aligned} \tag{8}$$

and defining the symmetric matrix

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

and the skew-symmetric matrix

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

Then if $q_n(t), p_n(t)$ solve (7), $L_F(t)$ solves the Lax-pair equation

$$\dot{L}_F = [L_F, B_F] \tag{9}$$

with $L_{F,0} = L_F(t = 0)$ given by $q_n(0), p_n(0)$. Again, the eigenvalues $\lambda_i(t)$ of $L_F(t)$ are constant and hence give N integrals for the open Toda lattice. In what follows, we will often simply refer to (7) as the Toda lattice, or the Toda system, or the Toda chain, and in cases where the periodic problem is under discussion, we will specifically refer to (5) as the periodic Toda system.

Just as in the periodic case, the Toda system can be solved explicitly, now in terms of rational functions of exponentials, as shown by J. Moser in [22]. Furthermore, Moser showed that the system has the following remarkable long-term scattering behavior:

$$q_n(t) = \alpha_n^{\pm} t + \beta_n^{\pm} + O(e^{-\delta|t|}),\ t \to \pm\infty,\ \ \delta > 0, 1 \le n \le N \tag{10}$$

with

$$\alpha_n^{+} \ =\ -2\lambda_n, \quad \alpha_n^{-} \ =\ -2\lambda_{N-n+1}, \quad 1 \le n \le N \tag{11}$$

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

$$\beta_{N-n+1}^{+} - \beta_n^{-} \ =\ \sum_{j \neq k} \ln(\alpha_j^{-} - \alpha_k^{+})^2\ . \tag{12}$$

Explicit expressions for the $\beta_n^{\pm}$'s themselves were derived later in the early 2000's (see [4]), and subsequently in [19] ; see (57) below. Here $\lambda_1 > \lambda_2 > \ldots > \lambda_N$ are the eigenvalues of $L_{F,0}$.

When one of the authors (PD) came across formula (12), he was astounded: he had just completed a PhD in abstract scattering theory in Hilbert space, and the idea that one could compute the scattering shifts (equivalently, the scattering matrix) for an N particle system explicitly, was beyond anything he had ever encountered. When he asked Moser how this was possible, Moser replied, somewhat mysteriously, that 'Every scattering system is integrable!'

What Moser meant was the following (see [23], Integrals via Asymptotics: the Störmer Problem): 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 $t \to \infty$,

$$\begin{aligned} p(t) &= p_\infty + o(1/t), \\ q(t) &= q_\infty + tp_\infty + o(1), \end{aligned}$$

for some constants (q_∞, p_∞). 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

$$\begin{aligned} p^0(t) &= p^0(0) \\ q^0(t) &= q^0(0) + p^0(0)t\ . \end{aligned}$$

Then

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

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,

$$U_s = W^{-1} \circ U^0_s \circ W \; . \tag{13}$$

Now $U^0_{-t} \circ U_t$ is symplectic for all t and so W, and hence W^{-1}, are symplectic. Thus (13) 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,

$$\{\beta_i, \beta_j\} = \{\alpha_i \circ W, \alpha_j \circ W\} = \{\alpha_i, \alpha_j\} \circ W = 0 \; . \tag{14}$$

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!'

In Moser's argument in [22] one finds that in addition to (10) one also has

$$p_n = \alpha^\pm_n + O(e^{-\delta|t|}) \quad \text{as} \;\; t \to \pm\infty \tag{15}$$

and so by Moser's integrability argument, the Toda lattice is integrable. Note further that

$$\alpha_i(q, p) = p_i \; , 1 \le i \le N$$

are commuting integrals of the motion for H^0 and so

$$\beta_i(q_0, p_0) = \alpha_i(W(q_0, p_0)) = \alpha_i(q_\infty, p_\infty) = p_{\infty,i}, \;\; 1 \le i \le N$$

are commuting integrals of the motion for H_F. But, from (10) and (11), up to a factor of -2, the $p_{\infty,i}$'s are just the eigenvalues of $L_{F,0}$, as they should be!

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!

Moser's argument can be used to prove the integrability of a variety of dynamical systems. For example, in [6] the authors showed, contrary to expectations, that the perturbed defocusing nonlinear Schrödinger equation on the line,

$$\begin{array}{l} iq_t + q_{xx} - 2|q|^2 q - \epsilon K(|q|^2) q = 0 \\ q(x,t=0) = q_0(x) \to 0 \ , \quad \text{as} \ \ |x| \to \infty \end{array}$$

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 $\ell > 2$.

Wave operators were first introduced in the context of quantum mechanical scattering theory, by C.Møller [21] . In particular, for two self-adjoint operators A and B in Hilbert space, with propagators e^{iAt} and e^{iBt}, Møller introduced the quantum mechanical wave operator

$$Wf = \lim_{t\to\infty} e^{-iAt} e^{iBt} f$$

for vectors f in the Hilbert space. Cook [1], and shortly thereafter Hunziker [15], were the first to use wave operators in the context of classical dynamics. Wave operators can also be used more generally to address problems in analysis: see, in particular, Nelson's proof in [24] of Sternberg's Linearization Theorem for non-resonant systems, and also the proof of Darboux's Theorem establishing the existence of local canonical coordinates for symplectic forms in [23]. A detailed treatment of classical two-body scattering theory in three dimensions using wave operators is given in [25]. A detailed treatment of classical and quantum mechanical N-particle scattering theory is given in [7].

In this paper we consider Toda's original system (4) 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

$$\begin{array}{lll} \dot{q}_n & = p_n \ , \quad 1 \le n \le N, & \\ \dot{p}_1 & = - e^{q_1 - q_2} - c, & \\ \dot{p}_n & = e^{q_{n-1} - q_n} - e^{q_n - q_{n+1}} \ , \quad 2 \le n \le N-1, & \\ \dot{p}_N & = e^{q_{N-1} - q_N} + c. & \end{array} \tag{16}$$

As opposed to the whole line case and the periodic case, the constant c, and in particular the sign of c, now plays a determining role. 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 of the lattice 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 study of H_c is motivated in part by the statistical mechanics of the Toda lattice. Here the statistics of the statistical mechanical ensemble is given by the canonical measure

$$\prod_{j=1}^{N} \mathrm{d}p_j \prod_{j=1}^{N} \mathrm{d}q_j \exp(-\beta H_c(q,p))$$

suitably normalized: This measure is clearly invariant under the flow generated by H_c. From [26] we learn that the case $c < 0$ arises most naturally, but the case $c > 0$ is also of interest. In general, the analysis of the thermodynamic limit, $N \to \infty$, of a statistical mechanical system with Hamiltonian H, is greatly simplified if H is known to be integrable. This motivates, in particular, the study of the integrability of H_c.

The numerical calculations below suggest strongly that in the case $c > 0$, H_c is integrable. And indeed, the main result in this paper 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, associated with the system.

As a benchmark, Figure 1 displays the solution of the Toda lattice with Hamiltonian H_F, $N = 20$ particles and randomly chosen initial data. As $t \to \infty$, $p(t) = p_\infty + o(1)$ and $q(t) = q_\infty + p_\infty t + o(1)$ for suitable constants q_∞ and p_∞ as in (10) and (15). Figure 2 displays the solution of the perturbed Toda lattice with Hamiltonian H_c, $c = 1, N = 20$ particles and randomly chosen initial data. As $t \to \infty$,

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

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.

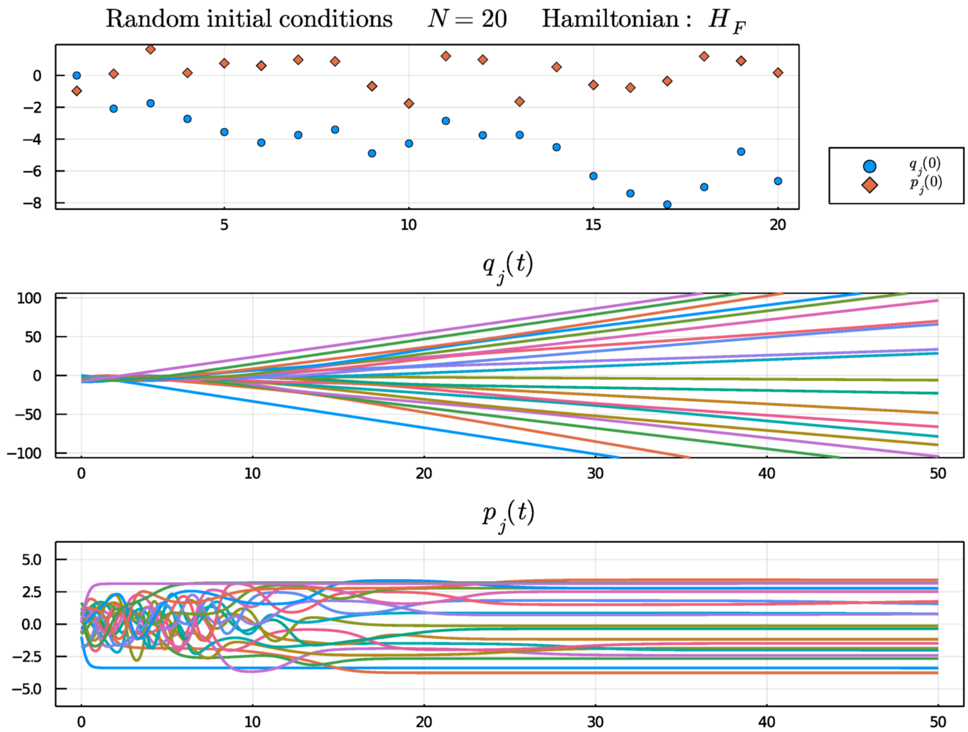

FIGURE 1. Numerical computations for the open Toda lattice. The system is integrated using a second-order accurate Störmer-Verlet method [2] with a time step of $\Delta t = 0.0001$. The initial conditions are generated by sampling $p_j(0), q_{j+1}(0) - q_j(0)$, $j = 1, \ldots, N$ as independent and normally distributed random variables.

Figure 3 displays the solution of the perturbed Toda lattice with Hamiltonian H_c and $c = -1$. Here there are N particles and the initial conditions are

$$q_i(0) = i \ , \quad 1 \le i \le 20 \ ,$$

with $\{p_i(0)\}$ random. In Figure 4, we again have $c = -1$, but now

$$q_i(0) = -i \ , \quad 1 \le i \le 20 \ ,$$

again with $\{p_i(0)\}$ random. In Figure 5, we again have $c = -1$, but now $\{q_i(0)\}$ and $\{p_i(0)\}$ are chosen randomly. In all three cases, the solution $q_i(t)$ appears to evolve almost periodically in time, modulo a slight gradient. In the first two cases, this behavior persists at least up to times $t \approx 300$, but in the third case the almost periodicity begins to unravel after $t \approx 200$.

This brings to mind the celebrated computations of E. Fermi, J. Pasta, S. Ulam and M. Tsingou [10], 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

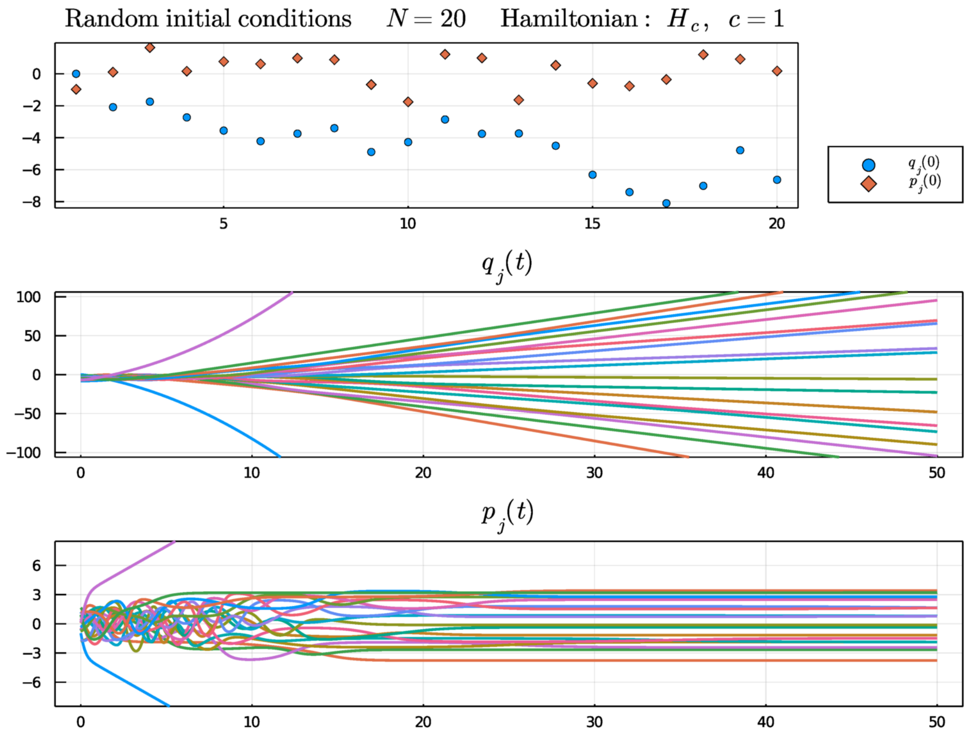

FIGURE 2. Numerical computations for the perturbed Toda lattice with $c = 1$. The system is integrated using a second-order accurate Störmer-Verlet method with a time step of $\Delta t = 0.0001$. The initial conditions are generated by sampling $p_j(0), q_{j+1}(0) - q_j(0)$, $j = 1, \ldots, N$ as independent and normally distributed random variables.

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. is given in [13]: 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., $Th^2 = \mathrm{O}(1)$, 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 $c < 0$? In Figure 5, in particular, when the almost periodicity unravels on a moderate time scale (the same is likely true regarding Figure 3 and Figure 4, but on a longer time scale), 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’.

One final comment: 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?

We will prove the integrability of H_c with $c > 0$ in steps. In Step 1, we prove that solutions of (16) with initial data $q_i(0), p_i(0), 1 \le i \le N$ are unique and exist globally, both for $c \ge 0$ and $c < 0$. In the remainder of the paper, we only consider the case $c > 0$. In Step 2, we will show that, as $t \to \infty$, the particle system under H_c splits up into two parts: a core Toda lattice $q_2, \dots, q_{N-1}, p_2, \dots, p_{N-1}$ obeying (7) up to super-exponentially small errors,

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

where $O_2(t) = e^{q_1 - q_2} = O(e^{-\gamma t^2}), O_{N-1}(t) = e^{q_{N-1} - q_N} = O(e^{-\gamma t^2})$ for some $\gamma > 0$, and a pair of decoupled particles q_1, q_N, p_1, p_N separating from the core lattice, $q_1(t) \to -\infty$ and $q_N(t) \to \infty$, as $t \to \infty$. In Step 3, for solutions $q_1(t), q_2(t), \dots, q_N(t), p_1(t), p_2(t), \dots, p_N(t)$ of (16), we obtain precise asymptotics for the inner core $q_2(t), \dots, q_{N-1}(t), p_2(t), \dots, p_{N-1}(t)$. Let $U_t(q_0.p_0) = ((q(t), p(t))$

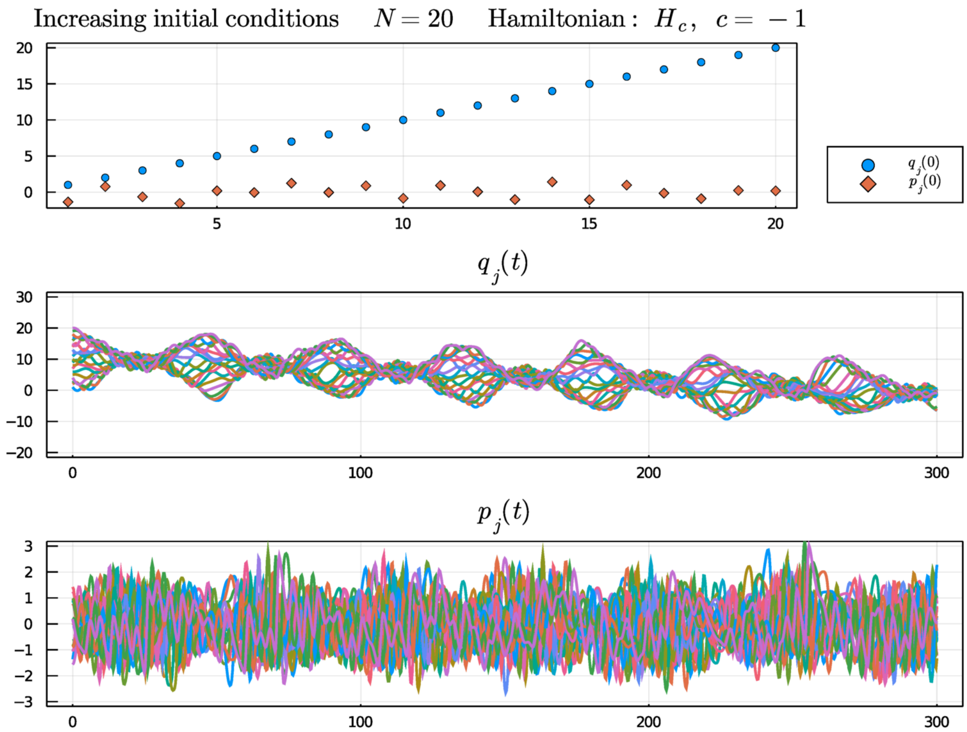

FIGURE 3. Numerical computations for the perturbed Toda lattice with $c = -1$. The system is integrated using a second-order accurate Störmer-Verlet method with a time step of $\Delta t = 0.0001$. The initial conditions are generated, for $j = 1, \ldots, N$, by sampling $p_j(0)$ as independent and normally distributed and setting $q_{j+1}(0) - q_j(0) = 1$.

denote the solution of the equations (16) generated by H_c. Let $\hat{U}_t(\hat{q}_0, \hat{p}_0) = (\hat{q}(t), \hat{p}(t))$ denote the solution generated by

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

in which the inner Toda core $(q_2, \ldots, q_{N-1}, p_2, \ldots, p_{N-1})$ is decoupled from particles q_1 and q_N. Finally, let $U_t^{\#}(q_0^{\#}, p_0^{\#}) = (q^{\#}(t), p^{\#}(t))$ denote the solution of the equation generated by the "free" decoupled Hamiltonian

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

Then in Step 4 we use the asymptotics obtained in Step 3 to show that as $t \to \infty$, solutions of (16) behave like "free" particles, and the convergence is sufficiently

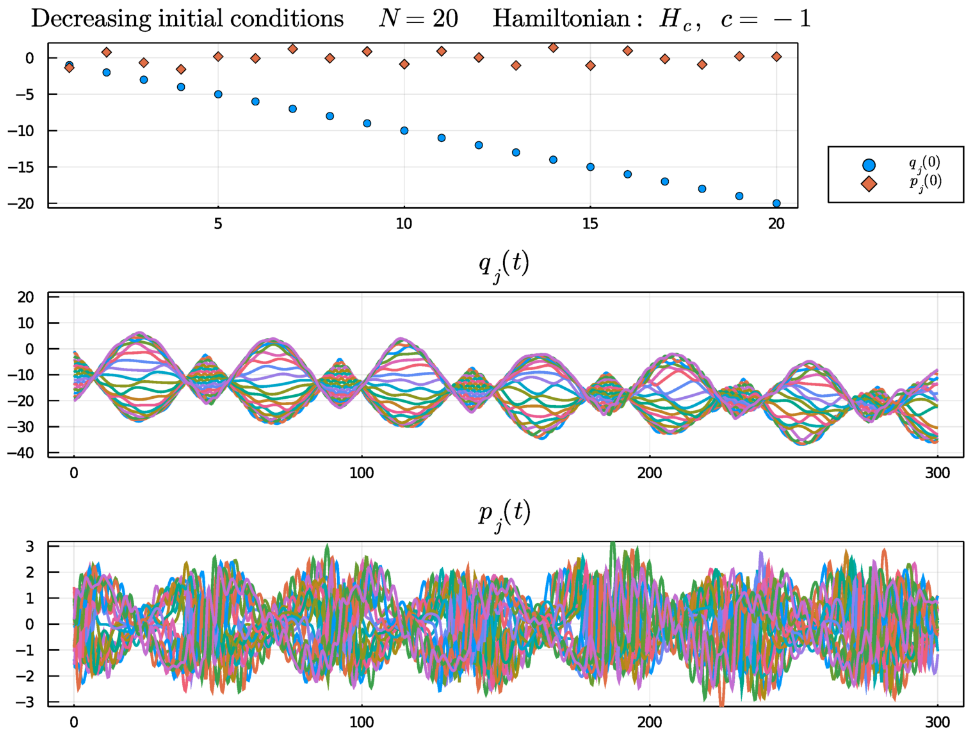

FIGURE 4. Numerical computations for the perturbed Toda lattice with $c = -1$. The system is integrated using a second-order accurate Störmer-Verlet method with a time step of $\Delta t = 0.0001$. The initial conditions are generated, for $j = 1, \dots, N$, by sampling $p_j(0)$ as independent and normally distributed and setting $q_{j+1}(0) - q_j(0) = -1$.

rapid so that Moser's argument applied and the wave operator

$$W^{\#}(q_0.p_0) = \lim_{t\to\infty} U^{\#}_{-t} \circ U_t(q_0, p_0)$$

exists. On the other hand, standard Toda asymptotics as in (10) and (15), also show that as $t \to \infty$, the solution $(\hat{q}(t), \hat{p}(t))$ of the equations generated by H^d_c, also behave like "free" particles, and the convergence is sufficiently rapid so that Moser's argument again applied and the wave operator

$$\hat{W}^{\#}(\hat{q}_0, \hat{p}_0) = \lim_{t\to\infty} U^{\#}_{-t} \circ \hat{U}_t(\hat{q}_0, \hat{p}_0)$$

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

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

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

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

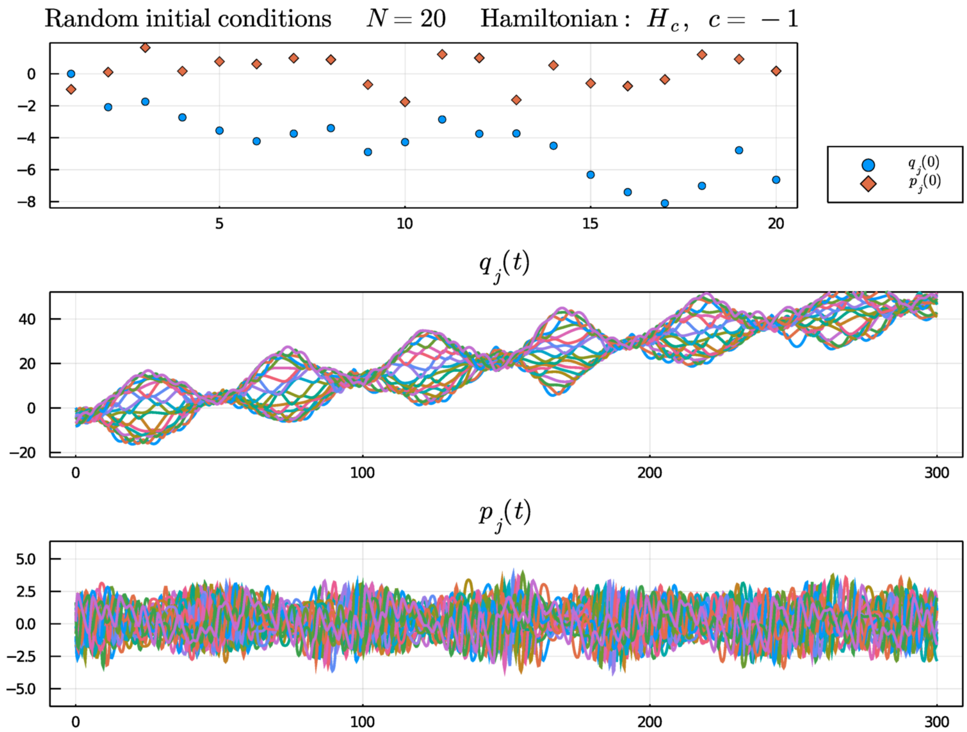

FIGURE 5. Numerical computations for the perturbed Toda lattice with $c = -1$. The system is integrated using a second-order accurate Störmer-Verlet method with a time step of $\Delta t = 0.0001$. The initial conditions are generated by sampling $p_j(0), q_{j+1}(0) - q_j(0)$, $j = 1, \dots, N$ as independent and normally distributed random variables.

and as H_c^d is integrable, the integrability of H_c follows. The intertwining relation is not enough, however, to show that as $t \to \infty$, the solutions U_t behave, as advertised above, like solutions $\hat{U}_t$ of the decoupled system: This is proved using a separate argument.

Note that we do not construct W directly as a wave operator

$$\lim_{t\to\infty} \hat{U}_{-t} \circ U_t(q_0, p_0).$$

The technical reason for this is discussed at the end of the section, together with a sketch of the argument that is needed to prove the existence of the limit. We leave the details to the interested reader.

Finally in Step 5 we display N independent, commuting integrals for the H_c flow and show how the flow can be written in Lax-pair form.

Step 1.

Standard ODE methods show that (16) has unique local solutions $(q(t), p(t))$ with $(q(0), p(0)) = (q_0, p_0)$ for which $H_c(q(t), p(t)) = h_0 \equiv H_c(q_0, p_0)$. Thus

$$\frac{1}{2}\sum_{n=1}^{N} p_n^2(t) + \sum_{n=1}^{N-1} e^{q_n(t)-q_{n+1}(t)} = h_0 - c(q_1(t) - q_N(t)) \tag{17}$$

and so in order to prove global existence it is enough to show, in particular, that

$$|q_1(t) - q_N(t)| \leq c_1 t^2 + c_2$$

for some constants, c_1, c_2. Indeed, by (17), we would then have, for $1 \leq n \leq N$, $|p_n(t)| \leq c_1' t + c_2'$ for some constants c_1', c_2' and so $|q_n(t)| \leq c_1'' t^2 + c_2''$, again for some constants c_1'', c_2''. Global existence for $(q(t), p(t))$ now follows, again by standard ODE methods. We derive stronger bounds on $q_n(t), p_n(t)$ in Step 2 below.

The following elementary calculation plays a crucial role in our analysis. From (17),

$$(p_1 - p_N)^2 \leq 2(p_1^2 + p_N^2) \leq 2\sum_{n=1}^{N} p_n^2 \leq 4(h_0 - c(q_1 - q_N)) \ .$$

Setting $q_1 - q_N = \Delta$, we have $(\dot{\Delta})^2 \leq 4(h_0 - c\Delta)$ and so

$$-2\sqrt{h_0 - c\Delta} \leq \dot{\Delta} \leq 2\sqrt{h_0 - c\Delta} \ . \tag{18}$$

Integrating we find

$$-t + c_3 \leq \frac{\sqrt{h_0 - c\Delta}}{-c} \leq t + c_4$$

for some constants c_3, c_4. For $c > 0$, this implies

$$0 \leq h_0 - c\Delta \leq (ct + c')^2 \tag{19}$$

where c' is some constant and so

$$\frac{h_0 - (ct + c')^2}{c} \leq q_1 - q_N \leq \frac{h_0}{c} \ .$$

There are, of course, similar bounds for $c < 0$.

Step 2.

From (16), we have

$$\frac{d}{dt}(p_N - p_1) = e^{q_{N-1}-q_N} + e^{q_1 - q_2} + 2c$$

which implies

$$p_N(t) - p_1(t) = p_N(0) - p_1(0) + \int_0^t (e^{q_{N-1}-q_N} + e^{q_1-q_2})\ ds + 2ct. \tag{20}$$

Now, from (18) and (19),

$$p_N - p_1 = (\dot{q}_N - \dot{q}_1) \leq 2\sqrt{h_0 + c(q_N - q_1)} \leq 2ct + 2c' \ . \tag{21}$$

Inserting (20) into (21), we conclude that

$$\int_0^\infty (e^{q_{N-1}-q_N} + e^{q_1-q_2})\, ds < \infty\ . \tag{22}$$

By (16),

$$p_1(t) = p_1(0) - \int_0^t e^{q_1-q_2}\, ds - ct$$

and so, as $t \to \infty$,

$$p_1(t) = p_{1,\infty} - ct + o(1) \tag{23}$$

for some constant $p_{1,\infty}$. Similarly, as $t \to \infty$,

$$p_N(t) = p_{N,\infty} + ct + o(1) \tag{24}$$

for some constant $p_{N,\infty}$ (note that $p_{i,\infty} \neq \lim_{t\to\infty} p_i(t)$, $i = 1, N$). We have

$$\frac{1}{2}p_1(t)^2 = \frac{1}{2}c^2\, t^2 - c\, t\, p_{1,\infty} + o(t) \tag{25}$$

and

$$\frac{1}{2}p_N(t)^2 = \frac{1}{2}c^2\, t^2 + c\, t\, p_{N,\infty} + o(t)\ . \tag{26}$$

Inserting (25) and (26) into

$$\frac{1}{2}\sum_{n=1}^N p_n^2 \leq h_0 + c\,(q_N - q_1),$$

and using (21), we find

$$c^2\, t^2 + c\, t\, (p_{N,\infty} - p_{1,\infty}) + \frac{1}{2}\sum_{n=2}^{N-1} p_n^2 + o(t)$$

$$\leq h_0 + c(q_N - q_1) \leq c^2\, t^2 + 2c\, c't + (c')^2\ .$$

We conclude that

$$|p_n| = O(t^{1/2})\ , \quad 2 \leq n \leq N-1 \tag{27}$$

and so

$$|q_n| \leq O(t^{3/2})\ , \quad 2 \leq n \leq N-1\ .$$

These bounds are sharper than those obtained in Step 1, and as

$$q_1(t) = \ -c\frac{t^2}{2} + O(t)\ , \quad q_N(t) = c\frac{t^2}{2} + O(t)$$

by (23) and (24), we see that the particles q_1 and q_N separate from the core $q_2, \ldots, q_{N-1}$. Moreover,

$$e^{q_1-q_2}\ , e^{q_{N-1}-q_N} = e^{-c\frac{t^2}{2}(1+O(t^{-1/2}))} = O(e^{-\gamma t^2}) \tag{28}$$

for some $\gamma > 0$.

Step 3.

Consider $H_F(q_2,\ldots,q_{N-1},p_2,\ldots,p_{N-1}) = \dfrac{1}{2}\sum_{n=2}^{N-1} p_n^2 + \sum_{n=2}^{N-2} e^{q_n-q_{n+1}}$, evaluated along the solutions $q_1(t), q_2(t),\ldots,q_{N-1}(t), q_N(t), p_1(t), p_2(t),\ldots,p_{N-1}(t), p_N(t)$ of (16), the flow induced by H_c. Then

$$\begin{aligned}
\frac{d}{dt}H_F(q_2,\ldots,q_{N-1},p_2,\ldots,p_{N-1}) = &\sum_{n=2}^{N-1} p_n\dot{p}_n + \sum_{n=2}^{N-2} e^{q_n-q_{n+1}}(p_n-p_{n+1}) \\
= &\sum_{n=2}^{N-1} p_n\ e^{q_{n-1}-q_n} - \sum_{n=2}^{N-1} p_n\ e^{q_n-q_{n+1}} \\
+ &\sum_{n=2}^{N-2} p_n\ e^{q_n-q_{n+1}} - \sum_{n=2}^{N-2} p_{n+1}\ e^{q_n-q_{n+1}} \\
= &\ - p_{N-1}\ e^{q_{N-1}-q_N} + p_2\ e^{q_1-q_2}\ .
\end{aligned}$$

It follows from (27) and (28) that

$$H_F(q_2,\ldots,q_{N-1},p_2,\ldots,p_{N-1}) \le \text{const.} \tag{29}$$

and hence

$$|p_n(t)| \le \text{const.}, \quad 2 \le n \le N-1 \tag{30}$$

which is a further strengthening of (27).

The argument now follows in analogy with Moser's convergence argument for the Toda lattice in [22]. From (16),

$$\frac{d}{dt}p_2 = e^{q_1-q_2} - e^{q_2-q_3},$$

and we obtain

$$\begin{aligned}
p_2(t) &= p_2(0) - \int_0^t e^{q_2-q_3}\,ds + \int_0^t e^{q_1-q_2}\,ds \\
&= p_2(0) - \int_0^t e^{q_2-q_3}\,ds + \int_0^\infty e^{q_1-q_2}\,ds + O(e^{-\gamma t^2})
\end{aligned}$$

by (28). Hence, as $|p_2(t)|$ is bounded by (30), we conclude that

$$\int_0^\infty e^{q_2-q_3}\ ds < \infty\ .$$

Thus

$$p_2(t) = p_{2,\infty} + o(1)\ . \tag{31}$$

Now

$$\frac{d}{dt}(p_2+p_3) = e^{q_1-q_2} - e^{q_3-q_4}$$

and as $p_2(t)$ and $p_3(t)$ are bounded, we conclude again as above that

$$\int_0^\infty e^{q_3-q_4}\, ds < \infty$$

and, using (31),

$$p_3(t) = p_{3,\infty} + o(1)\ .$$

In particular, we conclude that

$$q_2(t) - q_3(t) = t(p_{2,\infty} - p_{3,\infty}) + o(t)\ . \tag{32}$$

Using

$$\frac{d}{dt}(p_2 + \ldots + p_n) = e^{q_1-q_2} - e^{q_n-q_{n+1}}\ , \quad 2 \le n \le N-1$$

and proceeding by induction we find

$$\int_0^\infty e^{q_n-q_{n+1}}\, ds < \infty, \quad 2 \le n \le N-2\ . \tag{33}$$

(Of course the estimates

$$\int_0^\infty e^{q_{N-1}-q_N}\, ds, \int_0^\infty e^{q_1-q_2}\, ds < \infty$$

were obtained earlier.)

It follows that, as $t \to \infty$,

$$p_n(t) = p_{n,\infty} + o(1), \quad 2 \le n \le N-1$$

and hence

$$q_n(t) = q_{n,\infty} + p_{n,\infty} t + o(t), \quad 2 \le n \le N-1$$

and so

$$q_n(t) - q_{n+1}(t) = q_{n,\infty} - q_{n-1,\infty} + (p_{n,\infty} - p_{n+1,\infty})t + o(t), \quad 2 \le n \le N-2\ . \tag{34}$$

In particular, by (33), we must have

$$p_{n,\infty} - p_{n+1,\infty} \le 0, \quad 2 \le n \le N-2\ . \tag{35}$$

We will show shortly that the inequality in (35) is strict. But note first that by (29) and (30),

$$\frac{d}{dt} e^{q_n-q_{n+1}} = e^{q_n-q_{n+1}}(p_n - p_{n+1}), \quad 2 \le n \le N-2$$

is bounded, and so $e^{q_n-q_{n+1}}$ is globally Lipschitz in time, and in particular uniformly continuous in t, and it follows from (33) that

$$e^{q_n(t)-q_{n+1}(t)} \to 0 \tag{36}$$

pointwise as $t \to \infty$.

We now prove that the inequality in (35) is strict.

In terms of the variables introduced in (8), $a_n = -p_n/2, 1 \le n \le N$, and $b_n = e^{(q_n - q_{n+1})/2}/2,\ 1 \le n \le N-1$, the equations (16) take the form

$$\begin{aligned} \dot{a}_n &= 2(b_n^2 - b_{n-1}^2), \quad 2 \le n \le N-1, \\ \dot{b}_n &= b_n(a_{n+1} - a_n), \quad 2 \le n \le N-2 \ . \end{aligned} \tag{37}$$

Set $A_n = \lim_{t\to\infty} a_n = -p_{n,\infty}/2$, $2 \le n \le N-1$, and consider

$$S(t) \equiv \sum_{n=2}^{N-1} (a_n - A_n)^2 + 2 \sum_{n=2}^{N-2} b_n^2 \ .$$

From (37), we have

$$b_n(t) = b_n(0)\ e^{\int_0^t (a_{n+1} - a_n)\ ds} \ , \quad 2 \le n \le N-2$$

and as $b_n(t) = \frac{1}{2} e^{(q_n(t) - q_{n+1}(t))/2} \to 0$ by (36), we must have

$$\int_0^\infty (a_{n+1} - a_n)\ ds = -\infty \ , \quad 2 \le n \le N-2. \tag{38}$$

Using (37), we find after summing by parts

$$\begin{aligned} \frac{1}{4}\frac{d}{dt} S(t) = & \sum_{n=2}^{N-1} (a_n - A_n)(b_n^2 - b_{n-1}^2) + \sum_{n=2}^{N-2} b_n^2 (a_{n+1} - a_n) \\ &= (a_{N-1} - A_{N-1}) \sum_{n=2}^{N-1} (b_n^2 - b_{n-1}^2) \\ + \sum_{n=2}^{N-2} & (a_n - a_{n+1} - A_n + A_{n+1}) \sum_{i=2}^{n} (b_i^2 - b_{i-1}^2) + \sum_{n=2}^{N-2} b_n^2 (a_{n+1} - a_n) \\ &= (a_{N-1} - A_{N-1})(b_{N-1}^2 - b_1^2) \\ + \sum_{n=2}^{N-2} & (a_n - a_{n+1} - A_n + A_{n+1})(b_n^2 - b_1^2) + \sum_{n=2}^{N-2} b_n^2 (a_{n+1} - a_n) \\ &= \sum_{n=2}^{N-2} (A_{n+1} - A_n) b_n^2 + O(e^{-\gamma t^2}), \end{aligned}$$

where we have used (28),

$$b_1^2 = \frac{1}{4}\ e^{q_1 - q_2} \ , \quad b_{N-1}^2 = \frac{1}{4}\ e^{q_{N-1} - q_N} = O(e^{-\gamma t^2}) \ .$$

Now, if $A_{n+1} - A_n = -\frac{1}{2}(p_{n+1,\infty} - p_{n,\infty}) > 0$, then it follows from (34) that

$$b_n(t) = \frac{1}{2} e^{(q_n(t) - q_{n+1}(t))/2} = O(e^{-\mu t/2})$$

for some $\mu > 0$. As $A_{n+1} - A_n \geq 0$ by (35), it follows that

$$(A_{n+1} - A_n)b_n^2(t) = O(e^{-\mu t}), 2 \leq n \leq N-2 \ .$$

We conclude that, as $S(t) \to 0$ as $t \to \infty$,

$$S(t) = O(e^{-\mu t})$$

and hence

$$a_n = A_n + O(e^{-\mu t}), \quad 2 \leq n \leq N-1$$

as $t \to \infty$. Thus if $A_{n+1} - A_n = 0$ for some $2 \leq n \leq N-2$, we would have $a_{n+1}(t) - a_n(t) = O(e^{-\mu t})$ for some $2 \leq n \leq N-2$, which contradicts (38). Thus the inequality in (35) is strict,

$$p_{2,\infty} < p_{3,\infty} < \ldots < p_{N-1,\infty} \ . \tag{39}$$

In particular, it follows (use (34), or more directly $S(t) = O(e^{-\mu t})$) that, as $t \to \infty$,

$$e^{q_n(t) - q_{n+1}(t)} \equiv O(e^{-\mu t}), \quad 2 \leq n \leq N-2 \tag{40}$$

and hence, by the above induction argument we also have

$$p_n(t) = p_{n,\infty} + O(e^{-\mu t}) \ , \quad 2 \leq n \leq N-1, \tag{41}$$

and so

$$q_n = q_{n,\infty} + t\ p_{n,\infty} + O(e^{-\mu t}) \ , \quad 2 \leq n \leq N-1. \tag{42}$$

Equations (31) and (36) already imply that the core Toda matrix

$$L_F = \begin{pmatrix} a_2 & b_2 & \ldots & 0 \\ b_2 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & b_{N-2} \\ 0 & 0 & b_{N-2} & a_{N-1} \end{pmatrix} \tag{43}$$

converges to a diagonal matrix. By (40) and (41), the convergence is exponential.

Remark: If L_F evolved according to the (exact) Toda flow (9), then, as $t \to \infty$, $p_n(t) \to p_{n,\infty} = -2\lambda_n^F, 2 \leq n \leq N-1$, where the λ_n^F's are the eigenvalues of $L_F(t = 0)$. As $L_F(t = 0)$ is tridiagonal, the λ_n^F's are distinct and so the strict inequality in (35) is immediate. As $L_F(t)$ solves only a perturbed Toda flow, the strict inequality requires a more subtle analysis, as above.

Step 4.

From $p_1(t) = p_1(0) - \displaystyle\int_0^t e^{q_1 - q_2}\ ds - ct$ and (28), we see that

$$p_1(t) = p_{1,\infty} - ct + O(e^{-\gamma t^2}) \tag{44}$$

and similarly

$$p_N(t) = p_{N,\infty} + ct + O(e^{-\gamma t^2})$$

from which it follows that

$$q_1(t) = q_{1,\infty} - \frac{ct^2}{2} + tp_{1,\infty} + O(e^{-\gamma t^2})$$

and

$$q_N(t) = q_{N,\infty} + \frac{ct^2}{2} + tp_{N,\infty} + O(e^{-\gamma t^2}) \ .$$

From (41) and (42), we have for $2 \leq n \leq N-1$,

$$p_n(t) = p_{n,\infty} + O(e^{-\mu t})$$

and

$$q_n(t) = q_{n,\infty} + tp_{n,\infty} + O(e^{-\mu t}) \ . \tag{45}$$

Let $U_t(q_0, p_0) = (q(t), p(t))$ be the solution of (16) with $(q(0), p(0) = (q_0, p_0)$, and let $\hat{U}_t(\hat{q}_0, \hat{p}_0) = (\hat{q}(t), \hat{p}(t))$ be the solution of the Hamiltonian equations generated by the decoupled Hamiltonian

$$H_c^d(q,p) = \frac{1}{2}\sum_{n=1}^{N} p_n^2 + \sum_{n=2}^{N-2} e^{q_n - q_{n+1}} + c(q_1 - q_N) \ . \tag{46}$$

The Hamiltonian H_c^d is clearly completely integrable. We have

$$\dot{\hat{q}}_1(t) = \hat{p}_1(t) \ , \quad \dot{\hat{p}}_1 = -c$$

and so

$$\hat{p}_1(t) = \hat{p}_{1,0} - ct \ , \quad \hat{q}_1(t) = \hat{q}_{1,0} + \hat{p}_{1,0}t - \frac{ct^2}{2}$$

and similarly

$$\hat{p}_N(t) = \hat{p}_{N,0} + ct \ , \quad \hat{q}_N(t) = \hat{q}_{N,0} + \hat{p}_{N,0}t + \frac{ct^2}{2} \ .$$

By standard Toda asymptotics, (10) and (15), for $2 \leq n \leq N-1$, as $t \to \pm\infty$,

$$\hat{p}_n(t) = \alpha_n^{\pm} + O(e^{-\gamma|t|})$$

and

$$\hat{q}_n(t) = \beta_n^{\pm} + \alpha_n^{\pm} t + O(e^{-\gamma|t|}) \ .$$

Also let $U_t^{\#}(q_0^{\#}, p_0^{\#}) = (q^{\#}(t), p^{\#}(t))$ be the solution of the equations generated by the "free" decoupled Hamiltonian

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

Clearly

$$p_1^{\#}(t) = p_{1,0}^{\#} - ct \ , \quad q_1^{\#}(t) = q_{1,0}^{\#} + p_{1,0}^{\#}t - \frac{ct^2}{2}$$

and

$$p_N^{\#}(t) = p_{N,0}^{\#} + ct \ , \quad q_N^{\#}(t) = q_{N,0}^{\#} + p_{N,0}^{\#}t + \frac{ct^2}{2}$$

and

$$p_n^{\#}(t) = p_{n,0}^{\#}\ , \quad q_n^{\#}(t) = q_{n,0}^{\#} + p_{n,0}^{\#}t\ , \quad 2 \le n \le N-1\ . \tag{47}$$

Now

$$\hat{W}_t^{\#}(\hat{q}_0,\hat{p}_0) \equiv U_{-t}^{\#} \circ \hat{U}_t(\hat{q}_0,\hat{p}_0) = U_{-t}^{\#}\big(\hat{q}_{1,0} + \hat{p}_{1,0}t - \frac{ct^2}{2}, \hat{p}_{1,0} - ct,$$

$$\big(\beta_n^+ + \alpha_n^+ t + O(e^{-\gamma t}), \alpha_n^+ + O(e^{-\gamma t})\big)_{n=2}^{N-1}, \hat{q}_{N,0} + \hat{p}_{N,0}t + \frac{ct^2}{2}, \hat{p}_{N,0} + ct\big)$$

$$= \big((\hat{q}_{1,0} + \hat{p}_{1,0}t - \frac{ct^2}{2}) + (\hat{p}_{1,0} - ct)(-t) - \frac{c(-t)^2}{2}, (\hat{p}_{1,0} - ct) - c(-t)$$

$$\big(\beta_n^+ + \alpha_n^+ t + O(e^{-\gamma t}) + (\alpha_n^+ + O(e^{-\gamma t}))(-t), \alpha_n^+ + O(e^{-\gamma t})\big)_{n=2}^{N-1},$$

$$(\hat{q}_{N,0} + \hat{p}_{N,0}t + \frac{ct^2}{2}) + (\hat{p}_{N,0} + ct)(-t) + \frac{c(-t)^2}{2}, (\hat{p}_{N,0} + ct) + c(-t)\big)$$

$$= \big(\hat{q}_{1,0}, \hat{p}_{1,0}, \big(\beta_N^+ + O(e^{-\gamma t}), \alpha_n^+ + O(e^{-\gamma t})\big)_{n=2}^{N-1}, \hat{q}_{N,0}, \hat{p}_{N,0}\big)$$

$$\to \big(\hat{q}_{1,0}, \hat{p}_{1,0}, \big(\beta_N^+, \alpha_n^+\big)_{n=2}^{N-1}, \hat{q}_{N,0}, \hat{p}_{N,0}\big) \equiv (\hat{q}^{\#}, \hat{p}^{\#}),$$

where

$$\hat{q}^{\#} = (\hat{q}_{1,0}, \beta_2^+, \dots, \beta_{N-1}^+, \hat{q}_{N,0})\ , \quad \hat{p}^{\#} = (\hat{p}_{1,0}, \alpha_2^+, \dots, \alpha_{N-1}^+, \hat{p}_{N,0})\ . \tag{48}$$

Thus

$$\hat{W}^{\#}(\hat{q}_0,\hat{p}_0) = \lim_{t\to\infty} U_{-t}^{\#} \circ \hat{U}_t(\hat{q}_0,\hat{p}_0) = (\hat{q}^{\#}, \hat{p}^{\#}) \tag{49}$$

exists. A similar argument shows that

$$W^{\#}(q_0,p_0) = \lim_{t\to\infty} U_{-t}^{\#} \circ U_t(q_0,p_0) = (q^{\#}, p^{\#}) \tag{50}$$

exists, where we now use (44) and (45),

$$q^{\#} = (q_{1,\infty}, \dots, q_{N,\infty})\ , \quad p^{\#} = (p_{1,\infty}, \dots, p_{N,\infty})\ .$$

As

$$I_1(q,p) = \frac{1}{2}p_1^2 + cq_1\ , \quad I_n(q,p) = p_n,\ 2 \le n \le N-1\ , \quad I_N(q,p) = \frac{1}{2}p_N^2 - q_N$$

are commuting integrals for $U_t^{\#}$, it follows from (49), as in (14), that

$$J_n(q,p) = I_n \circ W^{\#}(q,p) = I_n(q^{\#}, p^{\#})\ , \quad 2 \le n \le N-1$$

are commuting integrals for U_t, i.e., for (16). In particular, this shows that H_c is integrable. However, we want to show more: we want to show that there is an intertwining operator W for $\hat{U}_t$ and U_t,

$$\hat{U}_t \circ W = W \circ U_t\ . \tag{51}$$

This will then allow us to display (16) in a convenient Lax-pair form, and hence as an isospectral deformation similar to the (unperturbed) Toda case. From (49) and (50), we have

$$U_t^\# \circ \hat{W}^\# = \hat{W}^\# \circ \hat{U}_t \quad \text{and} \quad U_t^\# \circ W^\# = W^\# \circ U_t \tag{52}$$

and so, if $(\hat{W}^\#)^{-1}$ exists, then (modulo domain issues, explained at the end of Step 4)

$$\hat{U}_t \circ (\hat{W}^\#)^{-1} \circ W^\# = (\hat{W}^\#)^{-1} \circ U_t^\# \circ W^\# = (\hat{W}^\#)^{-1} \circ W^\# \circ U_t$$

and so (51) holds with

$$W = (\hat{W}^\#)^{-1} \circ W^\# \ . \tag{53}$$

The proof that $(\hat{W}^\#)^{-1}$ exists requires detailed knowledge of $(\hat{q}^\#, \hat{p}^\#)$.

To prove that $(\hat{W}^\#)^{-1}$ exists, we use the following result from [4] (for an alternative proof, see Props. 5.2 and 3.6 in [19]). Let

$$(q(t), p(t)) = (q_2(t), \ldots, q_{N-1}(t), p_2(t), \ldots, p_{N-1}(t)) \tag{54}$$

solve the Toda equation generated by $H_F(q,p) = \dfrac{1}{2}\displaystyle\sum_{n=2}^{N-1} p_n^2 + \sum_{n=2}^{N-2} e^{q_n - q_{n+1}}$ with initial data (q_0, p_0). Then, as $t \to \infty$ (see (10)),

$$q_n(t) = \alpha_n^+ t + \beta_n^+ + O(e^{-\gamma t}) \ , \quad \gamma > 0, \ 2 \le n \le N-1, \tag{55}$$

where

$$\alpha_n^+ = \, -2\lambda_n \ , \quad 2 \le n \le N-1 \tag{56}$$

and

$$\beta_n^+ = \frac{1}{N-2}\sum_{j=2}^{N-1} q_{j,0} - \frac{2}{N-2}\sum_{j=2}^{N-1} \ln\left(\frac{u_n(2)}{u_j(2)} \frac{\Pi_{\ell=2}^{n-1} 2(\lambda_\ell - \lambda_n)}{\Pi_{\ell=2}^{j-1} 2(\lambda_\ell - \lambda_j)} \right) \ , \tag{57}$$

where $2 \le n \le N-1$, and $\Pi_{\ell=2}^{1} 2(\lambda_\ell - \lambda_2) \equiv 1$. Here $\lambda_2 > \lambda_3 > \ldots > \lambda_{N-1}$ are the eigenvalues of the core Toda matrix $L_F(q_0, p_0)$ in (43), where $a_i = \, -p_{i,0}/2$, $b_j = \dfrac{1}{2} e^{(q_{j,0} - q_{j+1,0})/2}$, $2 \le i \le N-1$, $2 \le j \le N-2$, and $u_2(2), \ldots u_{N-1}(2)$ are the first components of the normalized eigenvectors $u_n = (u_n(2), \ldots, u_n(N-1))^T$ of $L_F(q_0, p_0)$ corresponding to λ_n, $2 \le n \le N-1$. We have $\displaystyle\sum_{j=2}^{N-1} u_n^2(j) = 1$ and $u_n(2) > 0$ for all $2 \le n \le N-1$. It is well known (see e.g. [4]) that the map Φ from Jacobi matrices L_F with $b_i > 0$, $2 \le i \le N-1$, is a bijection onto

$$\{(\gamma_2, \ldots, \gamma_{N-1}, \mu_2, \ldots, \mu_{N-1}) \ : \ \gamma_2 > \gamma_3 > \ldots > \gamma_{N-1}, \\ \sum_{i=2}^{N-1} \mu_i^2 = 1, \quad \mu_i > 0, \quad 2 \le i \le N-1\}.$$

Let $U_t^F = (q(t), p(t))$ denote the solution of the Toda equations in (54) above and let U_t^0 denote the solution of the equations generated by $H^0(q,p) = \frac{1}{2}\sum_{n=2}^{N-1} p_n^2$. Then the argument leading to (49) shows that

$$W^F(q_0, p_0) = \lim_{t\to\infty} U_{-t}^0 \circ U_t^F(q_0, p_0)$$

exists and

$$W^F(q_0, p_0) = (\beta_2^+, \ldots, \beta_{N-1}^+, \alpha_2^+, \ldots, \alpha_{N-1}^+) \ . \tag{58}$$

We show first that W^F is one-to-one. Assume (58). From (56), the eigenvalues $\{\lambda_n\}$ of $L_F(q_0, p_0)$ are determined,

$$\lambda_n = -\alpha_n^+/2 \ , \quad 2 \le n \le N-1 \ .$$

From (57),

$$\sum_{n=2}^{N-1} \beta_n^+ = \sum_{j=2}^{N-1} q_{j,0} - \frac{2}{N-2}\sum_{n=2}^{N-1}\sum_{j=2}^{N-1} \ln\left(\frac{u_n(2)\,\Pi_{\ell=2}^{n-1} 2(\lambda_\ell - \lambda_n)}{u_j(2)\,\Pi_{\ell=2}^{j-1} 2(\lambda_\ell - \lambda_j)}\right) = \sum_{i=2}^{N-1} q_{j,0} \ , \tag{59}$$

as the double sum vanishes by oddness. It follows then from (57) that, for $2 \le n \le N-1$,

$$\sum_{j=2}^{N-1} \ln \frac{u_n(2)}{u_j(2)} = r_n \ , \tag{60}$$

where r_n is a function of $\{\beta_j^+\}_{i=2}^{N-1}$ and $\{\alpha_n^+ = -2\lambda_n\}$,

$$r_n = \frac{N-2}{2}\left(\frac{1}{N-2}\sum_{j=2}^{N-1} \beta_j^+ - \beta_n^+ - \frac{2}{N-2}\sum_{j=2}^{N-1} \ln\left(\frac{\Pi_{\ell=2}^{n-1}(\alpha_n^+ - \alpha_\ell^+)}{\Pi_{\ell=2}^{n-1}(\alpha_j^+ - \alpha_\ell^+)}\right)\right) . \tag{61}$$

Note that

$$\sum_{n=2}^{N-1} r_n = 0 \ . \tag{62}$$

From (60),

$$\prod_{j=2}^{N-1}\left(\frac{u_n(2)}{u_j(2)}\right) = e^{r_n}$$

and so

$$u_n(2) = \left(\prod_{j=2}^{N-1} u_j(2)\right)^{1/(N-2)} e^{r_n/(N-2)} \ .$$

Since $\sum_{n=2}^{N-1} u_n(2)^2 = 1$, this gives

$$\prod_{j=2}^{N-1} u_j(2) = \left(\sum_{n=2}^{N-1} e^{2r_n/(N-2)}\right)^{(2-N)/2} .$$

Thus

$$u_n(2) = \frac{e^{\frac{r_n}{N-2}}}{\left(\sum_{n=2}^{N-1} e^{\frac{2r_n}{N-2}}\right)^{1/2}} , \quad 2 \leq n \leq N-1 .$$

As $L_F(q_0, p_0)$ is determined by its eigenvalues and the first components of its normalized eigenvectors, it follows that $L_F(q_0, p_0)$ is determined by $\{\beta_i^+, \alpha_j^+\}, 2 \leq i, j, N-1$. But

$$p_{n,0} = -2a_n, \quad 2 \leq n \leq N-1$$

and

$$q_{n,0} - q_{n+1,0} = 2 \ln 2b_n , \quad 2 \leq n \leq N-2 .$$

As $\sum_{n=2}^{N-1} q_{n,0} = \sum_{n=2}^{N-1} \beta_n^+$, by (59), we thus see that (q_0, p_0) is determined by

$$(\beta_2^+, \ldots, \beta_{N-1}^+, \alpha_2^+, \ldots \alpha_{N-1}^+) = W^F(q_0, p_0) ,$$

i.e., W^F is one-to-one. We now show that W^F is onto

$$X = \{(x_2, \ldots, x_{N-1}, y_2, \ldots, y_{N-1}) \ : \ y_2 < \ldots < y_{N-1}\} \subset \mathbb{R}^{2(N-2)} .$$

Let $r_n = r_n(x, y)$ in (61) with β_n^+ replaced by x_n and α_n^+ by y_n, $2 \leq n \leq N-1$. Set

$$u_n(2) = \frac{e^{r_n/(N-2)}}{\left(\sum_{j=2}^{N-1} e^{2r_j/(N-2)}\right)^{1/2}} > 0 , \quad 2 \leq n \leq N-1 . \tag{63}$$

Then by (62),

$$\prod_{n=2}^{N-1} u_n(2) = \frac{e^{\frac{1}{N-2}\sum_{n=2}^{N-1} r_n}}{\left(\sum_{j=2}^{N-1} e^{2r_j/(N-2)}\right)^{(N-2)/2}} = \frac{1}{\left(\sum_{j=2}^{N-1} e^{2r_j/(N-2)}\right)^{(N-2)/2}} .$$

From (63),

$$\sum_{n=2}^{N-1} u_n(2)^2 = 1 \quad \text{and} \quad u_n(2) \geq 0, \ 2 \leq n \leq N-1, \tag{64}$$

and using (63), we see that

$$u_n(2) = \Big(\prod_{j=2}^{N-1} u_j(2)\Big)^{1/(N-2)} e^{r_n/(N-2)}$$

which implies

$$\prod_{i=2}^{N-1} \left(\frac{u_n(2)}{u_j(2)}\right) = e^{r_n(x,y)}$$

from which we conclude that

$$x_n = \frac{1}{N-2}\sum_{j=2}^{N-1} x_j - \frac{2}{N-2}\sum_{j=2}^{N-1} \ln\left(\frac{u_n(2)}{u_j(2)}\frac{\Pi_{\ell=2}^{n-1}(y_n-y_\ell)}{\Pi_{\ell=2}^{n-1}(y_j-y_\ell)}\right) .$$

Now, as Φ is a bijection, there exists a unique Toda matrix L_F (see (43)) with spectrum $\lambda_2 = -y_2/2 > \lambda_3 = -y_3/2 > \ldots > \lambda_{N-1} = -y_{N-1}/2$ and first components of the eigenvectors $u_2(2), \ldots, u_{N-1}(2)$.

Set

$$\begin{aligned} p_{n,0} &= -2a_n , \quad 2 \le n \le N-1, \\ q_{n,0} - q_{n+1,0} &= 2\ln(2b_n) , \quad 2 \le n \le N-1 . \end{aligned}$$

Then determine the $q_{n,0}$'s uniquely by requiring

$$\sum_{n=2}^{N-1} q_{n,0} = \sum_{n=2}^{N-1} x_n .$$

It then follows from the above calculations that

$$W^F(q_0, p_0) = (x_2, \ldots, x_{N-1}, y_2, \ldots, y_{N-1})$$

which completes the proof that W^F is a bijection from $\mathbb{R}^{2(N-2)}$ to X. Finally, we conclude from (48) that $\hat{W}^\#$ is a bijection from $\mathbb{R}^{2N}$ to

$$\hat{X}^\# = \{(x_1, x_2, \ldots, x_{N-1}, x_N, y_1, y_2, \ldots, y_{N-1}, y_N) \ : \ y_2 < y_3 < \ldots < y_{N-1}\} .$$

In order to derive (51) with W as in (53), we need to verify certain domain issues. For $(x, y) \in \hat{X}^\#$, we have from (52)

$$\hat{W}^\# \circ \hat{U}_t \circ (\hat{W}^\#)^{-1}(x, y) = U_t^\# \circ \hat{W}^\# \circ (\hat{W}^\#)^{-1}(x, y) = U_t^\#(x, y)$$

from which we see necessarily that $U_t^\#(x, y) \in \hat{X}^\#$, a fact that can be seen directly from (47). Hence

$$\hat{U}_t \circ (\hat{W}^\#)^{-1} = (\hat{W}^\#)^{-1} \circ U_t^\# \ \text{ on } \ \hat{X}^\# .$$

But it follows from (39) that for any $(x, y) \in \mathbb{R}^{2N}$, $W^\#(x, y) \in \hat{X}^\#$, and so

$$\hat{U}_t \circ (\hat{W}^\#)^{-1} \circ W^\#(x, y) = (\hat{W}^\#)^{-1} \circ U_t^\# \circ W^\# = (\hat{W}^\#)^{-1} \circ W^\# \circ U_t(x, y)$$

which verifies, indeed, that $W = (\hat{W}^\#)^{-1} \circ W^\#$ mapping $\mathbb{R}^{2N}$ to itself intertwines U_t, the propagator for the equations generated by H_c, and $\hat{U}_t$, the propagator for the equations generated by the completely integrable Toda-core Hamiltonian H_c^d.

As noted earlier, although the intertwining relation $\hat{U}_t \circ W = W \circ U_t$ is enough to prove integrability, it is not sufficient to prove that solutions generated by H_c behave asymptotically like solutions generated by the decoupled Toda core Hamiltonian H_c^d. In the quantum mechanical case , the fact that e^{iAt} is linear and unitary implies that $||e^{-iAt}e^{iBt}f - Wf|| = ||e^{iBt}f - e^{iAt}Wf|$, and so the convergence of the wave operator W is equivalent to showing that a solution $e^{iBt}f$ generated by the operator B, behaves like a solution $e^{iAt}g$ generated by the operator A, where $g := Wf$. In the case at hand, as $\hat{U}_t^{\#}$, is neither linear nor bounded, we cannot, in particular, immediately infer from the convergence $U_{-t}^{\#} \circ \hat{U}_t(q_0, p_0) - \hat{W}^{\#}(q_0, p_0) \to 0$, that $\hat{U}_t(q_0, p_0) - U_t^{\#}\hat{W}^{\#}(q_0, p_0) \to 0$, as desired. However, as we see from the calculations following (47), as $t \to \infty$,

$$U_{-t}^{\#} \circ \hat{U}_t(q_0, p_0) = \hat{W}^{\#}(q_0, p_0) + O(e^{-\gamma t})$$

it then follows from the explicit form, and polynomial growth, of $U_t^{\#}$ that

$$\hat{U}_t(q_0, p_0) = U_t^{\#}(\hat{W}^{\#}(q_0, p_0) + O(e^{-\gamma t})) = (U_t^{\#}\hat{W}^{\#}(q_0, p_0)) + O(e^{-\gamma t/2}).$$

A similar argument shows that

$$U_t(q_0, p_0) = U_t^{\#}(W^{\#}(q_0, p_0) + O(e^{-\gamma t})) = (U_t^{\#}W^{\#}(q_0, p_0)) + O(e^{-\gamma t/2}).$$

Now as $W^{\#}(q_0, p_0) \in \hat{X}^{\#}$, and as $\hat{W}^{\#}$ is a bijection onto $\hat{X}^{\#}$, it follows that there exist $(\hat{q}_0, \hat{p}_0)$ such that $\hat{W}^{\#}(\hat{q}_0, \hat{p}_0) = W^{\#}(q_0, p_0)$. Substitution into the above two relations shows that

$$U_t(q_0, p_0) = \hat{U}_t(\hat{q}_0, \hat{p}_0) + O(e^{-\gamma t/2})$$

where $(\hat{q}_0, \hat{p}_0) = W(q_0, p_0)$ as desired.

Finally, as noted before, we do not construct W directly as a wave operator $\lim_{t\to\infty} \hat{U}_{-t} \circ U_t(q_0, p_0)$. The reason for this is the following. In evaluating

$$\hat{U}_{-t} \circ U_t(q_0, p_0) = \hat{U}_{-t}(q(t), p(t))$$

we are facing a double scaling limit. The asymptotics of $\hat{U}_{-t}(\hat{q}_0, \hat{p}_0)$ as $t \to \infty$ is known for $(\hat{q}_0, \hat{p}_0)$ fixed, or in a compact set, but $q(t)$, in particular, grows linearly. This considerably complicates the analysis. The difficulty is avoided when we evaluate

$$\hat{U}_{-t}^{\#} \circ U_t(q_0, p_0) = \hat{U}_{-t}^{\#}(q(t), p(t))$$

as we have an explicit, and simple, formula for $\hat{U}_{-t}^{\#}(\hat{q}^{\#}, \hat{p}^{\#})$ for **all** $(\hat{q}^{\#}, \hat{p}^{\#})$, and so the double scaling limit is avoided. To avoid the problem of the double scaling limit in evaluating $\hat{U}_{-t}(q(t), p(t))$, we need to use an explicit formula for $\hat{U}_{-t}(\hat{q}_0, \hat{p}_0)$ for all $(\hat{q}_0, \hat{p}_0)$. This is most conveniently done by mapping the solution $(q_1(t), ..., q_N(t), p_1(t), ..., p_N(t))$ onto the eigenvalues $(\lambda_2(t), ..., \lambda_{N-1}(t))$ and first components of the associated normalized eigenvectors $(u_2(2)(t), ..., u_{N-1}(2)(t))$ of the core Toda matrix $L_F = L_F(t)$ in (43) . In [22], Moser used the Lax-Pair form (9) to show that under the Toda flow

$$\hat{\lambda}_i(t) = \hat{\lambda}_{i,0},\ i = 2, ..., N-1$$

and

$$\hat{u}_i(2)(t) = \frac{\hat{u}_{i,0}(2)e^{\hat{\lambda}_{i,0}t}}{(\sum_{j=2}^{N-1}(\hat{u}_{j,0}(2))^2 e^{2\hat{\lambda}_{j,0}t})^{1/2}},\ i = 2, ..., N-1$$

for any initial conditions $\hat{\lambda}_{i,0}$,$\hat{u}_{j,0}(2)$. The evolution of $L_F(t)$ is almost the same as in (9), except there is an additional diagonal driving term

$$\dot{L}_F = [L_F, B_F] + \mathrm{diag}(-2b_1^2, 0, 0, ..., 0, 2b_{N-1}^2)$$

where $b_1 = \frac{1}{2}e^{(q_1(t)-q_2(t))/2}$ and $b_{N-1} = \frac{1}{2}e^{(q_{N-1}(t)-q_N(t))/2}$. Now Moser's method to obtain the above formulae for $(\hat{\lambda}_i(t)$,$\hat{u}_j(2)(t))$, can be extended, using the driven Lax-Pair for $L_F(t)$, to obtain the asymptotics of $\lambda_i(t)$ and $u_j(2)(t)$. Then when we evaluate

$$\hat{U}_{-t} \circ U_t(q_0, p_0) = \hat{U}_{-t}(q(t), p(t))$$

now in the $(\lambda, u(2))$ variables, rather than the original (q, p) variables, we can use Moser's explicit formulae for $(\hat{\lambda}_i(t)$,$\hat{u}_j(2)(t))$, and the double scaling limit is avoided. Using the bijection between L_F and the $(\lambda, u(2))$ variables, we can then assert, after some algebra, the existence of

$$\lim_{t\to\infty} \hat{U}_{-t} \circ U_t(q_0, p_0)$$

directly in the original (q, p) variables. We leave the details to the interested reader.

Finally we note that the core Toda flow can also be solved explicitly for any time t in the bidiagonal formalism of [19], so that in evaluating

$$\lim_{t\to\infty} \hat{U}_{-t} \circ U_t(q_0, p_0)$$

we could just as easily have worked in bidiagonal coordinates.

Step 5.

We assert that $W = (\hat{W}^\#)^{-1} \circ W^\#$ is $C^1(\mathbb{R}^{2N})$. Indeed, $\hat{W}^\#$ is a diffeomorphism from $\mathbb{R}^{2N}$ onto $\hat{X}^\#$, as can be seen directly from (56) and (57) and the fact that Φ is a diffeomorphism, coupled with the fact that

$$(q_0, p_0) \mapsto \left(a_j = -p_{j,0}/2, b_j = \frac{1}{2}e^{(q_{j,0}-q_{j+1,0})/2}, 2 \le j \le N-1, \sum_{i=2}^{N-1} q_{i,0} \right),$$

is a diffeomorphism. At the analytical level, the fact that $\hat{W}^\# = \lim_{t\to\infty} U_{-t}^\# \circ \hat{U}_t$ is C^1 follows, alternatively, from the fact that $(q_0(t), p_0(t)) = U_{-t}^\# \circ \hat{U}_t(q_0, p_0)$ is a C^1 function of (q_0, p_0) for any finite t by standard ODE methods, and then noting from (7) that the derivative of $(q_0(t), p_0(t))$ with respect to (q_0, p_0) is a linear system with exponentially decaying coefficients. But the same is true for

(16), and so $W^{\#} = \lim_{t\to\infty} U^{\#}_{-t} \circ U_t$ is also C^1, and hence $W = (\hat{W}^{\#})^{-1} \circ W^{\#}$ is C^1. We leave the details to the interested reader.

For the core Toda system $(q, p) = (q_2, \ldots, q_{N-1}, p_2, \ldots, p_{N-2})$, let $\lambda_2 > \ldots > \lambda_{N-1}$ be the eigenvalues and $u_2(2), \ldots, u_{N-1}(2)$ be the first components of the normalized eigenvectors of the associated Toda matrix $L_F(q, p)$. Let $Z(\lambda) = \det(L_F(q,p) - \lambda)$. Then, as shown in [5], and also, more directly in [4] (action-angle variables for the Toda flow are also given in [17]),

$$\begin{aligned}
\theta_k &= \ln\left(\frac{u_k(2)}{u_{N-1}(2)}\left|\frac{Z'(\lambda_k)}{Z'(\lambda_{N-1})}\right|^{1/2}\right)\ , \quad 2 \le k \le N-2 \\
\theta_{N-1} &= \frac{1}{N-2}(q_2 + \ldots + q_{N-1}), \\
\tilde{\lambda}_k &= \lambda_k - \frac{1}{N-2}\sum_{j=2}^{N-1}\lambda_j\ , \quad 2 \le k \le N-2, \\
\tilde{\lambda}_{N-1} &= p_2 + \ldots + p_{N-1}
\end{aligned}$$

are action-angle variables for the core Toda flow,

$$\{\theta_i, \theta_j\} = 0\ , \{\tilde{\lambda}_i, \tilde{\lambda}_j\} = 0, \{\theta_i, \tilde{\lambda}_j\} = \delta_{ij}\ , 2 \le i, j \le N-1\ . \tag{65}$$

On the other hand, for additional variables q_1, p_1, q_N, p_N, if

$$\begin{aligned}
\theta_1 &= -\frac{1}{2}p_1\ , \quad \theta_N = \frac{1}{c}p_N, \\
\tilde{\lambda}_1 &= \frac{1}{2}p^2 + cq_1\ , \quad \tilde{\lambda}_N = \frac{1}{2}p_N^2 - cq_N,
\end{aligned}$$

it follows that (65) holds for $1 \le i, j \le N$. Also from (46),

$$H_c^d = \tilde{\lambda}_1 + \tilde{\lambda}_n + 2\sum_{i=2}^{N-1}\lambda_k^2\ . \tag{66}$$

Now, as $\tilde{\lambda}_{N-1} = -2(a_2 + \ldots + a_{N-1}) = -2\,\mathrm{tr}\,L_F = -2(\lambda_2 + \ldots + \lambda_{N-1})$, we see that $\lambda_k = \tilde{\lambda}_k - \frac{1}{2(N-2)}\tilde{\lambda}_{N-1}, 2 \le k \le N-2$, and then solving for λ_{N-1}, we find

$$\lambda_{N-1} = -\frac{1}{2(N-2)}\tilde{\lambda}_{N-1} - \sum_{j=2}^{N-2}\tilde{\lambda}_i\ .$$

Substitution into (66) gives

$$H_c^d = \tilde{\lambda}_1 + \tilde{\lambda}_N + 2\sum_{k=2}^{N-2}(\tilde{\lambda}_k)^2 + 2\left(\sum_{k=2}^{N-2}\tilde{\lambda}_k\right)^2 + \frac{1}{2(N-2)^2}\tilde{\lambda}_{N-1}^2$$

for which

$$\begin{aligned}\{\theta_i, H_c^d\} &= 1\ , \quad i = 1 \text{ or } N \\ \{\theta_i, H_c^d\} &= 4\left(\tilde{\lambda}_i + \sum_{j=2}^{N-2}\tilde{\lambda}_j\right)\ , \quad 2 \le i \le N-2, \\ \{\theta_{N-1}, H_c^d\} &= \frac{1}{(N-2)^2}\tilde{\lambda}_{N-1}\end{aligned} \tag{67}$$

so that the θ_i's move linearly under H_c^d. Also clearly,

$$\{\tilde{\lambda}_i, H_c^d\} = 0\ , \quad 1 \le i \le N\ . \tag{68}$$

Now for the flow $\hat{U}_t(\hat{q}_0, \hat{p}_0) = (\hat{q}(t), \hat{p}(t))$,

$$\frac{d}{dt}f(\hat{q}(t), \hat{p}(t)) = \{f, H_c^q\}(\hat{q}(t), \hat{p}(t))$$

for any $f : \mathbb{R}^{2N} \to \mathbb{R}$ and it follows from (67) and (68) that $\{\theta_i\}_{i=1}^N, \{\tilde{\lambda}_i\}_{i=1}^N$ are action-angle variables for H_c^d.

Set

$$\Theta_i = \theta_i \circ W\ , \quad \Lambda_i = \tilde{\lambda}_i \circ W\ , \quad 1 \le i \le N.$$

Then as in (14), Θ_i and Λ_i are canonically conjugate. Furthermore, under the flow U_t generated by H_c, for any $f : \mathbb{R}^{2N} \to \mathbb{R}$ and $F = f \circ W$,

$$\begin{aligned}\frac{d}{dt}F(U_t(q_0, p_0)) &= \frac{d}{dt}(f \circ W \circ U_t(q_0, p_0)) \\ &= \frac{d}{dt}(f \circ \hat{U}_t(\hat{q}_0, \hat{p}_0))\ ,\ (\hat{q}_0, \hat{p}_0) = W(q_0, p_0) \\ &= \frac{d}{dt}f(\hat{q}(t), \hat{p}(t))\ .\end{aligned} \tag{69}$$

Hence under U_t,

(70)

$$\begin{aligned}&\frac{d}{dt}\Theta_i(q_0, p_0) = \frac{d}{dt}\theta_i(W(q_0, p_0)) = 1\ , \quad i = 1, N, \\ &\frac{d}{dt}\Theta_i(q_0, p_0) = \frac{d}{dt}\theta_i(W(q_0, p_0)) = 4\left(\Lambda_i(q_0, p_0) + \sum_{j=2}^{N-2}\Lambda_j(q_0, p_0)\right), \quad 2 \le i \le N-2, \\ &\frac{d}{dt}\Theta_{N-1}(q_0, p_0) = \frac{1}{(N-2)^2}\Lambda_{N-1}(q_0, p_0)\ .\end{aligned}$$

Also,

$$\frac{d}{dt}\Lambda_i(q_0, p_0) = 0\ , \quad 1 \le i \le N\ .$$

Thus $\{\Theta_i\}_{i=1}^N$, $\{\Lambda_i\}_{i=1}^N$ are action-angle variables for H_c.

Note that by a general and simple argument, the relations $\{\Theta_i, \Lambda_j\} = \delta_{ij}$ imply that $\Lambda_1, \ldots, \Lambda_n$ are functionally independent, which is equivalent to the statement that their gradients are linearly independent on an open, dense set. Thus H_c is integrable in the sense of Liouville.

Finally note that every Hamiltonian of the form

$$H = \frac{1}{2}p^2 + V(q) \quad (q,p) \in \mathbb{R}^2$$

generates a flow that can be expressed in Lax-pair form. Indeed, for

$$\hat{L} = \begin{pmatrix} p & 2V(q) \\ 1 & -p \end{pmatrix} , \quad \hat{B} = \begin{pmatrix} 0 & V'(q) \\ 0 & 0 \end{pmatrix}, \tag{71}$$

a simple computation shows that

$$\dot{q} = p \ , \quad \dot{p} = \, - V'(q) \quad \Leftrightarrow \quad \frac{d}{dt}\hat{L} = [\hat{L}, \hat{B}] \ . \tag{72}$$

Let $(\hat{q}_k(t), \hat{p}_k(t), 1 \le k \le N$, solve the flow generated by H_c^d as above. Set

$$Q_k = \hat{q}_k \circ W \ , \quad P_k = \hat{p}_k \circ W \ , \quad 1 \le k \le N \ .$$

Then, for $2 \le k \le N-1$,

$$\frac{d}{dt}Q_k = \hat{p}_k \circ W = P_k,$$

$$\begin{aligned} \frac{d}{dt}P_k &= \left(e^{\hat{q}_{k-1}-\hat{q}_k} - e^{\hat{q}_k-\hat{q}_{k+1}}\right) \circ W \\ &= e^{Q_{k-1}-Q_k} - e^{Q_k-Q_{k+1}}, \end{aligned}$$

where $e^{Q_1-Q_2} = e^{Q_{N-1}-Q_n} = 0$. Also

$$\frac{d}{dt}Q_1 = P_1 \ , \quad \frac{d}{dt}P_1 = \, - c$$

$$\frac{d}{dt}Q_N = P_N \ , \quad \frac{d}{dt}P_N = c \ .$$

Finally, set

$$\mathcal{L} = \begin{pmatrix} A_1 & B_2 & & & & & & \\ B_2 & \ddots & \ddots & & & 0 & & \\ & \ddots & & B_{N-2} & & & & \\ & & B_{N-2} & A_{N-1} & 0 & & & \\ & & & 0 & P_1 & 2cQ_1 & & \\ & & & & 1 & -P_1 & 0 & 0 \\ & & 0 & & & & P_N & -2cQ_N \\ & & & & & & 1 & -P_N \end{pmatrix},$$

and

$$\mathcal{B} = \begin{pmatrix} 0 & -B_2 & & & & & & & \\ B_2 & \ddots & \ddots & & & & 0 & & \\ & \ddots & & -B_{N-2} & & & & & \\ & & B_{N-2} & 0 & 0 & & & & \\ & & & 0 & 0 & c & & & \\ & & & & 0 & 0 & 0 & & \\ & 0 & & & & & 0 & -c \\ & & & & & & 0 & 0 \end{pmatrix},$$

where

$$\begin{aligned} A_k &= -\frac{1}{2}P_k\ , \quad 2 \le k \le N-1, \\ B_k &= \frac{1}{2}e^{(Q_k - Q_{k+1})/2}\ , \quad 2 \le k \le N-2\ . \end{aligned}$$

Then

$$(q_k(t), p_k(t))_{k=1}^N \text{ solve (16)}$$

$$\Leftrightarrow$$

$$\frac{d}{dt}\mathcal{L} = [\mathcal{L}, \mathcal{B}]\ .$$

Thus the Hamilton equations for H_c have a Lax-pair form.

Remark: Instead of using (51), we could use (52), $U_t^{\#} \circ W^{\#} = W^{\#} \circ U_t$ to display (16) as a Lax-pair in another form. But now the analog $\mathcal{L}^{\#}$ and $\mathcal{B}^{\#}$ of $\mathcal{L}$ and $\mathcal{B}$ convey little information,

$$\mathcal{L}^{\#} = \begin{pmatrix} P_1 & 0 & & & & & & \\ 0 & P_2 & \ddots & & & 0 & & \\ & \ddots & \ddots & 0 & & & & \\ & & 0 & P_{N-1} & 0 & & & \\ & & & 0 & P_1 & 2cQ_1 & & \\ & 0 & & & 1 & -P_1 & 0 & \\ & & & & & & P_N & -2cQ_n \\ & & & & & & 1 & -P_N \end{pmatrix}$$

and

$$
\mathcal{B}^{\#} = \begin{pmatrix}
0 & 0 & & & & & & \\
0 & \ddots & \ddots & & & 0 & & \\
 & \ddots & & 0 & & & & \\
 & & 0 & 0 & 0 & & & \\
 & & & 0 & 0 & c & & \\
 & & & & 0 & 0 & & \\
 & 0 & & & & & 0 & -c \\
 & & & & & & 0 & 0
\end{pmatrix}
$$

where

$$
Q_k = q_k^{\#} \circ W^{\#} \ , \quad P_k = p_k^{\#} \circ W^{\#} \ , \quad 1 \leq k \leq N \ . \tag{73}
$$

Here $(q^{\#}(t), p^{\#}(t)) = U_t^{\#}(q_0^{\#}, p_0^{\#})$.

Acknowledgments. Luen-Chau Li acknowledges the support from the Simons Foundation through grant #585813. Tom Trogdon acknowledges the support of NSF grant DMS-1945652 and Carlos Tomei from CNPq and FAPERJ, Brazil. The authors would also like to thank Barry Simon for some helpful information.

References

[1] J. Cook, Banach algebras and asymptotic mechanics, in Cargese Lectures in Theoretical Physics (F.Lurchit, ed.) Gordon and Breach, New York, 1967.

[2] D. Bilman and T. Trogdon, Benchmarking numerical methods for lattice equations with the Toda lattice. Applied Numerical Mathematics, 141, 2019, 19-35.

[3] E. Date and S. Tanaka, Analogue of Inverse Scattering Theory for the Discrete Hill's Equation and Exact Solutions for the Periodic Toda Lattice, Prog. of Theor. Phys. 55, No.2, 1976, 457-465.

[4] P. Deift, G. Dubach and T. Trogdon, Universality in Numerical Computation, Courant Lecture notes, Wiley, 2021 (in preparation).

[5] P. Deift, L. C. Li, T. Nanda and C. Tomei, The Toda flow on a generic orbit is integrable, Comm. Pure Appl. Math. 39, 2, 1986, 183-232.

[6] P. Deift and X. Zhou, Perturbation Theory for Infinite Dimensional Integrable Systems on the Line, A Case Study, Acta Math. 188, 2002, 163-262.

[7] J. Dereziński and C. Gérard, Scattering Theory of Classical and Quantum N-Particle Systems, Springer-Verlag, Berlin Heidelberg, 1997.

[8] H. Flaschka, On the Toda Lattice II, Prog. Theor. Phys 51, 3, 1974, 703-716.

[9] H. Flaschka, The Toda Lattice I. Existence of Integrals. Phys. Rev. B 9, 4, 1974, 1924-1925.

[10] E. Fermi, J. Pasta, S. Ulam (and M. Tsingou[2]), Document LA-1940, Los Alamos Nat. lab. 1955.

[11] J. Ford, S. D. Stoddard and J.S. Turner, On the Integrability of the Toda Lattice, Prog. Theor. Phys 50, 5, 1973, 1547-1560.

[2]At the time, Mary Tsingou's name was omitted from the list of authors. Times have changed and her key contribution is no longer overlooked.

[12] J. Ford and J. Waters, Computer Studies of Energy Sharing and Ergodicity for Nonlinear Oscillator Systems, J. Math. Phys 4, 1963, 1293-1306.
[13] M. Gallone, A. Ponno and B. Rink, KdV and FPU: asymptotic integrability of quasi unidirectional waves. arXiv:2010.03520.
[14] M. Hénon, Integrals of the Toda Lattice, Phys. Rev. B 9, 4, 1974, 1921-1923.
[15] W. Hunziker, The S-matrix in classical mechanics, Comm. Math.Phys. 8 , 1968, 282-299.
[16] M. Kac and P. van Moerbeke, A Complete Solution of the Periodic Toda Problem, Proc. Nat. Acad. Sci. USA 72, 8, 1975, 2879-2880.
[17] I. Krichever and K. Vaninsky, The periodic and open Toda Lattice, Mirror Symmetry, IV (Montreal, QC, 2000), 139-158, AMS/IP Stud. Adv. Math. 33, Amer. Math. Soc, Providence, RI, 2002.
[18] P. D. Lax, Integrals of Nonlinear Equations of Evolution and Solitary Waves, Comm. Pure App. Math. 21, 5, 1968, 467- 490.
[19] R. Leite, N. Saldanha and C. Tomei, An atlas for tridiagonal isospectral manifolds, Lin. Alg. and its Applcations, 429, 2008, 387-402.
[20] S. V. Manakov, Complete Integrability and Stochastization of Discrete Dynamical Systems, Zh. Eksp. Ter. fiz. 67, 1974, 543-555 (Russian) English version: Sov. Phys. JETP 40, 2, 1975.
[21] C. Møller, General properties of the characteristic matrix in the theory of elementary particles, I, Danske. Vid. Selsk. Mat.-Fys. Medd. 23, 1945, 1-48.
[22] J. Moser, Finitely Many Mass Points on the Line Under the Influence of an Exponential Potential – an Integrable System, Dynamical Systems, Theory and Applications (Rencontres, Battelle, Res. Inst. Seattle, Wash. 1974), 467-497, Lecture Notes in Phys. 38, Springer, Berlin, 1975.
[23] J. Moser and E. Zehnder, Notes on Dynamical Systems, Courant Lecture Notes 12, American Mathematical Society, 2005.
[24] E. Nelson, Topics in Dynamics I : Flows, Princeton University Press and Tokyo University Press, Princeton, NJ, 1969.
[25] B. Simon, Wave operators for classical particle scattering, Comm. Math. Phys. 23, 1971, 37-48.
[26] M. Toda, Theory of Nonlinear Lattices, Springer Series in Solid-State Sciences, 20 (2ed), Berlin: Springer, 1989.
[27] M. Toda, Vibration of a Chain with Nonlinear Interaction, J. Phys. Soc. Japan 22, 2, 1967, 431-436.

Percy Deift, Courant Institute, 251 Mercer St., New York, NY 10012, USA
Email address: deift@cims.nyu.edu

Luen-Chau Li, Department of Mathematics, Pennsylvania State University, University Park, PA 16802, USA
Email address: luenli@math.psu.edu

Herbert Spohn, Zentrum Mathematik, Technische Universität München, Boltzmannstrasse 3, D-85748, Garching, Germany
Email address: spohn@ma.tum.de

Carlos Tomei, Depto. de Matemática, PUC-Rio, Rio de Janeiro, Brazil
Email address: carlos.tomei@gmail.com

Thomas Trogdon, Department of Applied Mathematics, University of Washington, Seattle, WA 98195, USA
Email address: trogdon@uw.edu