Stability of simple periodic orbits and chaos in a Fermi-Pasta-Ulam lattice

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We investigate the connection between local and global dynamics in the Fermi-Pasta-Ulam (FPU) β model from the point of view of stability of its simplest periodic orbits (SPO's). In particular, we show that there is a relatively high-q mode [$q=2(N+1)/3$] of the linear lattice, having one particle fixed every two oppositely moving ones (called SPO2 here), which can be exactly continued to the nonlinear case for $N=5+3m$, $m=0,1,2,\ldots$, and whose first destabilization E_{2u}, as the energy (or β) increases for *any* fixed N, practically *coincides* with the onset of a "weak" form of chaos preceding the breakdown of FPU recurrences, as predicted recently in a similar study of the continuation of a very low ($q=3$) mode of the corresponding linear chain. This energy threshold per particle behaves like $\frac{E_{2u}}{N}\propto N^{-2}$. We also follow exactly the properties of another SPO [with $q=(N+1)/2$] in which fixed and moving particles are interchanged (called SPO1 here) and which destabilizes at higher energies than SPO2, since $\frac{E_{1u}}{N}\propto N^{-1}$. We find that, immediately after their first destabilization, these SPO's have different (positive) Lyapunov spectra in their vicinity. However, as the energy increases further (at fixed N), these spectra converge to the *same* exponentially decreasing function, thus providing strong evidence that the chaotic regions around SPO1 and SPO2 have "merged" and large-scale chaos has spread throughout the lattice. Since these results hold for N arbitrarily large, they suggest a direct approach by which one can use local stability analysis of SPO's to estimate the energy threshold at which a transition to ergodicity occurs and thermodynamic properties such as Kolmogorov-Sinai entropies per particle can be computed for similar one-dimensional lattices.

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I. INTRODUCTION

The transition to widespread chaos in Hamiltonian systems of many degrees of freedom has been the subject of intense investigation for more than 50 years; see, e.g., Refs. [1–4]. It received great impetus following the pioneering work of Fermi, Pasta, and Ulam (FPU) [5], who were the first to study thermalization in one-dimensional lattices of N particles, with linear and nonlinear nearest-neighbor forces, as a parameter multiplying the nonlinear terms in the equations of motion becomes greater than zero. Surprisingly, they observed that when this parameter is relatively small, energy equipartition does *not* occur even after very long integration times, as only a small number of (low-q) modes of the corresponding linear lattice recurrently exchange the total energy among them. Of course, when the nonlinearity or the energy exceeds a certain threshold, these so-called FPU recurrences break down, large-scale chaos prevails, and a type of ergodicity sets in, whereby almost every orbit explores almost all of the available phase space of the system.

One of the first attempts to explain this phenomenon is due to Izrailev and Chirikov [6], who argued that the breakdown of FPU recurrences is related to the overlap of major resonances known to lead to large-scale chaos in N-degrees-of-freedom Hamiltonian systems [7]. As was later realized, however, a weaker form of chaos caused by the interaction of the first few FPU modes (with low q in Fourier space) appears to be sufficient for equipartition among all modes to occur [8,9]. Finally, very recently, Flach and coworkers [10] discovered that this transition to so-called "weak" chaos, in fact, coincides with the first destabilization of one of the lowest ($q=3$) normal mode of the linear lattice, as is continued by increasing the nonlinearity parameter. In fact, their results apply more generally to the lowest $q\ll N$ modes which also turn out to be highly localized in q space. These nonlinear modes represent examples of what we call simple periodic orbits (SPO's), where all particles return to their initial condition after only one oscillation; i.e., all their mutual rotation numbers are unity [11]. Such lowest-q-mode SPO's were actually termed q breathers due to their exponential localization in Fourier space [10].

In this paper, we investigate further the connection between local and global dynamics of the FPU lattice by studying the stability properties of its SPO's. In particular, we consider the FPU Hamiltonian

$$H=\frac{1}{2}\sum_{j=1}^{N}\dot{x}_j^2+\sum_{j=0}^{N}\left(\frac{1}{2}(x_{j+1}-x_j)^2+\frac{1}{4}\beta(x_{j+1}-x_j)^4\right)=E, \tag{1}$$

often called the FPU β model, as it only contains the term with quartic nonlinearities. The x_j represents the displacement of the jth particle from its equilibrium position, $\dot{x}_j$ is the corresponding velocity, β is a positive real constant, and E is the total energy. As with the original FPU problem, we will concern ourselves only with fixed boundary conditions, whereby particles with index $j=0,N+1$ are stationary for all time.

In particular, we will examine an SPO which keeps every *third* particle fixed, while the two in between are performing exactly opposite motions. This mode was studied in Ref. [12] where its stability was analyzed by means of Mathieu equations and has also been discussed in Ref. [13] in connection with the occurrence of sinusoidal waves in nonlinear lattices. This solution, called SPO2 from here on, will be compared to an orbit we call SPO1, which keeps every two particles fixed, with the ones in between executing exactly opposite oscillations. This latter one was originally mentioned in a paper by Ooyama *et al.* [14] and later studied analytically by Budinsky and Bountis [15] to determine its stability properties in the thermodynamic limit of large N and E with $\frac{E}{N}$ fixed. Recently, it was reexamined by Antonopoulos *et al.* [11], in a study of different SPO's and different Hamiltonians, from the viewpoint of connecting their local and global stability properties.

Our first result about the SPO2 orbit is that the energy per particle of its first destabilization goes to zero *faster* than SPO1, by a law $\frac{E_{2u}}{N} \propto N^{-2}$, in contrast to the SPO1 orbit whose law is $\frac{E_{1u}}{N} \propto N^{-1}$ as $N \to \infty$ [11,15]. This implies that if chaos is to spread in the nonlinear lattice as a result of the destabilization of SPO's, it might be more useful to look closely at the properties of SPO2, as that becomes unstable much earlier than SPO1, as N increases.

Remarkably enough, when we do this we discover that the energy (or β) values of the first destabilization as a function of N practically coincide with those found by Ref. [8,9] for the transition to "weak" chaos and Ref. [10] for destabilization of the $q=3$ mode. Our numerical results and their analytical formula are in excellent agreement.

We then examine the dynamics in more detail, following the first destabilization of SPO1 and SPO2 at $E=E_{1u}$ and $E=E_{2u}$, respectively, at high enough N. In particular, we choose initial conditions in the vicinity of these orbits and find that the (positive) Lyapunov exponents, at energies just above E_{1u} and E_{2u}, fall off to zero following distinct curves, both for SPO1, which destabilizes by a period-doubling type of bifurcation, and SPO2, which exhibits a *complex* instability with its monodromy eigenvalues exiting the unit circle in complex conjugate pairs. However, as the energy increases further, the Lyapunov spectra near SPO1 and SPO2 begin to *converge*, at some $E > E_{1u} > E_{2u}$, to the same functional form, implying that the chaotic regions of SPO1 and SPO2 have "merged" and large-scale chaos has spread in phase space.

The function to which the Lyapunov spectra converge is a nearly exponentially decaying curve of the form

$$L_i(N) \propto e^{-\alpha i/N}, \quad i = 1, 2, \ldots, K(N), \tag{2}$$

at least up to $K(N) \approx \frac{3N}{4}$, as we have discussed at length in a recent publication [11]. This function provides, in fact, an invariant of the dynamics, in the sense that, in the thermodynamic limit, we can use it to evaluate the average of the positive Lyapunov exponents (i.e., the Kolmogorov-Sinai entropy per particle) and find that it is a constant characterized by the value of the exponent α appearing in (2).

Thus, we argue that studying the local dynamics around some of the simplest periodic orbits which destabilize at low energies opens a "window" into the "global" dynamics of nonlinear lattices. Furthermore, by computing and comparing Lyapunov spectra in their vicinity, it is possible to gain valuable insight into the conditions for large-scale chaos and ergodicity, so that we may be able to define probability distributions and compute thermodynamic properties of the lattice, as E and N increase indefinitely with E/N fixed.

Our paper is organized as follows: In Sec. II we provide analytical expressions of the SPO1 and SPO2 solutions under study and describe in detail their stability properties for an arbitrarily large number of particles of the FPU β model with fixed boundary conditions. Comparing with similar findings in the literature, we observe that our results accurately predict the onset of "weak" chaos preceding the breakdown of FPU recurrences, although the reasons for this agreement are still under investigation. In Sec. III, we use our results on the convergence of Lyapunov spectra, as the energy is increased beyond the destabilization thresholds of SPO1 and SPO2 to estimate the onset of large-scale chaos and thermodynamic behavior in the lattice and in Sec. IV we present our conclusions. We thus believe that today, 50 years after its famous discovery, the Fermi-Pasta-Ulam problem and its transition from recurrences to globally chaotic behavior is still very much alive as a topic of intense research into some truly fundamental questions connecting classical and statistical mechanics [16].

II. SIMPLE PERIODIC ORBITS AND STABILITY ANALYSIS

A. Analytical results for SPO1

Let us start by describing briefly some analytical results concerning SPO1, as this particular mode has been studied recently by Antonopoulos *et al.* [11] and also previously in Refs. [14,15].

We consider, for this reason, a one-dimensional lattice of N particles with equal masses and nearest-neighbor interactions with quartic nonlinearities (β model) which is given by the FPU Hamiltonian (1), with fixed boundary conditions

$$x_0(t) = x_{N+1}(t) = 0, \quad \forall\, t. \tag{3}$$

For $\beta=0$, Hamiltonian (1) describes a system of coupled harmonic oscillators and hence all solutions can be written as combinations of N independent normal modes whose individual energies are constant in time. Since, in that case, the spectrum has frequencies $\omega_q = 2\sin[\pi q/2(N+1)]$, which are rationally independent, all solutions are quasiperiodic, and hence the only strictly periodic solutions are the normal modes, with frequencies ω_q, $q=1,2,\ldots,N$ [6,10,16]. That these modes can be continued for $\beta>0$ is a consequence of a famous theorem by Lyapunov [17], based on the assumption that no ratio of linear frequencies ω_q/ω_r is an integer, for $q,r=1,2,\ldots,N$, which holds in this case. These solutions are examples of what we call SPO's, in which all particles return to their starting point after one maximum (and one minimum) in their oscillation [11].

Let us consider one such orbit—we shall call SPO1—which is specified by the conditions

$$\hat{x}_{2j}(t) = 0, \quad \hat{x}_{2j-1}(t) = -\hat{x}_{2j+1}(t) \equiv \hat{x}(t), \quad j = 1, \ldots, \frac{N-1}{2}, \tag{4}$$

and exists for all odd N, keeping every even particle stationary at all times. It is not difficult to show that this is, in fact,

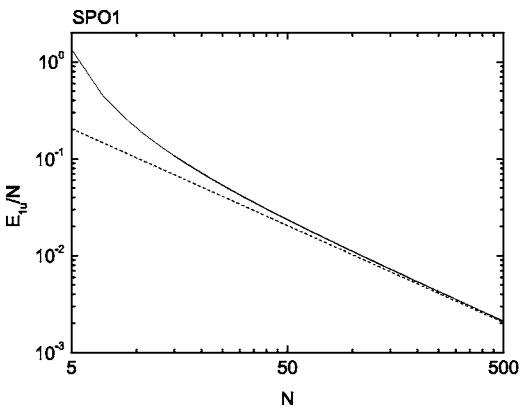

FIG. 1. The solid curve is the energy per particle, $\frac{E_{1u}}{N}$, of the first destabilization of the SPO1 for $\beta=1$ while the dashed line is the function $\propto\frac{1}{N}$.

the $q=(N+1)/2$ mode of the linear lattice with frequency $\omega_q=\sqrt{2}$. The remarkable property of this solution is that it is continued in precisely the same spatial configuration in the nonlinear lattice as well, due to the form of the equations of motion associated with Hamiltonian (1),

$$\ddot{x}_j(t) = x_{j+1} - 2x_j + x_{j-1} + \beta((x_{j+1}-x_j)^3 - (x_j - x_{j-1})^3), \quad j = 1, \ldots, N, \tag{5}$$

which reduce, upon using Eq. (4) with Eq. (3), to a single second-order nonlinear differential equation for $\hat{x}(t)$,

$$\ddot{\hat{x}}(t) = -2\hat{x}(t) - 2\beta\hat{x}^3(t), \tag{6}$$

describing the oscillations of all moving particles of SPO1, with $j=1,3,5,\ldots,N$. For the stationary particles $j=2,4,6,\ldots,N-1$, of course, we have $\hat{x}(t)=0$, $\forall t\geq 0$. The solution of Eq. (6) is well known in terms of Jacobi elliptic functions [18] and can be written as

$$\hat{x}(t) = \mathcal{C}\,\mathrm{cn}(\lambda t, \kappa^2), \tag{7}$$

where

$$\mathcal{C}^2 = \frac{2\kappa^2}{\beta(1-2\kappa^2)}, \quad \lambda^2 = \frac{2}{1-2\kappa^2}, \tag{8}$$

and κ^2 is the modulus of the cn elliptic function. The energy per particle of SPO1 is then found to be

$$\frac{E}{N+1} = \frac{1}{4}\mathcal{C}^2(2+\mathcal{C}^2\beta) = \frac{\kappa^2(1-\kappa^2)}{\beta(1-2\kappa^2)^2} \tag{9}$$

by substituting simply the solution $\hat{x}(t)$ of Eq. (7) in Hamiltonian (1).

The linear stability analysis of the SPO1 mode is straightforward and was carried out recently in Ref. [11] using Lamé equations, Hill's determinants, and Floquet theory. Plotting the first destabilization energy for this orbit as a function of N with solid lines in Fig. 1, we observe that the corresponding energy density threshold $\frac{E_{1u}}{N}$ decreases with N following a simple power law $\propto 1/N$ (dashed line). Following such an approach, we find, for example, for $\beta=1$ and $N=11$, that SPO1 destabilizes for the first time when $E_{1u}\approx 1.93$.

B. Solution of SPO2

Let us now turn to the second simple periodic orbit studied in this paper, which we call SPO2. We impose again fixed boundary conditions and consider lattices consisting of $N=5+3m$, $m=0,1,2,\ldots$, particles, in which every third particle is fixed, while the two in between move in opposite directions as follows:

$$x_{3j}(t) = 0, \quad j = 1,2,3, \ldots, \frac{N-2}{3}, \tag{10}$$

$$x_j(t) = -x_{j+1}(t) = \hat{x}(t), \quad j = 1,4,7, \ldots, N-1. \tag{11}$$

This solution, in fact, corresponds to the $q=2(N+1)/3$ normal mode with frequency $\omega_q=\sqrt{3}$ of the linear system and can also be continued in exactly the same form in the nonlinear case $\beta>0$, due to the symmetry of the equations of motion,

$$\ddot{x}_j(t) = x_{j+1} - 2x_j + x_{j-1} + \beta((x_{j+1}-x_j)^3 - (x_j - x_{j-1})^3), \quad j = 1, \ldots, N, \tag{12}$$

which, under the above conditions (10) and (11) collapse to a single second-order nonlinear differential equation very similar to (6):

$$\ddot{\hat{x}}(t) = -3\hat{x}(t) - 9\beta\hat{x}^3(t). \tag{13}$$

As before, this equation describes the moving particles of the lattice, while the stationary ones satisfy $\hat{x}(t)=0$, $\forall t\geq 0$, for $j=3,6,9,\ldots,N-2$. The solution of Eq. (13) is again given in terms of the Jacobi elliptic functions [18] and is written in the form

$$\hat{x}(t) = \mathcal{C}\,\mathrm{cn}(\lambda t, \kappa^2), \tag{14}$$

where

$$\mathcal{C}^2 = \frac{2\kappa^2}{3\beta(1-2\kappa^2)}, \quad \lambda^2 = \frac{3}{1-2\kappa^2}, \tag{15}$$

and κ^2 is, again, the modulus of the cn elliptic function. The energy per particle of the SPO2 mode is found now to be

$$\frac{E}{N+1} = \frac{2\kappa^2(1-\kappa^2)}{3\beta(1-2\kappa^2)^2} \tag{16}$$

by simply substituting the solution $\hat{x}(t)$ of Eq. (13) in Hamiltonian (1).

In order to perform the linear stability analysis of the SPO2 mode we set $x_j=\hat{x}_j+y_j$ in the equations of motion (12) and keep up to linear terms in the small displacement variable y_j. We thus get the variational equations for this orbit in the form

$$\ddot{y}_j(t) = A_3 y_{j-1} + A_1 y_j + A_2 y_{j+1}, \quad j = 1,4,7, \ldots, N-1, \tag{17}$$

$$\ddot{y}_j(t) = A_2 y_{j-1} + A_1 y_j + A_3 y_{j+1}, \quad j = 2,5,8, \ldots, N, \tag{18}$$

$$\ddot{y}_j(t) = A_3(y_{j-1} - 2y_j + y_{j+1}), \quad j = 3,6,9, \ldots, N-2, \tag{19}$$

where $y_0 = y_{N+1} = 0$ and

$$A_1 = -2 - 15\beta\hat{x}^2(t), \tag{20}$$

$$A_2 = 1 + 12\beta\hat{x}^2(t), \tag{21}$$

$$A_3 = 1 + 3\beta\hat{x}^2(t). \tag{22}$$

Unfortunately, it is not as easy to uncouple the above linear system of differential equations and study the stability of the SPO2, in terms of independent Lamé equations, as we were able to do with SPO1 [11]. We can, however, compute numerically with arbitrary accuracy and for every given $N = 5+3m$, $m = 0,1,2,\ldots$, the complex eigenvalues λ_i, $i = 1,\ldots,2N$, of the corresponding monodromy matrix and characterize the stability of the SPO2 by their position on the complex plane with regard to the unit circle.

We have thus computed, for many values of $N = 5+3m$, $m = 0,1,2,\ldots,98$, the energy $E_{2u}(N)$ of the first destabilization of the SPO2 for $\beta = 1$ and have plotted the results with solid lines in Fig. 2(a). As we see, the energy density $\frac{E_{2u}}{N}$ at the first instability decreases following a power law $\propto 1/N^2$ (dashed line) which is faster than the SPO1 solution we discussed earlier; see Fig. 1. Following this approach, we find, for $\beta = 1$ and $N = 11$, that SPO2 destabilizes for the first time when $E_{2u} \approx 0.153$.

Interestingly enough, if we calculate the eigenvalues of the monodromy matrix of the SPO2 for greater energies, we find that it becomes again stable, beyond a new critical energy $E_{2s}(N)$. In Fig. 2(b) we plot this restabilization energy density of SPO2 as a function of $\log N$ and observe that it approaches a constant as N tends to infinity.

Pursuing further this restabilization phenomenon, we have estimated the "size" of the islands of stability around SPO2 for energies above the energy threshold $E_{2s}(N)$, using the method of the smaller alignment index (SALI) [19–22]. This index has proved to be very efficient for distinguishing rapidly and with certainty regular versus chaotic orbits, as it exhibits completely different behavior in these two cases: It fluctuates around nonzero values for regular orbits, while it converges exponentially to zero for chaotic orbits. SALI is particularly useful in the case of many degrees of freedom, where very few such methods are available beyond the cumbersome and often inconclusive calculation of the maximal Lyapunov exponent.

We thus observe the following: As the energy E increases beyond the restabilization threshold $E_{2s}(N)$, for fixed N, the "size" of the island around SPO2 changes very little, compared with the growth of the system's available phase space. Moreover, if we keep $\frac{E}{N}$ fixed, thus holding the "radius" of the energy surface nearly constant, we find that the "radius" of the SPO2 island diminishes as a function of E. This is done by changing one of the particles' position and momentum by Δx and Δp_x away from its SPO2 values while keeping the energy constant and using SALI to estimate Δx_{max} at which we reach chaos (e.g., with $\frac{E}{N} = 4$ and $N = 5,8,11,14$,

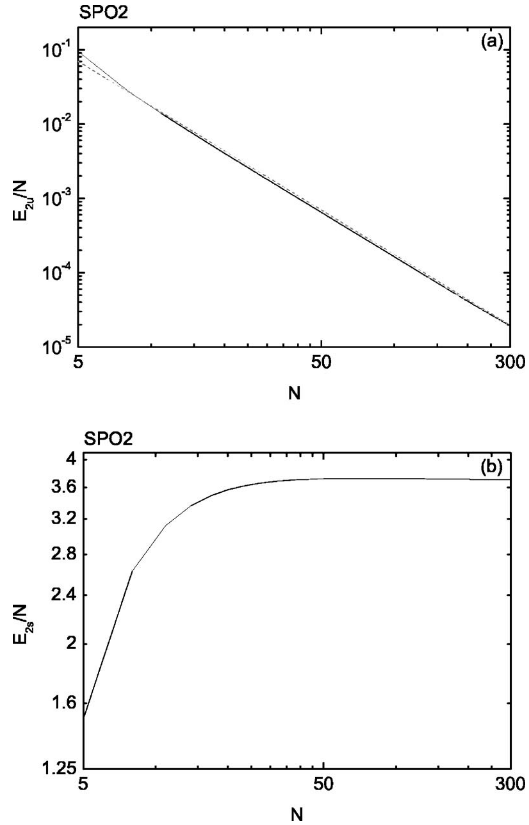

FIG. 2. (a) The solid curve is the energy density $\frac{E_{2u}}{N}$ of the first destabilization of the SPO2 obtained by numerical evaluation of the eigenvalues of the monodromy matrix, while the dashed line is $\propto \frac{1}{N^2}$. (b) The energy density $\frac{E_{2s}}{N}$ of the first restabilization of the SPO2 obtained by the same method as in (a). In this figure $\beta = 1$.

we find, respectively, $\Delta x_{max} \approx 0.01, 0.005, 0.0025, 0.002$). We therefore conclude that the island of ordered motion around the SPO2 solution should be of no consequence to the statistical properties of the lattice, such as ergodicity and the definition of thermodynamic quantities.

Moreover, as we observe in Figs. 3(a) and 3(c), the kinds of bifurcation leading to instability for these SPO's are very different: In the case of SPO1, Fig. 3(a) shows that the bifurcation is of the period-doubling type, as one pair of real eigenvalues is seen to exit the unit circle at -1, while Fig. 3(c) shows that we have complex instability in the case of SPO2. This is also indicated by the positive Lyapunov exponents in the *immediate* vicinity of the SPO's (about 10^{-12} from them), which are closely connected with the eigenvalues of the corresponding variational equations and are shown in Figs. 3(b) and 3(d) with solid lines. Of course, moving away from the two modes (within a range of about $10^{-11}-10^{-2}$), the Lyapunov spectra change into the familiar form of two smoothly decaying, evidently different curves, plotted with dashed lines in Figs. 3(b) and 3(d). This fact suggests that the chaotic regions near these modes are separated from each other in phase space.

It is quite interesting to observe that the chaotic region about an unstable SPO can be isolated in phase space from the chaotic motion occurring in different domains. In fact, there may be several such domains embedded into each

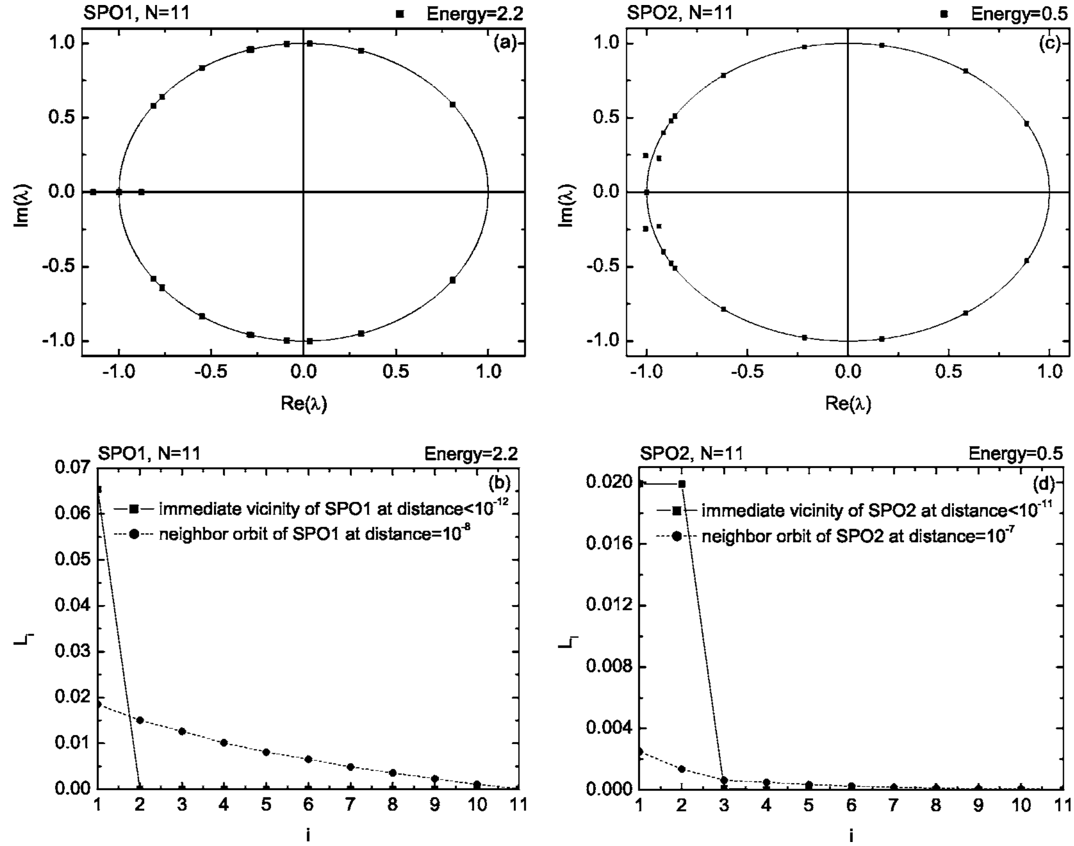

FIG. 3. (a) The period-doubling bifurcation of SPO1 for $N=11$ at the energy $E=2.2$. (b) The Lyapunov spectrum of two orbits, one starting very close to SPO1 and another a little farther away, for the same N and E as in panel (a). (c) The complex instability of SPO2 for $N=11$ at the energy $E=0.5$ after its first destabilization. (d) The Lyapunov spectrum of two similar orbits, one in the immediate vicinity and another more distant from SPO2 for the same N and E as in panel (c). In this figure $\beta=1$.

other. For example, in the $N=5$ FPU β model, when SPO1 becomes unstable, a "figure-8" chaotic region becomes clearly visible in its immediate neighborhood, on a Poincaré surface of section $(x_1,\dot{x}_1)$ taken at times when $x_3=0$ (see Fig. 4). Even though the SPO1 mode is unstable, nearby orbits oscillate about it for very long times, forming eventually the figure-8 we see in the picture.

More surprisingly however, starting at points a little farther away, a different chaotic domain is observed which bears a vague resemblance to the figure-8 and does not spread to the full energy surface. Of course, if one chooses more distant initial conditions, a large-scale chaotic region becomes evident on the surface of section of Fig. 4.

We have checked that the Lyapunov exponents in these regions are quite different from each other, at least when one integrates the equations of motion up to $t=10^5$. Of course, if an orbit lies on the "boundary" between two of these domains, if integrated long enough, it may drift from the inner to the outer chaotic region, where its Lyapunov exponents are expected to change accordingly.

In Sec. III, we will study in more detail the relative location of chaotic domains in phase space and argue that these will "overlap" when their respective Lyapunov spectra begin to converge as a function of increasing energy for fixed N.

C. Comparison with results in the literature

It was shown very recently in Ref. [10] that the linear modes of the FPU β model can be continued as SPO's of the corresponding nonlinear lattice—i.e., as exact, time periodic solutions—having nearly the same spatial configuration and frequency as in the linear case. These new solutions are characterized by exponential localization in the q space of the normal modes $Q_j(t)$, $j=1,\ldots,2N$, and preserve their stability for small enough $\beta>0$. In fact, the energy threshold for the destabilization of the $q=3$ solution found by Ref. [10] coincides with the "weak"-chaos threshold determined by De Luca, Lichtenberg, and Lieberman [8].

In this section, we show that the energy threshold found in Refs. [8] and [10] also appears to coincide with the instability threshold of the SPO2 mode. This is somewhat surprising since, in all studies of the breakdown of FPU recurrences so far, the wave number q of the periodic solutions responsible for the transition to "weak" chaos is low ($q\leq 4$), while our SPO2 mode has a considerably higher wave number $q=2(N+1)/3$.

Thus, using different approaches, the authors of Refs. [8] and [10] report an approximate formula, valid to order $O(\frac{1}{N^2})$, for the destabilization energy of the q-breather solution with wave number $q=3$ given by

$$E_c \approx \frac{\pi^2}{6\beta(N+1)}. \tag{23}$$

In Fig. 5 we compare the approximate formula (23) (dashed line) with our destabilization threshold for SPO2

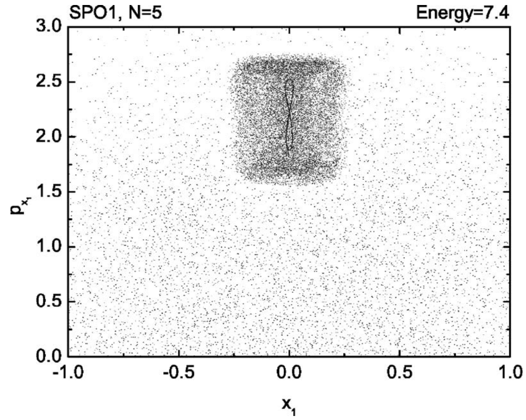

FIG. 4. The figure-8 chaotic region for initial conditions in the immediate vicinity of SPO1 ($\simeq 10^{-5}$), a vague resemblance to the figure-8 for initial conditions a little farther away ($\simeq 10^{-1}$) and a large-scale chaotic region in the energy surface for initial conditions more distant ($\simeq 1$) for $N=5$ particles, when it is unstable, on the Poincaré surface of section $(x_1, \dot{x}_1)$ computed at times when $x_3=0$. In this picture we integrated our orbits up to $t_n=10^5$ in the energy surface $E=7.4$.

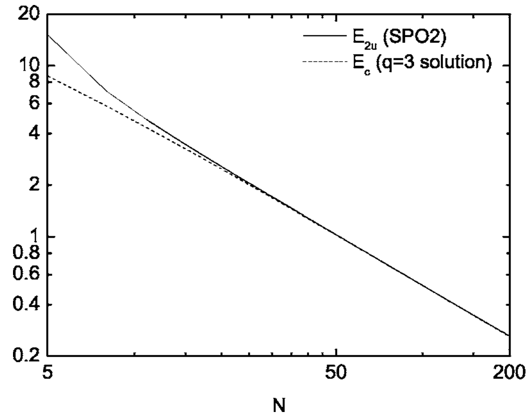

FIG. 5. The solid curve corresponds to the energy $E_{2u}(N)$ of the first destabilization of the SPO2 for $\beta=0.0315$ obtained by numerical evaluation of the eigenvalues of the monodromy matrix, while the dashed line corresponds to the approximate formula (23) for the q-breather solution.

obtained by the monodromy matrix analysis of Sec. II B (solid line), for $\beta=0.0315$, following Ref. [10]. We clearly observe very good agreement between our numerical results and those of (23).

The reasons for this agreement are not yet clear to us. Of course, if one wanted to look for a chaotic transition via the destabilization of SPO's, it would be natural to analyze first SPO2 rather than SPO1, since SPO2 becomes unstable for lower energies. Perhaps the power law $\frac{E_{2u}}{N} \propto 1/N^2$ is important as it is the same in formula (23) as well as our SPO2 stability results. Still, the agreement between the two curves in Fig. 5 cannot be due only to the coincidence of power laws. The proportionality factors in the corresponding formulas must also be nearly the same.

III. CONVERGENCE OF LYAPUNOV SPECTRA

Let us now start from the neighborhood of the SPO1 and SPO2 modes and examine systematically the onset of large-scale chaos in the system as the energy is increased above the instability thresholds $E_{1u}(N)$ and $E_{2u}(N)$. To do this, we need to evaluate the Lyapunov exponents L_i, $i=1,\ldots,2N$, near the SPO's (ordered as $L_1 > L_2 > \cdots > L_{2N}$), which measure the rate of exponential divergence of nearby orbits in different directions of phase space as time goes to infinity [1,23,24].

Note that Fig. 3 reveals that when one calculates Lyapunov exponents starting very close ($<10^{-12}$) to a periodic orbit, one finds that they are closely related to the eigenvalues of the monodromy matrix of the local dynamics. In Figs. 3(c) and 3(d), we have plotted these quantities for the SPO2 mode at an energy where it has undergone a complex bifurcation and has two pairs of eigenvalues off the unit circle on the complex plane.

For comparison, we have also calculated in Fig. 3(a) the eigenvalues of the monodromy matrix of the SPO1 mode at an energy where it is unstable with only one pair of eigenvalues off the unit circle on the real negative axis. As we see in Fig. 3(b), very near this orbit the Lyapunov spectrum is again in close agreement with the local results. Of course, in both cases, starting with initial conditions a little farther away yields the true spectrum, as a smoothly decaying curve, which is an invariant of the dynamics in that region [see the dashed lines in Figs. 3(b) and 3(d)].

Thus, in the neighborhood of unstable SPO's, one can easily find evidence of "small"-scale chaos, which is visible at energies where these orbits have just destabilized. This, however, is only a local effect, which may have nothing to do with the chaotic behavior anywhere else in the system. How could we use the dynamics near SPO's to obtain more global properties of the motionlike, e.g., the onset of large-scale chaos in phase space?

One way to answer might be to test whether the chaotic regions of the two SPO's become "connected" in phase space, above a certain value of the energy. Evidence that such "merging" of chaotic regions in phase space indeed occurs can be provided by their maximal (L_1) Lyapunov exponents becoming equal and, more specifically, by the convergence of the corresponding Lyapunov spectra in their vicinity to an exponential function with a characteristic exponent.

To see this, let us proceed to exhibit in Fig. 6(a) the Lyapunov spectra of two neighboring orbits of the SPO1 and SPO2 modes (all orbits in this figure start at distances $\simeq 10^{-2}$ from the SPOs in phase space), for $N=11$ degrees of freedom and energy values $E_1=1.94$ and $E_2=0.155$, respectively, where the SPO's have just destabilized. As expected, in this case, the maximum Lyapunov exponents L_1 are very small ($\approx 10^{-4}$) and the corresponding Lyapunov spectra are quite distinct.

Turning now to Fig. 6(b), we observe that at the energy value $E=2.1$, the Lyapunov spectra for both SPO's are much closer to each other, even though their maximal Lyapunov exponents L_1 are still different. Furthermore, in Fig. 6(c), at $E=2.62$, we see that the two spectra have nearly converged to the same exponentially decreasing function,

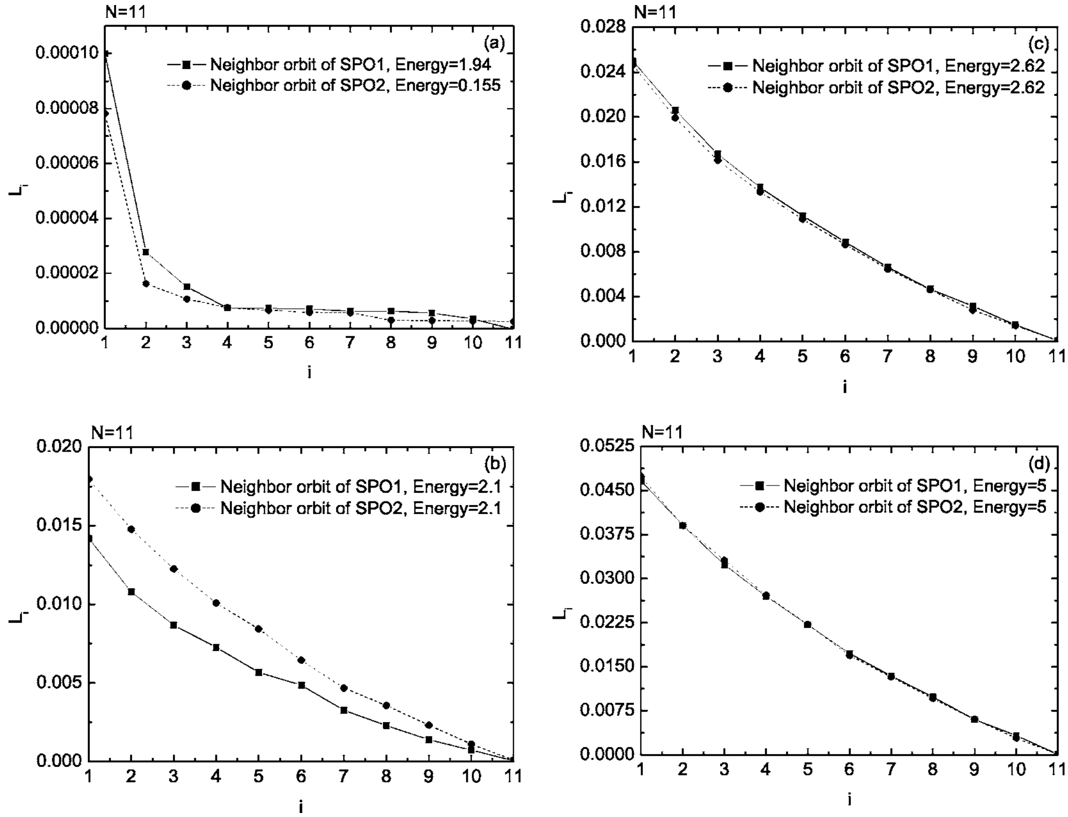

FIG. 6. (a) Lyapunov spectra of neighboring orbits of SPO1 and SPO2, respectively, for $N=11$ at energies $E=1.94$ and $E=0.155$, where they respectively have just destabilized. (b) Same as in panel (a) at energy $E=2.1$ for both SPO's, where the spectra are still distinct. (c) Convergence of the Lyapunov spectra of neighboring orbits of the two SPO's at energy $E=2.62$ where both of them are unstable. (d) Coincidence of Lyapunov spectra continues at higher energy $E=4$. All initial distances between nearby trajectories are $\simeq 10^{-2}$.

$$L_i(N) \propto e^{-\alpha i/N}, \quad i=1,2,\ldots,K(N), \tag{24}$$

at least up to $K(N) \approx \frac{3N}{4}$, while their maximal Lyapunov exponents are virtually the same. The α exponents of (24) for the SPO1 and SPO2 are found to be approximately 2.3 and 2.32, respectively. Finally, Fig. 6(d) shows that this coincidence of Lyapunov spectra persists at higher energies.

We regard this coincidence as an indication that the chaotic regions of the two SPO's have "merged" in phase space in the sense that they "communicate," as orbits starting initially in the vicinity of one SPO may now visit the chaotic region of the other. This is strong evidence of the existence of large scale chaos in the FPU lattice, at least over the part of phase space traveled by the SPO1 and SPO2 orbits, during their time evolution.

IV. CONCLUSIONS

In this paper we investigated the connection between local and global dynamics in the FPU β model from the point of view of stability of its SPO's. Initially, we showed that a relatively high-q mode of the linear lattice, with one particle fixed every two oppositely moving ones, called SPO2, is stable for low energies until it undergoes complex instability. In parallel, we also studied the properties of another mode called SPO1, which keeps every two particles fixed, with the ones in between executing exactly opposite oscillations.

Our first result concerning these orbits is that the energy threshold of the first destabilization of SPO2 goes to zero faster than that of SPO1. Additionally, we discovered that, as a function of N, the SPO2 destabilization threshold coincides with the one found by other researchers for the transition to "weak" chaos and the destabilization of the $q=3$ mode. This implies that if chaos is to spread as a result of the destabilization of SPOs in the FPU lattice, one might as well look closely at the properties of the SPO2, as that becomes unstable much earlier than SPO1, as N increases arbitrarily.

In order to examine their local dynamics in more detail, we raised the energy above the destabilization of SPO1 and SPO2 and calculated the Lyapunov spectra in their neighborhood. We thus found that, as E increases, the Lyapunov spectra in the neighborhood of these SPO's appear to converge, at some relatively low-energy value, to the same functional form, implying that their chaotic regions have "merged" and large-scale chaos has spread in the FPU lattice.

We therefore argue that by studying local dynamics near some of the simplest periodic orbits which destabilize at low energies, one can gain a better view of the "global" dynamics of nonlinear lattices. Furthermore, by computing and comparing Lyapunov spectra in the vicinity of such orbits, it is possible to obtain valuable insight into the conditions for (or obstructions to) full-scale chaos and ergodicity, so that we may be able to define probability distributions and compute thermodynamic properties of the lattice, as the energy and number of degrees of freedom increase indefinitely, while the energy density is kept fixed.

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