



On the Role of the Integrable Toda Model in One-Dimensional Molecular Dynamics

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Abstract

We prove that the common Mie–Lennard–Jones (MLJ) molecular potentials, appropriately normalized via an affine transformation, converge, in the limit of hard-core repulsion, to the Toda exponential potential. Correspondingly, any Fermi–Pasta–Ulam (FPU)-like Hamiltonian, with MLJ-type interparticle potential, turns out to be $1/n$ -close to the Toda integrable Hamiltonian, n being the exponent ruling repulsion in the MLJ potential. This means that the dynamics of chains of particles interacting through typical molecular potentials, is close to integrable in an unexpected sense. Theoretical results are accompanied by a numerical illustration; numerics shows, in particular, that even the very standard 12–6 MLJ potential is closer to integrability than the FPU potentials which are more commonly used in the literature.

Keywords Fermi–Pasta–Ulam · Mie–Lennard–Jones · Toda model · Molecular dynamics · Pre-thermalization

1 Introduction

The study of both the dynamical and the statistical behavior of particle chains is a research topic essentially started by the celebrated numerical experiment of Fermi, Pasta and Ulam (FPU) [1], whose aim was to study in the simplest possible examples the time of approach to equilibrium of weakly nonlinear systems. As is well known, on the available computation

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time they did not observe any trend to equilibrium, and this is commonly named, after the authors, the FPU problem, or paradox.

The existing literature on the subject is huge, see e.g. the collection of papers [2, 3] or the more recent and short reviews [4, 5]. The revival of physical interest in such an old problem has been also stimulated, in recent years, by the experiments on arrays of cold atoms or ions, i.e. arrays of trapped quantum particles cooled down to extremely low temperatures, where the lack or the slow down of thermalization is also observed [6–8]. In the current literature, the FPU phenomenology is referred to as *pre-thermalization* [9, 10].

Nowadays, it is quite well understood that, at least on the classical side, no paradox exists at all, the FPU problem being a manifestation of closeness to (nonlinear) integrability, when the energy is low and the observation time is not long enough, which means a matter of separation of time-scales; see for example [11–17]. More precisely, denote by q_i the displacement of the i -th particle from its reference equilibrium position (the crystal configuration), and let $\phi(\xi)$, $\xi = q_{i+1} - q_i$, be the interaction potential between nearby particles. A common way (started by FPU) to express ϕ for small ξ is

$$\phi(\xi) = \frac{\xi^2}{2} + \alpha \frac{\xi^3}{3} + \beta \frac{\xi^4}{4} + \gamma \frac{\xi^5}{5} + \dots, \tag{1}$$

with suitable constants α, β and so on. Now, as pointed out in [18], widely developed in [19], and reconsidered in recent years for example in [12–15], the Toda exponential potential

$$\mathcal{T}(\xi) = \frac{e^{\lambda\xi} - \lambda\xi - 1}{\lambda^2} \tag{2}$$

for $\lambda = 2\alpha$ has a contact of order three with ϕ . But the Toda chain is an integrable Hamiltonian system [18–22], so it is interesting to rewrite

$$\phi(\xi) = \mathcal{T}(\xi) + (\beta - \beta_T)\xi^4 + \dots, \quad \beta_T = \frac{1}{6}\lambda^2 = \frac{2}{3}\alpha^2,$$

and consider the particle chain at hand as a perturbation $O(\xi^4)$ of the integrable Toda chain [12, 15, 23], rather than a perturbation $O(\xi^3)$ of the harmonic chain. Since in typical non-localized states (equilibrium, or excitation of some bunch of modes) it is $q_{i+1} - q_i \sim \sqrt{\varepsilon}$, where $\varepsilon = E/N$ is the specific energy of the system (the ratio of the total energy E to the number of particles N), the particle chain (1) is ε -close to Toda, and only $\sqrt{\varepsilon}$ -close to the harmonic chain.

Having in mind Toda as the reference integrable system, the scenario is as follows. On short terms, the dynamics of the nonlinear chain stays close to the Toda dynamics: trajectories run on the Toda torus corresponding to the same initial data, phases fill ergodically the torus, while the motion transversal to tori is negligible. Normal modes apparently interact, producing in particular the strange energy distribution originally observed by FPU, but this is in a sense an illusion due to the difference between linear normal modes and conserved nonlinear Toda actions, and has nothing to do with thermal equilibrium. On a much larger time scale the drift transversal to tori gets important, and diffusion in the whole phase space, eventually leading to thermalization, does occur. Time scales are inverse powers of ε , so are well separated for small ε : for the standard FPU model, already on times $O(\varepsilon^{-3/8})$ the nonuniform energy distribution observed by FPU (the apparent paradox) starts to be evident [24, 25], while times $O(\varepsilon^{-5/2})$ look necessary to observe full diffusion [12]. An intermediate time scale also exists, namely the Lyapunov time (the inverse of the maximal Lyapunov exponent), see [13, 15, 26]; however, on such a time scale the diffusion of actions is not affected, since chaos turns out to be tangent to tori. So, if the observation time is sufficiently large, the FPU

paradox disappears, and in general, pre-thermalization scenarios turn out to be a matter of interplay between observation time and dynamical time-scales of the given physical system.

The order of contact between the pair potential (1) and the Toda potential (2) can be increased of course by choosing $\beta = \beta_T$ and possibly $\gamma = \gamma_T = \alpha^3/3$ and so on. Similar exotic choices of the potential obviously lengthen the pre-thermal scenario and the thermalization times [11, 27]. Another possibility to approach Toda would be considering coefficients $\beta, \gamma \dots$ depending on a parameter, in such a way that in a convenient limit they all suitably converge to the corresponding Toda values. Similar potentials might appear even more artificial and exotic: why should physical potentials share such a bizarre property?

In this paper we address precisely this problem, and show that, somehow unexpectedly, this latter possibility is not at all bizarre, but is the case of a class of molecular potentials among the most used ones, namely the Mie–Lennard-Jones potentials, and the limit in question is that of hard-core repulsion. This means that the above outlined FPU scenario, with its quite long pre-thermalization times and well separated time scales, is realistic and relevant to physics.

The Mie–Lennard-Jones (MLJ) potentials are known to model the short-range interaction between neutral atoms or molecules [28, 29]. A possible expression is

$$\Phi_{nm}(r) = \frac{\epsilon_0}{n-m} \left[m \left(\frac{a}{r} \right)^n - n \left(\frac{a}{r} \right)^m \right], \quad (3)$$

where r denotes the inter-particle distance, $r = x_{i+1} - x_i > 0$ in dimension one, a is the zero-pressure equilibrium distance, i.e. $\Phi'_{nm}(a) = 0$, and $\Phi_{nm}(a) = -\epsilon_0$ is the depth of the potential well, whereas m and $n > m$ are positive integers. As is well known, the exponent m rules the attractive part of the potential due to Van der Waals charge fluctuation forces, its value ranging from 6 to 7 depending on whether electromagnetic retardation effects are taken into account [30]. In the present paper we treat m as a not much relevant parameter (as remarked below, we might also allow for more general attractive tails). On the other side, the exponent n , which rules the repulsive part of potential (3) due to the Pauli exclusion principle, cannot be determined from first principles, and should be just chosen large enough to fit the experimental data on cohesion energies [31, 32]. It is then natural to explore the limit $n \rightarrow \infty$ in order to see whether an asymptotic, universal form of the interaction somehow emerges. Such a limit amounts to model the repulsion between nearby atoms with a hard-core barrier.

Results, in short. In the present paper we show that, if the potential Φ_{nm} is rescaled around the minimum (via an affine transformation) and put in a “normal form” V_{nm} such that the minimum is in the origin, the second derivative (determining the time scale) is one, and the third derivative (determining the energy scale)¹ fits the chosen value λ entering (2), then it is $V_{nm} = T + O(1/n)$. Correspondingly, in the phase space there is an affine canonical transformation depending on the free parameter λ , which maps the Hamiltonian of the particle chain with pairwise potential (3) into a new Hamiltonian which is $1/n$ -close to the integrable Toda Hamiltonian.

Remark (*Toda and hard spheres: Hénon’s view*). Ref. [21], by M. Hénon, is one of the three almost simultaneous papers proving integrability of the Toda chain. It is a short paper, in which the author does not explain how he did guess the form of the integrals of motion. This was explained by him during a lecture in Nice, which one of us attended. The idea was writing

¹ For a harmonic system, motions on any constant energy surface are similar to each other up to a trivial length rescaling, so a natural energy scale does not exist. Similarity is instead broken if the third derivative is different from zero. If λ is the third derivative at equilibrium, the dominant term at small ϵ is $\lambda\sqrt{\epsilon}$; in this sense we say the third derivative determines the energy scale. The parameter ϵ_0 in MLJ is also a reference energy, but has a different meaning (a binding energy), is not immediately connected to the dynamics in the bottom of the potential well, and does not exist in general for potentials like (1) or (2).

down the integrals of motion for the hard-sphere gas, which do not include potential energy and can be written as convenient extensive combinations of velocities, and then understanding how to compensate the lack of constancy of velocities, for the exponential potential, by suitable mixed terms (containing products of exponentials and velocities). Details are not relevant to our purposes, but it is remarkable that, in the Hénon thought, the Toda model was considered to be a perturbation of the hard-sphere gas (see also [22], line 12). Having this in mind, it is not as surprising that MLJ potentials, in the limit of hard-core repulsion, get close to Toda, and a window opens to possible generalizations.

2 The Normal form of the MLJ Potentials

2.1 Rescaling Potentials

Putting a potential in normal form, as outlined above, is not specific of MLJ. Consider the class of analytic functions $f(r)$ which display a generic minimum, namely are such that, for some a ,

$$f^{(1)}(a) = 0, \quad f^{(2)}(a) > 0, \quad f^{(3)}(a) \neq 0, \tag{4}$$

where $f^{(j)}$, $j \geq 1$, denotes the j -th derivative of f . We say that two functions f and \tilde{f} are *equivalent*, if they differ just by the scale, more precisely, if they are brought one into the other by an affine transformation:

$$\tilde{f}(\xi) = Af(C\xi + D) + B; \quad A > 0, \quad C \neq 0. \tag{5}$$

Such transformations form a group, and the class of functions defined above gets partitioned into equivalence classes. The transformed function \tilde{f} will be said to be the λ -*normal form* of f (shortly *normal form*), if the minimum is carried to the origin and the second and third derivatives are normalized:

$$\tilde{f}(0) = 0, \quad \tilde{f}^{(1)}(0) = 0, \quad \tilde{f}^{(2)}(0) = 1, \quad \tilde{f}^{(3)}(0) = \lambda. \tag{6}$$

The following Lemma is easily proved:

Lemma *For any f as above there exists an affine transformation (5) which gives the transformed function \tilde{f} the normal form (6). Explicitly it is*

$$\tilde{f}(\xi) = \frac{f(a + \lambda f^{(2)}(a)\xi / f^{(3)}(a)) - f(a)}{\lambda^2 [f^{(2)}(a)]^3 / [f^{(3)}(a)]^2} = \frac{\xi^2}{2} + \lambda \frac{\xi^3}{6} + \sum_{j \geq 4} k_j \lambda^{j-2} \frac{\xi^j}{j!}, \tag{7}$$

with

$$k_j = \frac{[f^{(2)}(a)]^{j-3}}{[f^{(3)}(a)]^{j-2}} f^{(j)}(a). \tag{8}$$

If in addition $f(r) = cg(r/a)$ with $g(1) = -1$, then (7) and (8) become

$$\tilde{f}(\xi) = \frac{g(1 + g^{(2)}(1)\xi / g^{(3)}(1)) + 1}{[g^{(2)}(1)]^3 / [g^{(3)}(1)]^2} \tag{9}$$

and

$$k_j = \frac{[g^{(2)}(1)]^{j-3}}{[g^{(3)}(1)]^{j-2}} g^{(j)}(1). \tag{10}$$

The last statement is clearly adapted to MLJ, since $\Phi_{nm}(r) = \varepsilon_0 g_{nm}(r/a)$ with

$$g_{nm}(\rho) = \frac{1}{n - m} (m\rho^{-n} - n\rho^{-m}) . \tag{11}$$

Proof The four constants A, B, C, D are promptly determined so as to fit the four requirements (6); expressions (7) and (8) are immediate as well. Expression (9) and (10) obviously follow from (7) and (8), using $f^{(j)}(r) = ca^{-j}g^{(j)}(r/a)$. \square

Remark (on the peculiarity of Toda potential). Each equivalence class is characterized by the sequence $\{k_j\}_{j \geq 4}$; the class of the Toda potential (2) has $k_j = 1$ for any $j \geq 4$. The Toda potential has another deep property, actually used in an essential way by Dubrovin [33] to show that the Toda chain is the unique nonlinear integrable chain (with nearest neighbours interaction). Let us extend the coefficient k_4 to the function $k_4(r)$, just by replacing a with r in (8). For Toda it is $k_4(r) = 1$ identically in r , and this characterizes Toda, namely imposing $k_4(r) = 1$ gives a differential equation that picks up the exponential.

2.2 The Main Result

The result we shall prove is the following:

Proposition Consider the MLJ potential Φ_{nm} , let V_{nm} be its normal form and let $k_{nm,j}$ be the coefficients entering the series expansion (7). For any fixed m and any fixed $j \geq 4$ it is

$$k_{nm,j} = 1 + O(1/n) . \tag{12}$$

For any fixed m and any fixed neighborhood I of the origin it is

$$V_{nm}(\xi) = \mathcal{T}(\xi) + O(1/n) , \tag{13}$$

uniformly for $\xi \in I$.

Proof It is just a computation. Using (10) with $g = g_{nm}$ as in (11), immediately gives

$$k_{nm,j} = \frac{(n + 1) \cdots (n + j - 1) - (m + 1) \cdots (m + j - 1)}{(n - m)(n + m + 3)^{j-2}} = \frac{n^{j-1}(1 + O(1/n))}{n^{j-1}(1 + O(1/n))} \tag{14}$$

and (12) follows. There is no uniformity in j , so this is not enough to get (13). From (9) and (11), however, we promptly obtain

$$V_{nm}(\xi) = \frac{\left(1 - \frac{\lambda\xi}{n+m+3}\right)^{-n} - \frac{n}{m} \left(1 - \frac{\lambda\xi}{n+m+3}\right)^{-m} + \frac{n}{m} - 1}{\lambda^2 \frac{n(n-m)}{(n+m+3)^2}} . \tag{15}$$

The denominator is clearly $\lambda^2 + O(1/n)$. The first term at the numerator, profiting of the very definition of the Euler number, gives $e^{\lambda\xi}(1 + O(1/n))$, while the remaining part of the numerator gives $-\lambda\xi - 1 + O(\xi/n)$. The conclusion follows. \square

Remark (on the tail of MLJ potentials). By following the proof, it clearly appears that the first term inside the square bracket entering the MLJ potential (3) produces, in the limit $n \rightarrow \infty$, the exponential $e^{\lambda\xi}$ entering Toda potential, while the second term provides the subtraction $-\lambda\xi - 1$. The power form of the former looks indeed essential to work out the exponential, while the detail of the latter looks not as relevant, and the subtraction $-\lambda\xi - 1$ is generally expected, since the normal form (for each n and in the limit) must satisfy (6). This means that

the precise expression of the attractive tail in MLJ is irrelevant, and in fact, it is a trivial matter to check that the power $(r/a)^{-m}$ can be replaced by any function $\varphi_m(r/a)$, independent of n , provided Φ_{nm} has a critical point in a ; for this it is enough $\varphi(1) = 1, \varphi^{(1)}(1) = -m$ (the critical point is automatically a minimum for large n).

Remark (on the limit at constant m/n). As a curiosity, we can study the normal form V_{nm} of the MLJ potential, as $n \rightarrow +\infty$, not at fixed m , but at fixed ratio $\delta = m/n < 1$. It is not difficult to see that

$$V_{n,\delta n}(\xi) \longrightarrow \frac{(1 + \delta)^2}{\lambda^2 \delta (1 - \delta)} \left[\delta e^{\frac{\lambda \xi}{1+\delta}} - e^{\frac{\delta \lambda \xi}{1+\delta}} + 1 - \delta \right]. \tag{16}$$

An interesting choice is $\delta = 1/2$, which gives

$$V_{n,n/2}(\xi) \longrightarrow \frac{9}{2} (e^{\lambda \xi/3} - 1)^2, \tag{17}$$

i.e. the Morse potential. For $\delta \rightarrow 0$, as is not surprising, the Toda potential is recovered.

2.3 Canonical Completion of the Normalization

The above normalization involves only the coordinates of the particles, but it naturally extends to momenta, also in the limit $n \rightarrow \infty$, so as to have a canonical transformation. The Hamiltonian of a particle chain with nearest neighbours potential (3) is

$$H(x, p) = \sum_{i=0}^{N-1} \left[\frac{p_i^2}{2m} + \Phi_{nm}(x_{i+1} - x_i) \right]; \tag{18}$$

to fix the ideas let us think of fixed ends, i.e. $x_0 = 0$ and $x_N = L$, with $L = Na$ so as to have zero pressure, and correspondingly $p_0 = p_N = 0$.

The canonical transformation can be divided into two steps. First, a translation followed by a rescaling of coordinates x_i, p_i and time variable t , namely

$$\begin{aligned} x_i &= a(i + Q_i), & p_i &= a\sqrt{m\Phi^{(2)}(a)} P_i, \\ t &= \sqrt{\frac{m}{\Phi^{(2)}(a)}} \tau, & H &= a^2\Phi^{(2)}(a) K(Q, P) + N\Phi_{nm}(a), \end{aligned}$$

which is canonical with valence $a^2\sqrt{m\Phi^{(2)}(a)}$; the new boundary conditions are $Q_0 = Q_N = 0, P_0 = P_N = 0$. The new Hamiltonian reads

$$K(Q, P) = \sum_{i=0}^{N-1} \left[\frac{P_i^2}{2} + \frac{\Phi_{nm}(a(1 + Q_{i+1} - Q_i)) - \Phi_{nm}(a)}{a^2\Phi_{nm}^{(2)}(a)} \right].$$

The second step consists in rescaling coordinates and momenta by a further factor $w = \lambda a^{-1} \Phi_{nm}^{(2)}(a) / \Phi_{nm}^{(3)}(a)$, namely

$$Q_i = w\zeta_i, \quad P_i = w\eta_i, \quad K = w^2\mathcal{H}(\zeta, \eta);$$

this is canonical with valence w^2 , and the new Hamiltonian \mathcal{H} is

$$\mathcal{H}(\zeta, \eta) = \sum_{i=0}^{N-1} \left[\frac{\eta_i^2}{2} + V_{nm}(\zeta_{i+1} - \zeta_i) \right] = \sum_{i=0}^{N-1} \left[\frac{\eta_i^2}{2} + \mathcal{T}(\zeta_{i+1} - \zeta_i) \right] + O(1/n).$$

Use has been made of (12) and (15). This proves that the Hamiltonian (18) is, up to a canonical normalization, $1/n$ -close to the integrable Toda one. Starting with a generalized MLJ potential, with a tail $\varphi_m(r/a)$ as discussed above, leads to the same conclusion.

3 Numerical Illustration

The purpose of this numerical section is to show quantitatively, and visually, how quickly, by increasing n at fixed m , the normalized MLJ potentials V_{nm} approach the Toda potential, and correspondingly, the dynamics gets close to integrable. Comparison will be made with the first polynomial approximations of Toda, denoted by \mathcal{T}_j , obtained by truncating the Taylor series of \mathcal{T} at order j . Concerning λ , we shall use $\lambda = -2$ (λ should be negative, if we wish the steeper wall of the Toda potential to stay on the left, as in MLJ potentials; $\lambda = -2$ corresponds to the quite common choice $\alpha = -1$ in FPU).

3.1 Some Coefficients

Preliminarily, let us give a glance at the values of the first few coefficients $k_{nm,j}$ entering the series expansion of V_{nm} . At small energy, the difference $V_{nm} - \mathcal{T}$ is dominated by the fourth order term; correspondingly, the most relevant quantity to look at is the difference $\Delta_4 = k_{nm,4} - 1$. From (14), that we met in the proof of the Proposition, it follows

$$\Delta_4 = \frac{2 - nm}{(n + m + 3)^2} .$$

Computation shows that already for the classical values $m = 6$ and $n = 12$, Δ_4 is rather small, namely $\Delta_4 \simeq -0.16$, and raising n/m to 4 or 8 lowers Δ_4 to -0.131 or -0.088 . Such values should be compared with the typical constants used in FPU studies. In the standard FPU language, it is

$$\Delta_4 = \frac{\beta}{\beta_T} - 1 = \frac{3\beta}{2\alpha^2} - 1 ;$$

common values of Δ_4 , deduced from typical values of α and β used in the literature, are much larger,² namely Δ_4 between 2 and 6 ($\Delta_4 = -2/3$ in the original FPU study, where $\beta = 0$). Concerning the next coefficient $k_{nm,5}$, a similar computation shows that the difference to 1 is $\Delta_5 \simeq 0.30$ already for $n = 12$, while in typical FPU papers the choice is $\gamma = 0$, that is $\Delta_5 = -1$. We see that even for not much large n , MLJ potentials are closer to integrability than typical FPU models. Figure 1 shows the behavior of Δ_j , $j = 4, \dots, 7$, for $m = 6$ and n/m up to 32.

3.2 The Shape of the Normalized Potential

Figure 2, left panel, shows how V_{nm} (colored curves) converges to \mathcal{T} (black curve) by increasing n at fixed $m = 6$; n grows there from 12 to 192 ($2m$ to $32m$), in geometric progression. The right panel exhibits, on the same scale, Toda and its truncations \mathcal{T}_j , $j = 3, \dots, 10$. The figure shows that, for example, for potential energy around 1, even the common $12 - 6$ MLJ potential approximates Toda much better than very exotic high order truncations

² This is not surprising, since larger Δ_4 accelerates the thermalization process and decreases the computational effort.

Fig. 1 The differences $\Delta_j = k_{nm,j} - 1$ vs. n/m , for fixed $m = 6$; $j = 4, \dots, 7$

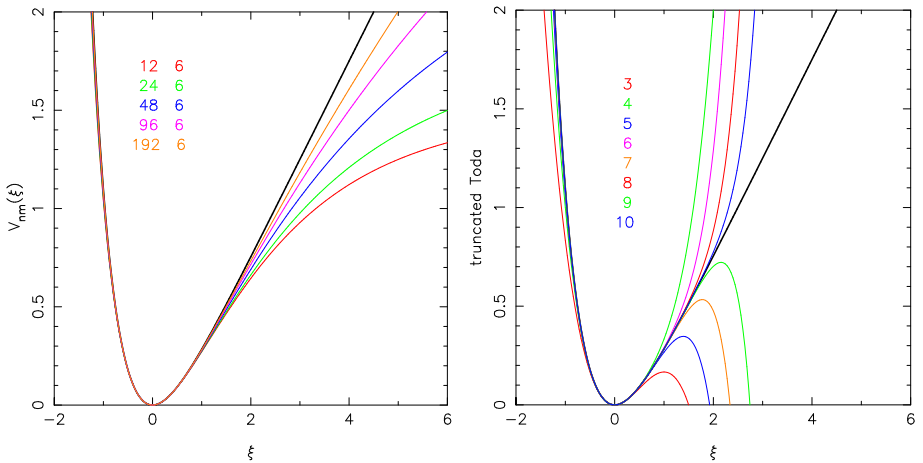
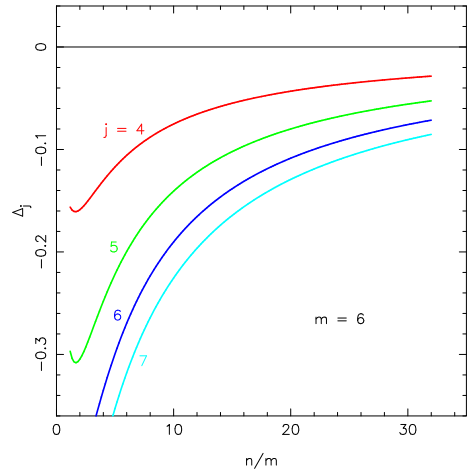


Fig. 2 Left panel: Toda potential \mathcal{T} (black) and normalized MLJ potential V_{nm} , for fixed $m = 6$ and $n = 12, 24, 48, 96, 192$ (bottom to top, colored curves); $\lambda = -2$. Right panel: Toda potential and its Taylor truncations \mathcal{T}_j , $j = 3, \dots, 10$

\mathcal{T}_j . The superiority becomes striking by growing energy. Let us stress that high energies can localize in a single bond, even at small specific energy, if the number of particles is large.

3.3 Dynamics: Three particles on a Ring

We come now to dynamics, and consider the model of three particles on a ring:

$$H(\zeta, \eta) = \sum_{i=0}^2 \left[\frac{\eta_i^2}{2} + V(\zeta_{i+1} - \zeta_i) \right],$$

with periodic boundary condition, baricenter at rest, two effective degrees of freedom. This model was used in the celebrated paper [20], with $V = \mathcal{T}$, to provide a strong numerical indication that the Toda model is integrable. The method, as is typical after [34] for systems

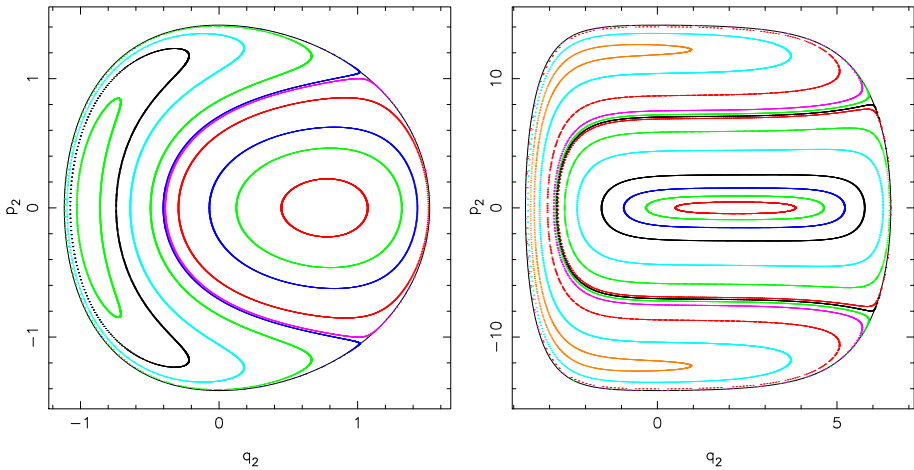


Fig. 3 The Poincaré section of the model of three particles on a ring, with Toda potential. Left panel $E = 1$, right panel $E = 100$

with two degrees of freedom, consisted in analyzing the Poincaré section. We do not provide details and refer to [20] for the choice of the Poincaré section and the coordinates on it; everything is indeed absolutely standard.

Figure 3, left panel, concerns the Toda model ($V = T$) and shows the Poincaré section for total energy $E = 1$. The right panel shows the same section for much higher energy $E = 100$. The absence of any chaotic region, no matter which is the value of E , convinced the scientific community that the Toda model was integrable, and prompted for mathematical proofs that soon arrived [18, 21, 22]. Figure 4 refers to Taylor truncations T_j of Toda, $j = 3, 4, 6, 8$ (see the labels inside panels), at energy $E = 1$. Let us recall that T_3 coincides with the celebrated Hénon-Heiles Hamiltonian, up to a trivial rescaling of energy by a factor 6 (the first panel is indeed the celebrated figure of Ref. [34], at $E = 1/6$). Figure 5 refers instead to the normalized MLJ potentials V_{nm} , for $m = 6$ and $n = 12$ (left), $n = 48$ (right; very similar), at energy $E = 1$. Not only, at this energy, the chaotic region is absent, but the similarity with Toda, already for $n = 12$, is striking. At high energy, even high order truncations of Toda behave completely differently from Toda; see Fig. 6, left panel, which represents the Poincaré section of T_{12} at $E = 100$. Instead, at the same energy, V_{nm} maintains an excellent similarity with Toda even for $m = 6$ and $n = 12$; see the right panel of the figure.

3.4 Lyapunov Exponents for Large N

Finally, we come to the dynamics for large N , actually $N = 1024$. The purpose is to quickly compare the dynamics of MLJ potentials V_{nm} , and of Toda truncations T_j , with the integrable Toda dynamics, using as an easy tool the Lyapunov exponents (for a recent extensive study of Lyapunov exponents in truncated Toda and other FPU models, see [13, 26]).

Consider any initial datum z in the phase space, let $F^t(z)$ be its evolution at time t , and for any tangent vector u in z , let $DF_z^t u$ be the evolved tangent vector. As is well known, the Lyapunov exponent $\chi(z, u)$ is defined as

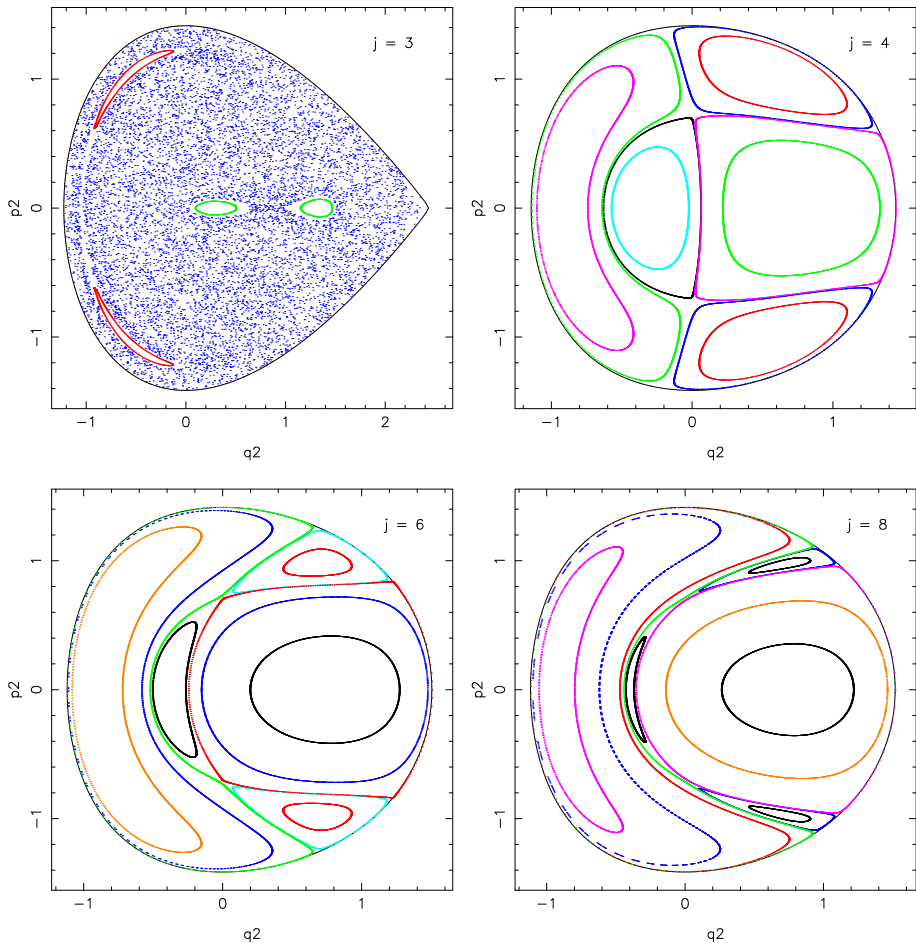


Fig. 4 The Poincaré section of the model of three particles on a ring, with truncated Toda potential T_j , $j = 3, 4, 6, 8$ (see the labels inside panels); energy $E = 1$

$$\chi(z, u) = \lim_{t \rightarrow \infty} \chi(t, z, u), \quad \chi(t, z, u) = \frac{1}{t} \log \frac{\|DF_z^t u\|}{\|u\|}.$$

For given z , essentially all vectors u provide in the limit one and the same value of $\chi(z, u)$, namely the maximal one. In fact, very quickly the finite time quantity $\chi(t, z, u)$ loses the dependence on u , so we shall disregard it. Unless there is fully developed chaos, the dependence on z is instead effective. Experience however shows [13] that taking an average even on a limited sample of points in phase space, smooths significantly the z dependence, and provides a reliable finite time indicator $\bar{\chi}(t)$. We shall average on 24 randomly chosen points, as in [13].

Our aim here is not to perform a complete study, but just to exemplify the theory, so we shall limit ourselves only to one value of the specific energy, namely $\varepsilon = 0.1$. Figure 7 shows $\bar{\chi}(t)$ vs. t for Toda (black), for FPU with $\beta = 2$ (blue) which has a contact of order 3 with Toda, for T_4 (pink) and T_6 (green); then for MLJ potentials V_{nm} with $m = 6$ and

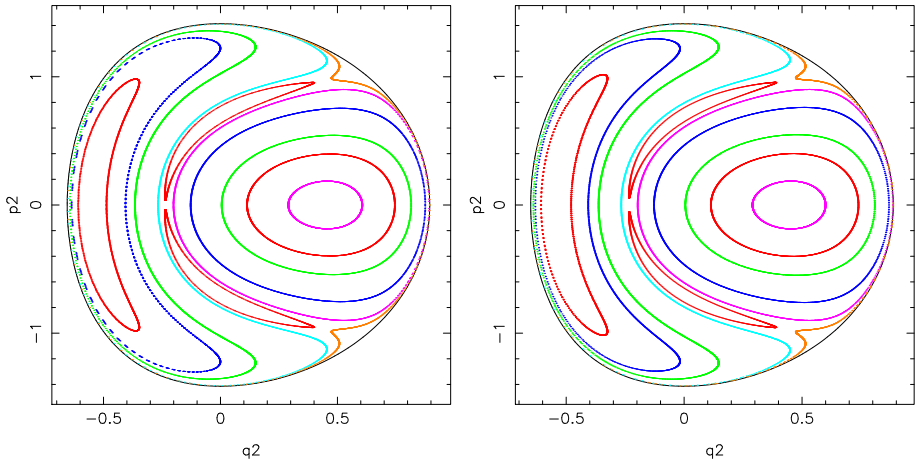


Fig. 5 The Poincaré section of the model of three particles on a ring, with normalized MLJ potential V_{nm} ; $m = 6$ and $n = 12$ (left) and 48 (right). Energy $E = 1$

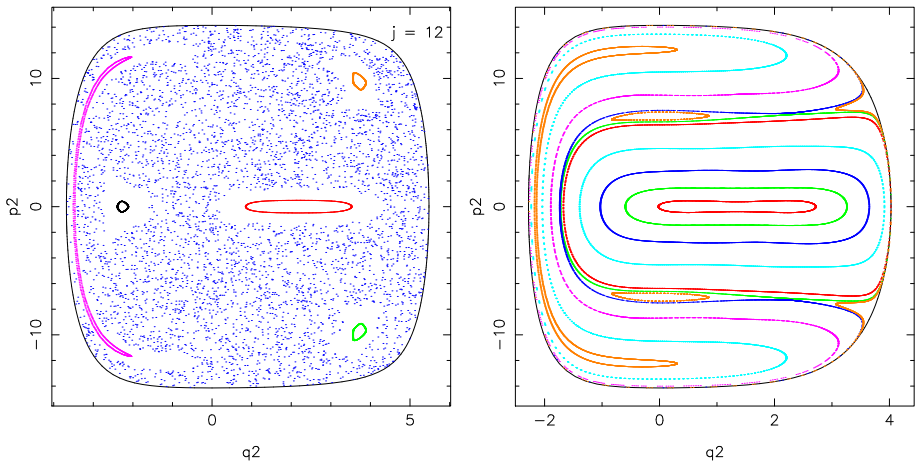
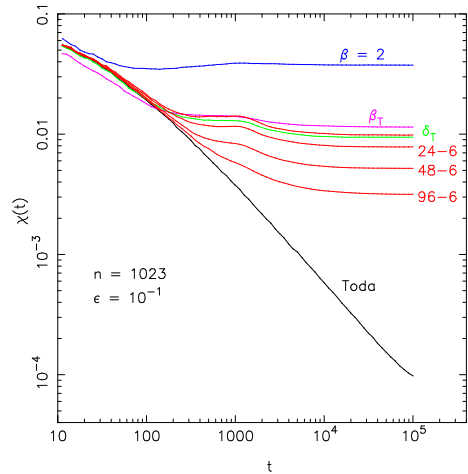


Fig. 6 The Poincaré section of the model of three particles on a ring, at high energy $E = 100$. Left: truncated Toda \mathcal{T}_{12} . Right: MLJ potential V_{nm} with $m = 6, n = 12$

$n = 12, 24, 48, 96$ (red; $n = 12$, almost coinciding with \mathcal{T}_6 , is not marked in the figure for lack of space).

For Toda, like for all integrable systems, $\bar{\chi}(t)$ goes to zero as $\log t/t$. The other models reach instead a nonzero limit. By increasing n , MLJ potentials V_{nm} follow Toda for a longer while. At this value of energy, even the $12 - 6$ MLJ approaches Toda better than standard FPU, and similarly to the rather exotic potential \mathcal{T}_6 . For lower energies, however, the situation gets complicated: the basic fact we aimed to illustrate, namely that by increasing n MLJ potentials approach better and better Toda, is observed, and moreover, even for low n they are closer to Toda than standard FPU. But higher order truncations \mathcal{T}_j , by lowering energy, become

Fig. 7 The finite time Lyapunov indicator $\bar{\chi}(t)$ vs. t , for Toda (black), FPU with $\alpha = -1$ and $\beta = 2$ (blue), truncations \mathcal{T}_4 and \mathcal{T}_4 of Toda (pink and green, respectively), then for MLJ potentials V_{nm} with $m = 6$ and $n = 12, 24, 48, 96$ (red) (Color figure online)



competitive, with a sort of cross-over. We do not think it is worthwhile to further investigate this point.

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Data Availability Data sharing is not applicable to this article as no datasets were generated or analysed during the current study.

Declarations

Competing interest The authors have no competing interests to declare that are relevant to the content of this article.

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