On the numerical integration of FPU–like systems

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Abstract

This paper concerns the numerical integration of systems of harmonic oscillators coupled by nonlinear terms, like the common FPU models. We show that the most used integration algorithm, namely leap–frog, behaves very gently with such models, preserving in a beautiful way some peculiar features which are known to be very important in the dynamics, in particular the “selection rules” which regulate the interaction among normal modes. This explains why leap–frog, in spite of being a low order algorithm, behaves so well, as numerical experimentalists always observed. On the same time, we show how the algorithm can be improved by introducing, at low cost, a “counterterm” which eliminates the dominant numerical error.

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1 Introduction

This paper is addressed to the wide community of researchers who are interested in numerical results for systems of many coupled harmonic oscillators. The model we shall explicitly take into consideration is the well known one-dimensional fixed-ends Fermi–Pasta–Ulam (FPU) α–model:

\[ H(q, p) = K(p) + V(q) , \quad K(p) = \sum_{i=1}^{n} \frac{p_i^2}{2} , \quad V(q) = \sum_{i=0}^{n} U(q_{n+1} - q_n) , \]  

where \( q_0 = q_{n+1} = 0 \) and

\[ U(x) = \Omega^2 \left( \frac{x^2}{2} + \alpha \frac{x^3}{3} \right) ; \]  

everything however extends in an obvious way to the β or α + β–models, to all common lattice models like Klein–Gordon or discrete \( \varphi^4 \) with any boundary conditions, as well as to their two or three–dimensional extensions; let us say to all systems of many harmonic oscillators, weakly coupled by nonlinear terms. A quick view to the very abundant literature on the subject, shows that in most papers, at least in the last decades, the algorithm used for the numerical integration is the so–called “leap–frog” (or Störmer–Verlet), namely the splitting algorithm

\[ \Psi_\tau = \Phi^{\tau/2}_K \circ \Phi^{\tau/2}_V \circ \Phi^{\tau/2}_K \]  

where \( \tau \) is the integration step and \( \Phi^t_K, \Phi^t_V \) denote the Hamiltonian flows of, respectively, \( K \) and \( V \); thanks to the fact that \( K \) depends only on \( p \) while \( V \) depends only on \( q \), implementing (3) is straightforward. The algorithm is only of order 2, that is

\[ \Psi_\tau - \Phi^\tau_H = O(\tau^3) , \]

nevertheless the common experience is that it works excellently.

It is not at all obvious why a simple algorithm like (3) behaves so well. Indeed the algorithm is symplectic, and this is well known to be a great advantage, but this is not enough to explain its performance. As shown in [1, 2] (see for an illuminating review and further results [3]), whenever a symplectic algorithm of order \( s \) is used to integrate a Hamiltonian system, what concretely happens is that the Hamiltonian \( H \) is replaced by a “modified Hamiltonian” (depending on the integration step and more generally on the chosen algorithm)

\[ H^m_\tau(p, q) = H(p, q) + \tau^s \Delta(p, q, \tau) , \]

with suitable regular \( \Delta \), and then the algorithm integrates \( H^m_\tau \) essentially exactly: precisely, a theorem states that

\[ \Psi_\tau(p, q) - \Phi^\tau_{H^m_\tau}(p, q) = O(e^{-\tau_s/\tau}) , \]

with some \( \tau_s > 0 \); practically, for very reasonable \( \tau \), the r.h.s. becomes (much) smaller than the round–off errors and as negligible as them (for a multi–precision numerical illustration of this game, see [4]).

Now, models like (1) have the structure

\[ H = H^0 + \alpha V^1 , \quad \text{with} \quad H^0 = K + V^0 , \]

\( V^j \) denoting the term of \( V \) of degree \( 2 + j \); \( \alpha V^1 \) is usually considered as a perturbation of \( H^0 \), actually as small as \( \alpha \sqrt{\varepsilon} \) where \( \varepsilon \) is the specific energy. In the following, to be definite, we shall
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think that $\alpha$ is small while $\varepsilon$ is of order one. Correspondingly, the modified Hamiltonian assumes the form

$$H^m = H^0 + \alpha V^1 + \tau^2 \Delta,$$  \hspace{1cm} (4)

and the evident risk appears that for small $\alpha$ the additional perturbation $\tau^2 \Delta$ due to the algorithm gets as important, or more important, than $\alpha V^1$: unless for small $\alpha$ the time step $\tau$ is suitably reduced, but such a need was never pointed out in the literature.

This is only one of the problems. Other delicate questions arise if we go more inside the structure of the Hamiltonian and look at its expression in terms of the linear normal modes. As is well known, the change of variables from $p, q$ to the normal mode variables $P, Q$ is

$$P_j = C \sum_{i=1}^{n} p_i \sin \frac{\pi i j}{n+1}, \quad Q_j = C \sum_{i=1}^{n} q_i \sin \frac{\pi i j}{n+1},$$

with $C = \sqrt{2/(n+1)}$; denoting (from here on) by $\tilde{F}(P, Q)$ the transformed of a generic function $F(p, q)$, so that

$$\tilde{H}(P, Q) = \tilde{H}^0(P, Q) + \alpha \tilde{V}^1(Q),$$

it turns out that both $\tilde{H}^0$ and $\tilde{V}^1$ have very peculiar properties, which are essential in the dynamics of the system and need to be saved in the modified Hamiltonian. Concerning $\tilde{H}^0$, it is

$$\tilde{H}^0(P, Q) = \frac{1}{2} \sum_{j=1}^{n} (P_j^2 + \omega_j^2 Q_j^2)$$

with dispersion relation

$$\omega_j = 2\Omega \sin \frac{\pi j}{2(n+1)}, \quad j = 1, \ldots, n;$$

the details of the dispersion relation are of great importance, since they determine the resonances in the problem and thus the energy exchanges among modes. In particular the acoustic resonance

$$j \omega_1 - \omega_j = O\left(\left(\frac{j}{n}\right)^3\right) = \Omega \frac{\pi^3}{24} \frac{j^3 - j}{(n+1)^3} + \left(\left(\frac{j}{n}\right)^5\right),$$

from the early studies by Izrailev and Chirikov [5] to the most recent papers on FPU (see for example the theoretical analysis in [6, 7]), has been shown to play an absolutely crucial role.

Concerning $\tilde{V}^1$, its expression is

$$\tilde{V}^1(Q) = \frac{1}{3} C \sum_{jlm=1}^{n} S_n(j, l, m) \omega_j \omega_l \omega_m Q_j Q_l Q_m,$$  \hspace{1cm} (7)

the “selector” $S_n$ being a sum of a few Kronecker $\delta$’s:

$$S_n(j, l, m) = \delta_{j+l, m} + \delta_{l+m, j} + \delta_{m+j, l} - \delta_{j+l+m, 2n+2}.$$

So, the overwhelming majority of the three–body interactions in the perturbation are switched off, and this is obviously a crucial fact in the dynamics.

It is not a priori evident if, and to which extent, the modified Hamiltonian preserves such essential features of the model. As a matter of fact, in the everyday practice of numerical experimentalists, leap-frog always appeared to work smoothly, and no difficulties, as far as we know,
have ever been raised: but clearly, something needs to be understood. This paper addresses these delicate questions, with a twofold purpose. On the one hand we show, by a direct analysis of the modified Hamiltonian produced by the leap–frog algorithm (3), why leap–frog behaves so gently; this is done in Section 2, where we recall some known results concerning $H_0$ and the dispersion relation, complete them, and then study the effect of leap–frog on the nonlinear part. On the other hand, in Section 3, we show how the leap–frog algorithm can be improved, at quite low cost, simply by adding to the FPU Hamiltonian $H$, in the particle coordinates, suitable easy “counterterms”. Section 4 is devoted to concluding remarks. We are confident our paper will be useful to strengthen the link between experts in numerical algorithms (who are not always aware of the subtle physical peculiarities the algorithms are expected to save) and experts in FPU (who are not always aware of the subtle details of geometrical integration).

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2 Analysis of the leap–frog

Let

$$k = \{., K\}, \quad v = \{., V\}, \quad h_r = \{., H^m_r\};$$

the modified Hamiltonian $H^m_r$ is implicitly defined, for leap–frog, by

$$e^{\tau h_r} = e^{\frac{\tau}{2} k} e^{\frac{\tau}{2} v} e^{\frac{\tau}{2} k}.$$

The Baker–Campbell–Hausdorff (BCH) formula, specifically its symmetric version which is obviously adapted to leap–frog, gives

$$h_r = k + v + \tau^2 h_2 + \tau^4 h_4 + \cdots ,$$

with [9]

$$h_2 = \frac{1}{24} [[k, v], k] + \frac{1}{12} [[k, v], v]$$

$$h_4 = -\frac{1}{360} [[[k, v], k], k] - \frac{1}{360} [[[k, v], k], k] + \frac{1}{120} [[[k, v], v], k]$$

$$+ \frac{1}{120} [[[k, v], v], v] + \frac{1}{360} [[[k, v], v], k] - \frac{1}{120} [[[k, v], k], v] ;$$

the commutators $[.,.]$ among operators turn into the Poisson brackets of the corresponding functions, and this leads quite easily to express the modified Hamiltonian in the form of an even series in $\tau^2$:

$$H^m_r = H + \tau^2 \Delta_2 + \tau^4 \Delta_4 + \cdots ;$$

in particular,

$$\Delta_2 = \frac{1}{24} \{K, V\} , K + 2V .$$

A further development in powers of $\alpha$ gives

$$H^m_r = H^0 + \tau^2 \Delta_2^0 + \tau^4 \Delta_4^0 + \cdots$$

$$+ \alpha V^1 + \alpha \tau^2 \Delta_2^1 + \cdots$$

$$+ \alpha^2 \tau^2 \Delta_2^2 + \cdots ,$$

\footnote{The literature on BCH is rather abundant; we found particularly useful [3] (chapter 3) and [8].}
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and from (11) it is

\[ \Delta_2^0 = \frac{1}{2!} \{ \{ K, V^0 \}, K + 2V^0 \} \]
\[ \Delta_2^1 = \frac{1}{2!} \{ \{ K, V^1 \}, K + 2V^0 \} + \frac{1}{2!} \{ \{ K, V^0 \}, V^1 \} . \]

All these relations are obviously independent of the chosen (canonical) coordinates, and hold in particular among the corresponding quantities expressed in the normal modes variables. In such coordinates the analysis gets trivial, and the result for \( \Delta_2^0 \) is

\[ \Delta_2^0(P, Q) = -\frac{1}{24} \sum_{j=1}^{n} \omega_j^2 (P_j^2 - 2\omega_j^2 Q_j^2) ; \]

 correspondingly, the modified unperturbed Hamiltonian \( \tilde{H}_r^0 \) (that is, \( H_r^m \) for \( \alpha = 0 \)) is

\[ \tilde{H}_r^0 = \frac{1}{2} \sum_{j=1}^{n} \left[ (1 - \frac{1}{12}\tau^2 \omega_j^2)P_j^2 + \omega_j^2 (1 + \frac{1}{6}\tau^2 \omega_j^2)Q_j^2 \right] + \mathcal{O}(\tau^4) . \]

This shows that the dominant term of the correction is very inessential, indeed:

i. \( \tilde{H}_r^0 \) remains quadratic, and moreover no coupling among different oscillators is introduced (quite clearly, any small coupling would have a strong impact in the dynamics).

ii. The only effect is a small change in the dispersion relation: the original frequencies \( \omega_j \) are indeed replaced by \( \tilde{\omega}_j \) given by

\[ \tilde{\omega}_j^2 = \omega_j^2 (1 - \frac{1}{12}\tau^2 \omega_j^2)(1 + \frac{1}{6}\tau^2 \omega_j^2) , \]

so that

\[ \tilde{\omega}_j = \omega_j \left( 1 + \frac{1}{24}\tau^2 \omega_j^2 + \mathcal{O}(\tau^4) \right) . \]

Quite clearly, for small \( \tau \) (compared to the \( \omega_j \)'s at hand) the resonance properties are essentially unaltered, and in particular the great acoustic resonance is practically not affected: indeed, a direct computation gives

\[ j\tilde{\omega}_j - \omega_j = \Omega \frac{\pi^3}{24} \frac{j^3 - j}{(n+1)^3} \left( 1 - \tau^2 \Omega^2 \right) + \mathcal{O} \left( \left( \frac{j}{n} \right)^5 \right) \]
\[ = (j\omega_j - \omega_j)(1 - \tau^2 \Omega^2) + \mathcal{O}((j/n)^5) , \]

so the “small divisor” \( j\omega_j - \omega_j \) is modified, at the dominant order, in a trivial way.

One might wonder about the corrections of order \( \tau^4 \) in \( \tilde{H}_r^0 \). Using (10), it is not difficult to find

\[ \tilde{\Delta}_4^0 = -\frac{1}{120} \sum_{j=1}^{n} \omega_j^4 (P_j^2 - 4\omega_j^2 Q_j^2) , \]

and the conclusions do not change. Apart from the precise values of the coefficients, the form (18) of \( \tilde{\Delta}_4^0 \) is quite obvious, since the Poisson brackets of quadratic functions remain quadratic, and do not mix different degrees of freedom; the presence of the coefficient \( \omega_j^4 \) in front of each term in (18) is clearly necessary for dimensional reasons. It is obvious as well that similar considerations hold at any order in \( \tau \).
Remark. We found convenient to produce this simple analysis for completeness and for later use, but the main point, namely the fact that leap–frog, for a set of harmonic oscillators, results in a shift of their frequencies — not only at first order in $\tau$, but as an exact result — is known in the literature, see for example [10, 11]; moreover ref. [12], devoted to FPU, includes (up to a typo) the dispersion relation (17).

It is worthwhile to continue the analysis of the dominant correction by translating $\hat{\Delta}^0_2$ into the original particle coordinates, i.e. by writing explicitly $\Delta^0_2$. Indeed a straightforward computation, made either by antitransforming $\hat{\Delta}^0_2$ or by directly computing the Poisson bracket in (13), gives the result

$$\Delta^0_2(p,q) = -\frac{1}{24} \Omega^2 \sum_{i=0}^{n} (p_{j+1} - p_j)^2 + \frac{1}{12} \Omega^4 \sum_{i=1}^{n} (q_{i+1} - 2q_i + q_{i-1})$$

(with $p_0 = p_{n+1} = 0$). This expression shows that the dominant effect of the correction entering the modified Hamiltonian $H^m_p$ is just the introduction of a next–nearest-neighbours coupling among coordinates and a nearest-neighbours coupling among momenta, with coefficients small as $\tau^2$. So, the leading correction preserves the locality of the interaction among particles, without introducing long range couplings among particles. A little reflection shows that the next correction $\Delta^1_2$ further increases the range of the interaction by one unity, and so on. Expression (19) will also be the starting point of the next Section 3.

We now come to the further (and crucial) question raised in the Introduction, namely how the correction to the Hamiltonian affects the structure of the interaction term $\hat{V}$, and specifically the selection rules expressed by $S_n$. Practically, this means looking at the structure of the correction term $\Delta^1_2$ in (12), or to its analog $\hat{\Delta}^1_2$ in the $P,Q$ variables. Using (14), the computation is easy; once more, the key element is the fact that $\hat{K}$ and $\hat{V}^0$ are quadratic, so that the Poisson bracket saves the order, and different degrees of freedom are not mixed. One easily finds

$$\{\hat{K}, \hat{V}^1\} = \left\{\frac{1}{2} \sum_{j=1}^{n} P_j^2, \frac{1}{3} C \sum_{jlm=1}^{n} S_n(j,l,m) \omega_j \omega_l \omega_m Q_j Q_l Q_m\right\}$$

$$= -C \sum_{jlm=1}^{n} S_n(j,l,m) \omega_j \omega_l \omega_m P_j Q_l Q_m ,$$

and then

$$\{\{\hat{K}, \hat{V}^1\}, \hat{K}\} = -2C \sum_{jlm=1}^{n} S_n(j,l,m) \omega_j \omega_l \omega_m P_j P_l Q_m .$$

Similarly one finds

$$\{\{\hat{K}, \hat{V}^1\}, \hat{V}^0\} = 2C \sum_{jlm=1}^{n} S_n(j,l,m) \omega_j^3 \omega_l \omega_m Q_j Q_l Q_m ,$$

and the conclusion is

$$\hat{\Delta}^1_2(P,Q) = 2C \sum_{jlm=1}^{n} S_n(j,l,m) \omega_j \omega_l \omega_m \left(-P_j P_l Q_m + 2\omega_j^2 Q_j Q_l Q_m\right) .$$

(20)

This shows that the selection rules (no matter which they are!) are preserved by the algorithm, as is required to save one of the most relevant features of the FPU Hamiltonian.
Figure 1: The relative error in energy conservation for the original Hamiltonian $H$ (left) and for the Hamiltonian $H_r$ corrected with counterterms (right), plotted versus $1/\tau$. The values of $\alpha$ are reported in the figure. The dashed lines in the left panel do not refer to $E$, but to the corrected energy $E'$, see the text. Parameters: $n = 512$, energy per particle 1; random initial data on the particle velocities.

3 Eliminating the dominant correction $\Delta^0_2$.

A well known way to improve the accuracy of an integration algorithm, is the so-called backward analysis (see [3] for a review). In a language more familiar to physicists, this means introducing “counterterms” in the original Hamiltonian, which exactly compensate the dominant correction entering the modified Hamiltonian, in such a way that the new modified Hamiltonian gets closer to the original one. Conceptually the idea is very simple, but practically there is a feasibility problem: the addition of the counterterms should not complicate too much the numerical algorithm. In particular, for FPU, the wish is that the Hamiltonian remains separate, and the number of operations per time step remains of order $n$.

In our case, the counterterm we can conveniently add to $H$ is the opposite of $\tau^2 \Delta^0_2$; this means integrating numerically, in place of $H$, the “pre-modified Hamiltonian”

$$H_r(p, q) = H(p, q) - \tau^2 \Delta^0_2(p, q).$$

The new modified Hamiltonian obviously looses the correction $\Delta^0_2$, and gets the structure

$$H^m_r(p, q) = H(p, q) + \tau^2 \alpha \Delta^1_2(p, q) + \tau^4 \Xi^0_4(p, q) + \cdots$$

(the term $O(\tau^4)$ is not the same as before). The expression (19) of $\Delta^0_2$ shows that (21) remains separate, and the number of operations per time step grows rather moderately; in fact, a test shows that the cpu–time increases by a factor (slightly less than) two.
The improved accuracy can be seen by looking at the energy conservation. Figure 1 refers to an FPU $\alpha$–model with $n = 512$; the left and right panels refer, respectively, to the original Hamiltonian $H$ and to the Hamiltonian with counterterms $\mathcal{H}_\tau$. The initial data are $q_i = 0$ and random $p_i$, $i = 1, \ldots, n$, normalized in such a way that the energy per particle is one. On the left panel, the solid line represents the maximal relative error $\delta E(t)/E(0)$ in the energy conservation, where $E(t) = H(p(t), q(t))$ and $\delta E(t) = E(t) - E(0)$, up to $t = 10^5$ (with $\Omega = 1$), plotted vs. $\tau^{-1}$; $\alpha$ here is $10^{-2}$. The “error” $\delta E$ just expresses the difference between $H$ and $H^m_\tau$, more precisely it is
\[
\delta E(t) = H(p(t), q(t)) - H^m_\tau(p(t), q(t)) + H^m_\tau(p(0), q(0)) - H(p(0), q(0)),
\]
and is dominated by
\[
\tau^2 (\Delta^0_2(p(t), q(t)) + \Delta^0_2(p(0), q(0)) ;
\]
correspondingly, the slope $\gamma$ of the line is 2 (a numerical best fit gives $\gamma = 2.00$). The dominant correction clearly disappears if, in place of $E = H(p, q)$, we measure $E' = E + \tau^2 \Delta^0_2(p, q)$, which is constant up to
\[
\alpha \tau^2 \Delta^1_2 + \tau^4 \Delta^0_4 + \cdots
\]
For $\alpha = 10^{-2}$ and $\tau$ in the range appearing in the figure, the former term dominates, and $\gamma$ remains 2 (the computation gives $\gamma = 2.02$): see, in the same panel, the upper dashed line, interpolating the squares. For $\alpha = 0$, instead, the latter term obviously dominates, and the slope becomes 4 (the numerical value is $\gamma = 3.98$); see the lower dashed line, interpolating the small dots. For $\alpha$ in between, by lowering $\tau$ one observes a crossover from one behavior to the other; see the circles and triangles, without interpolating line, which refer respectively to $\alpha = 10^{-3}$ and $10^{-4}$.

The right panel refers to the numerical integration of $\mathcal{H}_\tau$, but the computed energy is $E = H(p, q)$. Thanks to the counterterms, the previously dominating term $\tau^2 \Delta^0_2$ is not present anymore, and the error $\delta E$, which is plotted in the figure (normalized to $E(0)$), is expected to be as large as
\[
\alpha \tau^2 \Delta^1_2 + \tau^4 \Xi^0_4 + \cdots
\]
For not too small $\alpha$, the dominant contribution to $\delta E$ is the former, and this is shown by the three lines in the figure, interpolating squares, circles and triangles, which refer respectively to $\alpha = 10^{-2}$, $10^{-3}$ and $10^{-4}$. The computed slope is effectively 2 (numerical values: 2.02, 2.00 and 2.00); it could also be seen that at fixed $\tau$ the error is, as expected, proportional to $\alpha$. For $\alpha = 0$, the expected $\delta E$ is $O(\tau^4)$, but this is not revealed by the numerics: indeed the computed slope is not 4, but 6, see the lowest line in the figure interpolating the dots (the numerical value is $\gamma = 6.00$). This surprised us, till we understood the reason after writing, on the basis of the symmetric BCH (10), the exact form of $\Xi^0_4$ in (22). The computation is more easily done in the $P, Q$ variables, and the result is
\[
\Xi^0_4 = - \frac{1}{120} \sum_{j=1}^n \omega_j (P_j^2 + \omega_j^2 Q_j^2) ;
\]
correspondingly it is
\[
\mathcal{H}^m_\tau(P, Q) = \frac{1}{2} \sum_{j=1}^n \left( 1 + \frac{\tau^4 \omega_j^4}{60} \right) (P_j^2 + \omega_j^2 Q_j^2) + O(\tau^6)
+ \alpha V^1 + \alpha \tau^2 \Delta^1_2(P, Q) + O(\alpha \tau^4).
\]
Quite clearly, for vanishing $\alpha$, the energies $\frac{1}{2} (P_j^2 + \omega_j^2 Q_j^2)$ of the different degrees of freedom are separately constant, and consequently $\mathcal{H}^m_\tau$ is constant up to order $\tau^6$, as numerical computations...
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correctly make evident. The very minor correction $1 + \tau^4 \omega_j^4/60$ in (23) results in a very negligible change of frequency of the different oscillators. In the $p, q$ coordinates, the correction $\tau^4 \Xi_4^0$ corresponds to a coupling among third neighbours for the particle positions, and among second neighbours for their momenta. A corresponding counterterm of fourth order in $H$ would eliminate this term too from the modified Hamiltonian, at not too large computational cost: nevertheless, introducing a similar correction is, in our opinion, useless.

4 Concluding remarks

A. Other models. It should be clear that all considerations we made in Sections 2 and 3 extend in a trivial way to all FPU–like models. Consider for example the $\beta$ model, i.e. the model with $U(x) = \Omega^2 (x^2/2 + \beta x^4/4)$ in place of (2). Concerning $\Delta_0^2$ and $\Delta_1^0$, they do not depend on the nonlinearity, and thus such corrections, as well as the counterterm eliminating $\Delta_0^0$, do not change. Concerning the correction to the interaction term $\tilde{V}(Q)$, let us recall that for the $\beta$ model it is

$$\tilde{V}(Q) = \frac{1}{4} C^2 \sum_{jlmr=1}^n S_n(j, l, m, r) \omega_j \omega_l \omega_m \omega_r Q_j Q_l Q_m Q_r,$$

the selector $S_n$ being a natural generalization of (8) which is not worthwhile to write in detail; the rather obvious result is that, for such a model, the expression (20) of $\tilde{\Delta}_1^2(P, Q)$ is replaced by

$$\tilde{\Delta}_1^2(P, Q) = 3C \sum_{jlmr=1}^n S_n(j, l, m, r) \omega_j \omega_l \omega_m \omega_r (-P_j P_l Q_m Q_r + 2 \omega_j^2 Q_j Q_l Q_m Q_r),$$

and the conclusions do not change. The extension to models where $U$ is a full series, like the Lennard–Jones model, is trivial as well.

Other models, like Klein–Gordon, have a different dispersion relation and consequently different resonances among oscillators; but clearly, (16) continues to hold, and the dispersion relation, whatever it is, remains nearly unchanged. The other considerations (observing that the form of (19), and consequently the counterterm, is independent of the dispersion relation) are not affected.

Finally, we remark that the extension to higher dimensional models, as for example those studied in [13] or in [14], does not deserve relevant novelties, even for the nonperiodic models studied in [13] for which the normal modes are not known analytically. For what concerns $\Delta_2^0$, giving the frequency shift and the counterterms, the normal modes coordinates are not necessary to compute the Poisson brackets. An easy computation shows that in general, if the quadratic part of the potential is

$$V^0(q) = \frac{1}{2} \sum_{ij=1}^n v_{ij} q_i q_j$$

(with $v$ symmetric), then

$$\Delta_2^0(p, q) = -\frac{1}{12} \sum_{ij=1}^n v_{ij} p_i p_j + \frac{1}{6} \sum_{ij=1}^n (v^2)_{ij} q_i q_j.$$

This generalizes (19) and shows that in any case $\Delta_2^0$ produces a shift of order $\tau^2$ to the frequencies, and nothing else; moreover (as is important to use the opposite of $\Delta_2^0$ as counterterm) the interaction, if short range, remains short range.
Concerning instead the selection rules in the coupling among normal modes, let us observe that even if the normal modes coordinates \( P, Q \) cannot be explicitly written, they nevertheless do exist and give the Hamiltonian \( \tilde{H}(P, Q) \) the form (5), with \( \tilde{H}^0 \) as in (6) and nonlinear term as in (7), for some \( S_n \). The above analysis then applies, leading in any case to \( \Delta_2^1 \) of the form (20); this shows that the selection rules, whatever they are, are preserved. The generalization to nonlinearities higher than cubic is straightforward.

B. Yoshida algorithms. As first observed in [9], by suitably composing three second–order steps of the form (3) it is possible to obtain a fourth–order algorithm; the rule is

\[
\Psi^{(4)}_r = \Psi r_{1\tau} \circ \Psi r_{2\tau} \circ \Psi r_{1\tau},
\]

with

\[
\gamma_1 = \frac{1}{2 - 2^{1/3}}, \quad \gamma_2 = -\frac{2^{1/3}}{2 - 2^{1/3}}.
\]

Similar algorithms are not much diffused among numerical experimentalists on FPU, but have been occasionally used as for example in [13, 7]. For such algorithms, (12) is replaced by

\[
H^m_r = H^0 + \alpha V^1 + \alpha^2 \Delta_4^1 + \cdots
\]

and an analysis similar to the one exhibited in sections 2 and 3 can be performed, using carefully the symmetric BCH formula.

Concerning the dominant term \( \Delta_4^0 \), or better the corresponding term \( \tilde{\Delta}_4^0 \) in the normal modes coordinates, the result, skipping details, is

\[
\tilde{\Delta}_4^0 = \sum_{j=1}^n \omega_j^4 (\lambda_p p^2_j + \lambda_q q^2_j),
\]

with

\[
\lambda_p = -\frac{1}{120} (2\gamma_1^5 + \gamma_2^5), \quad \lambda_q = \frac{1}{120} (2\gamma_1^5 + \gamma_2^5) + \frac{1}{12} \gamma_1 \gamma_2 (\gamma_1 + \gamma_2)^2 (\gamma_1 - \gamma_2).
\]

The obvious conclusion is that the dispersion relation and all resonances remain almost unchanged.

Concerning instead the interaction term \( \alpha^4 \Delta_4^1 \), it should be evident that it is the sum of a certain number of terms, each of them being a suitable chain of nested Poisson brackets involving \( K, V^0 \) and \( V^1 \), with just one \( V^1 \). But clearly, \( K \) and \( V^0 \) being quadratic, any Poisson bracket simply replaces one of the \( Q_s \)’s in \( V^1 \) by the corresponding \( P_s \), \( s = j,l,m \), or conversely turns one of the \( P_s \) back in the corresponding \( Q_s \), without ever mixing the degrees of freedom. This implies that the selection rules in any case are preserved.

Finally, the form (24) of \( \tilde{\Delta}_4^0 \), with \( \omega_j^4 \) in front of \( P_j^2 \) and \( \omega_j^6 \) in front of \( Q_j^2 \), shows that the corresponding term \( \Delta_4^0 \) in the \( p,q \) coordinates includes (as is not surprising) second neighbours interaction for the momenta and third neighbours interaction for the positions. Suitable counterterms could be introduced to eliminate this term, so as the dominant correction in the modified Hamiltonian gets proportional to \( \alpha \). We do not enter the details.

C. Resonant normal form and KdV equation. It is well known, since the seminal paper [15], that the dynamics of the \( \alpha \)–model, for long wavelength initial conditions, is well modeled by the
Korteweg-de Vries (KdV) equation. Quite recently, a very precise relation between KdV and \( \alpha \)-model has been drawn [7], namely the Fourier-Galerkin truncation of order \( n \) of a suitable KdV equation is the leading order resonant normal form for the \( \alpha \)-model; moreover, on the basis of such analysis, some peculiar properties of the FPU dynamics have been deduced, and the results have been tested numerically with very good agreement. The natural question arises, whether the modified Hamiltonian \( H^m r \), as produced by the numerical integration, does maintain the same relation with KdV. Without entering the details, let us stress here that the answer is affirmative. The point is that the term \( \tau^2 \Delta^0_2 \), entering \( H^m r \), has the only effect of multiplying the dispersion coefficient in the KdV equation by a factor \( (1 - \tau^2 \Omega^2) \), close to one if \( \tau \) is small, while the term \( \alpha \tau^2 \Delta^1_2 \) goes into the remainder of the perturbation construction leading to the normal form, so that the normal form is not affected. No other changes are introduced.

References


