

The Fermi-Pasta-Ulam problem: 50 years of progress

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Abstract

A brief review of the Fermi-Pasta-Ulam (FPU) paradox is given, together with its suggested resolutions and its relation to other physical problems. We focus on the ideas and concepts that have become the core of modern nonlinear mechanics, in their historical perspective. Starting from first numerical results of FPU, both theoretical and numerical findings are discussed in close connection with the problems of ergodicity, integrability, chaos and stability of motion. New directions related to the Bose-Einstein condensation and quantum systems of interacting Bose-particles are also considered.

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I. INTRODUCTION

The goal of this paper is two-fold. First, we evaluate and summarize the most interesting results related to the FPU model, after the seminal paper [1] appeared in 1955. Second, we discuss new directions in the study of many-body chaos, that are related, directly or indirectly, to the FPU problem. We hope that our analysis will help future investigations of nonlinear classical and quantum systems of interacting particles.

Numerous attempts to resolve the FPU paradox have resulted in a burst of analytical and numerical studies of nonlinear effects in physical systems. The primary interest of FPU was the observation of energy sharing in one-dimensional lattices with nonlinear coupling among rigid masses. For E. Fermi this study was directly related to his first paper of 1923 [2] in which he tried to rigorously prove the ergodicity hypothesis which lies at the core of traditional statistical mechanics. For a long time, the ergodicity was assumed to serve as the only mechanism needed for the foundation of statistical mechanics. Specifically, by assuming the ergodic motion of classical trajectories on the surface of constant energy, one can expect statistical behavior of a system and apply well developed statistical methods. Symbolically, the first and last papers of E. Fermi deal with the problem of the foundations of statistical mechanics.

In view of the result of Fermi [2], and in accordance with wide-spread expectations, any weak nonlinear interaction between particles in a system with very many degrees of freedom causes ergodic behavior of a system. In fact, this point is used in the derivation of statistical distributions in the thermodynamic $N \rightarrow \infty$ limit for systems of non-interacting particles. Therefore, it is natural to expect that a system of 32 or 64 particles, as in the FPU numerical study, would reveal ergodic behavior provided the nonlinearity is not extremely small. To the great surprise of FPU, the result was opposite: the long-time dynamics of the studied model appeared to be periodic, with almost perfect returns to the initial conditions. Having extraordinary intuition, Fermi noted that this effect may have very important consequences [3]. About ten years later, two alternative explanations of the FPU paradox were suggested, giving rise to new phenomena, the integrability of nonlinear equations and dynamical (deterministic) chaos.

One of the discoveries triggered by the FPU results was the complete integrability of a class of nonlinear differential equations. The first indication of this unexpected fact was

due to numerical integration of the Korteweg-de-Vries equation in 1965 by N. Zabusky and M. Kruskal [4]. As was demonstrated, stable solitary waves (*solitons*) emerged from generic initial conditions and traveled through the media, interacting with each other without losing their identities. This effect was suggested as an explanation of the remarkable recurrence in the FPU model, with the claim of its closeness to a completely integrable model.

Another approach in resolving the FPU paradox was developed by B. Chirikov on the basis of his criterion of *stochasticity* (or *dynamical chaos*) [5]. As was already known from the study of nonlinear systems in applications to accelerator and plasma physics, the motion of a dynamical nonlinear system with few degrees of freedom can exhibit strong chaotic behavior. Thus, the description of these systems can be given in terms of conventional statistical mechanics. The mechanism of chaotic behavior of dynamical systems was found to be an exponential instability of motion for a wide range of initial conditions. The essential role in the emergence of this kind of instability is played by interacting nonlinear resonances. By 1965, the relatively simple criterion of resonance overlap enabled one to determine the conditions for the onset of stochasticity for various low-dimensional systems. Therefore, it was natural to apply the same approach to nonlinear systems of the FPU type. As a result, the threshold of stochasticity was found analytically in Ref.[6] and later confirmed numerically [7]. According to these studies, the initial conditions used by FPU in their numerical simulations were chosen below the stochasticity threshold, just in the region corresponding to stable quasi-periodic motion. Above this threshold, the FPU model was shown to behave in accordance to the original expectations of FPU, revealing strong statistical properties, such as energy equipartition among the linear modes.

In fact, the FPU study gave birth to a new method to study the physical laws of nature. The two first methods are well-known: theoretical and experimental physics. The new approach was predicted by S. Ulam and discussed in his mathematical book [8]. Expecting a future burst of computer technology, he proposed a new kind of *synergetic* cooperation between a physicist and computer (see, also, [9]). Apart from the normal use of computers as a tool for calculations of integrals, functions, differential equations etc., the new role for computers consists of the study of physical systems *ab initio*, starting from given models and investigating their properties by varying parameters, forces, initial conditions etc. This kind of activity was marked in the FPU paper as “numerical experiments”. Later, this term has been widely used by B. Chirikov to stress the difference of the new approach from both

theoretical and experimental studies.

The FPU problem may be treated as a perfect example of this approach. Specifically, first, the model was set up in the form of equations of motion. Then, “numerical experiments” were performed to see how rapidly the thermalization occurs due to the nonlinear interactions. And, unexpectedly, a new phenomenon was discovered, initiating further theoretical studies. Afterwards, theoretical predictions were checked and further numerical studies gave new insight in the problem. Thus, the “synergetic” approach progresses. Since the time of the first “numerical experiments” of FPU many physical discoveries have been found first numerically, then explained theoretically and confirmed by real experiments. An exciting story of first twenty years of studies of the FPU paradox can be found in the book of T.Weissert [10].

II. THE FPU MODEL

The primary aim of the authors of Ref.[1] was to observe thermal equilibrium in a non-linear string, and to establish the rate of approach to the equipartition of energy among different degrees of freedom. In order to treat this problem numerically, the continuum was represented by a large number of masses interacting with each other via nonlinear forces.

The corresponding partial differential equations were approximated by a linear chain of particles of equal masses M connected by elastic springs. The linear part of the forces is determined by the constant K , resulting in harmonic frequencies $\omega_0 = \sqrt{2K/M}$ for all particles. (Following many papers we assume, for simplicity, $M = K = 1$). For the nonlinear part, in Ref.[1] main attention was paid to simplest cases of quadratic and cubic additional terms, although some alternative forms of the interaction have been also discussed. For the quadratic force (called the α -*model*) the corresponding equations of motion are

$$\ddot{x}_n = (x_{n+1} - 2x_n + x_{n-1}) + \alpha[(x_{n+1} - x_n)^2 - (x_n - x_{n-1})^2]. \quad (1)$$

Correspondingly, the chain of particles with additional cubic forces (called the β -*model*) is governed by the equations,

$$\ddot{x}_n = (x_{n+1} - 2x_n + x_{n-1}) + \beta[(x_{n+1} - x_n)^3 - (x_n - x_{n-1})^3] \quad (2)$$

Here x_n denotes the displacement of the n -th particle from its original position, and the parameters α and β are the strengths of nonlinear interactions between particles.

In the absence of nonlinear forces the exact solution can be written in the form of normal modes $Q_k(t)$ that are essentially the Fourier representation of the displacements $x_n(t)$ (for fixed ends of the chain, $x_0 = x_N = 0$),

$$Q_k(t) = \sqrt{\frac{2}{N}} \sum_{n=1}^N x_n(t) \sin \frac{\pi kn}{N} \quad (3)$$

With this representation one can see that for any initial conditions $x_n(0)$ and $\dot{x}_n(0)$ the energy

$$E_k = \frac{1}{2}(\dot{Q}_k^2 + \omega_k^2 Q_k^2) \quad (4)$$

of every k -th mode is constant. Therefore, the model is trivially integrable and energy equipartition among normal modes is not possible. As a result, the motion of this model is quasi-periodic in time, with the discrete spectrum determined by the normal frequencies ω_k ,

$$\omega_k = 2 \sin \left(\frac{\pi k}{2N} \right). \quad (5)$$

In the normal mode representation, the equations of motion take the form,

$$\ddot{Q}_k + \omega_k^2 Q_k = \alpha \sum_{i,j=1}^N C_{ij} Q_i Q_j \quad (6)$$

for the α -model (1) and

$$\ddot{Q}_k + \omega_k^2 Q_k = \beta \sum_{i,j,l=1}^N D_{ijl} Q_i Q_j Q_l \quad (7)$$

for the β -model (2). Here $C_{i,j}$ and $D_{i,j,l}$ are coefficients of the complicated dependence on the indexes i, j and l , defined by the nonlinear forces.

Having in mind the predictions of conventional statistical mechanics, the authors of Ref.[1] expected that by switching on the nonlinear terms in Eqs.(1-2) (or equivalently Eqs.(6-7)), energy initially concentrated in a particular mode, will flow into all other modes, thus demonstrating the transition to equilibrium. In particular, analytical arguments were given in Ref.[11], according to which after a long time the systems of coupled anharmonic oscillators have to approach thermal equilibrium. Thus, it was a general belief that any kind of nonlinearity in a system with large number of degrees of freedom would give rise to ergodicity (see, e.g., [2]). And the latter was assumed to serve as the mechanism for the onset of statistical behavior in dynamical systems.

The numerical studies in Ref.[1] were performed on Metropolis' new MANIAC computer with $N = 32$ or $N = 64$ and with sufficiently small values of the nonlinear parameters α and β , for zero initial conditions, $x_0 = x_N = 0$. The first results refer to 1953-1954, with some additional runs that have been done after the death of E.Fermi in December 1954. Typically, the first mode with $k = 1$ was initially excited, for which most details are given. The time dependence of the energies $E_k(t)$ of all modes was studied for many fundamental periods $T_1 = 2\pi/\omega_1$ (for more details, see, e.g. [12]).

To the great surprise of the authors of Ref.[1], the results of a numerical simulation were quite astonishing. The behavior of both models was at first as expected: the energy spread to higher harmonics but after about 1000 oscillation periods T_1 , the flow of the energy into other modes stops, and the dynamics reversed, with the energy flowing back into the first mode. This recurrence of energy was found to be almost complete, with a decrease in energy of only about 2% of the total energy. In time, this periodic behavior persisted, thus demonstrating the absence of the expected statistical thermalization. The surprise was enhanced by the fact that the period of a recurrence was found to decrease with increasing coefficients of nonlinearity. Therefore, the nonlinear effects are significant and can not be neglected. The time evolution did not lead to equipartition of energy, rather, it demonstrated the existence of “quasi-modes” consisting of a number of linear modes. According to J.Tuck ([3]), Fermi became really excited about this phenomena and thought that “something new and important might be at hand”.

A few possible reasons for this observed effect were discussed during the first stage of the story. Initially, the accuracy of the numerics was questioned, with a hint that more accurate calculations would show thermalization, although a very weak one. This point was somehow supported by the observation of a non-complete return of the energy in the originally excited mode. However, further more accurate computations of Tuck in 1961 (see in Refs.[3, 13]) revealed an even more exciting effect. It was found that at later times, the recurrence of the energy becomes more nearly complete. Specifically, a “super period” was found that is about 80,000 linear cycles, T_1 . The energy recurrence after this super period was more than 99 % of the total energy. In general, these results of Tuck, although not discussed in the literature until much later [13], confirmed the phenomena of the recurrence in the FPU-model.

Of special interest was whether or not the energy recurrence can be associated with

Poincaré cycles that occur for ergodic systems. The estimate of the Poincaré cycle for a chain of linear oscillators was derived in Ref.[14]. This estimate shows that the recurrence time in a chain of linear oscillators increases in an approximately exponential way with the number of degrees of freedom. Therefore, it is clear that the Poincaré cycles have no relation to the observed recurrence in the FPU-model. Careful analysis [15] of this estimate in application to the FPU-problem shows, however, that one should distinguish the FPU-recurrence from the Poincaré cycles. The point is that the latter are defined for trajectories in phase space, rather than for the energy of a system. Obviously, the energy recurrence time will usually be much less than the Poincaré time. Moreover, the estimate was given for a harmonic lattice, and there is no way, apart from direct computation, to determine this recurrence time in the presence of nonlinear coupling. This remark, however, does not change the conclusion that the FPU-recurrence is of a different nature than Poincaré cycles.

In view of the many discussions about the mechanism of irreversibility in the systems of interacting particles, it is instructive to mention some of the computations of Tuck. To see the influence of numerical errors, he performed the following check. After few thousand cycles, the dynamics of the model was numerically reversed by the change of time and velocities of all particles. It was then found that 100% of the energy returns to the first mode. This fact was underestimated in early sixties. Now it can be treated as a direct (numerical) proof of the *regular* dynamics in the above models.

As is now well known, dynamical chaos is characterized by an exponential sensitivity of the dynamics to the initial conditions. As a result, the unavoidable round-off errors in numerical simulations give rise to a drastic change for individual chaotic trajectories. Because of this exponential sensitivity and the round-off errors it is not possible to reach numerically the initial state, unless the reversal time is very small. This fact leads to the very important conclusion that chaotic systems can not be treated as isolated ones since any weak external perturbation is essentially strong (see the discussion in [16, 17]). Therefore, this local instability serves as a mechanism for apparent irreversibility in dynamical systems, although any dynamical system is reversible in principle (here, we do not discuss dissipative or noisy systems).

For about a decade after the publication of the FPU preprint, discussions of the FPU paradox were restricted to a trivialization of the results, attempting to explain the recur-

rence effect as simply as due to numerical errors, insufficient computation time, Poincarè recurrence, or the specific choice of nonlinear forces which prevents the ergodicity. It was still not well recognized that the FPU results initiated a new era in physics, associated with nonlinear phenomena.

III. PERTURBATIVE APPROACHES

The first analytical studies of the FPU paradox were described in the paper of J. Ford [18]. It was argued there that the absence of ergodicity in the FPU calculations may be due to the arithmetic properties of the unperturbed spectrum determined by Eq.(5). By making use of the perturbation theory of Kryloff and Bogoliuboff [19], it was claimed that appreciable energy sharing among normal modes for a very weak coupling nonlinear interaction occurs only if the frequencies ω_k of the unperturbed motion are linearly dependent (or, only if $\sum_k m_k \omega_k = 0$ for some nonzero collection of integers $\{m_k \neq 0\}$). As for the FPU numerical data, they refer to the value of N as a power 2, therefore, to linearly independent frequencies (see details in Ref. [18]). For this reason, only few (low) modes in the FPU simulation could share the energy. Therefore, one should have multiple resonance conditions, in order to expect widespread energy sharing. However, as was shown in Ref.[20], this idea, although quite useful in the description of weakly nonlinear oscillations, turned out to fail to explain the FPU paradox. Numerical experiments with many other values of N confirmed irrelevance of linear resonance conditions to the FPU recurrence.

The numerical data of Ref.[1] describe a relatively weak interaction between particles. This fact has triggered analytical studies of the FPU dynamics utilizing perturbation theories. In an attempt to explain the quasi-period for the normal modes, in Ref.[21] standard perturbation methods were examined in the light of application to long-time dynamics of nonlinearly coupled oscillators. As is known, the main problem is the small divisors that arise due to resonances between unperturbed oscillators. In the large N -limit the frequencies become dense and the frequency differences approach zero, causing all terms containing the small divisors to become infinite. Another problem is related to the appearance of secular terms that are proportional to a power of time t , and, therefore, restrict the application of time-dependent expressions to finite times. In order to avoid these secular terms, the Kryloff-Bogoliubov method [19] was modified [21] and applied [20] to the FPU model.

Specifically, second-order perturbation theory was found to give an accurate estimate (within 15%) of the recurrence time and amount of energy exchange in the FPU problem. On the other hand, it was revealed that for some cases numerically studied in Ref.[1], higher-order analysis is required due to a relatively large nonlinearity (when the nonlinear term is of the order of one-tenth of the linear term, in energy units). The important conclusion of these studies is that, strictly speaking, the FPU model does not belong to the category of weak coupling.

It was also indicated [20] that when discussing the limit $N \rightarrow \infty$, one should distinguish two different limits. The first one considered in Ref.[22] (see discussion below), assumes that the length $L = Na$ of the chain remains constant due to the decreasing spacings, a , between the particles. Correspondingly, the effective coupling $\bar{\alpha}$ decreases with N as $2\alpha/N$ (correspondingly, $\bar{\beta} = 3\beta/N^2$). In this way, by normalizing time $t \rightarrow tN$ and the spacial coordinate $z \rightarrow zL^{-1}$, one can obtain the following partial differential equations,

$$\frac{\partial^2 x}{\partial t^2} = \left[1 + \bar{\alpha} \frac{\partial x}{\partial z} \right] \frac{\partial^2 x}{\partial z^2} \quad (8)$$

and

$$\frac{\partial^2 x}{\partial t^2} = \left[1 + \bar{\beta} \left(\frac{\partial x}{\partial z} \right)^2 \right] \frac{\partial^2 x}{\partial z^2}. \quad (9)$$

The corresponding initial conditions are prescribed over the range $0 < z < 1$ as $x(z, 0) = x_0(z)$ and $\partial x / \partial t|_{t=0} = 0$.

The other possible limit assumes the parameters of the chain are constant. Therefore, as $N \rightarrow \infty$, the length L becomes infinite and the frequency spectrum becomes dense. This is the limit typically discussed in the literature, especially, for the study of irreversible processes. One of the main questions is how the statistical properties of this system depends on the number N of interacting particles.

As is shown in Ref.[20], the phenomenon of recurrence in nonlinearly coupled oscillators is quite robust. Namely, assuming the coupling constant in Eq.(1) to be different for different particles (a kind of imperfection), one can 'kill' the recurrence only with a sufficiently strong imperfection. This important fact indicates that the FPU recurrence is not an artifact of the chosen forces between particles.

The meaning of the FPU recurrence and its relevance to the problem of ergodicity was thoroughly discussed in Ref.[23]. Taking the results of FPU to be fundamental, it was suggested that ergodicity may not be required for the onset of thermalization in dynamical

systems. In fact, this was a new insight into the problem of the foundations of statistical mechanics. In support of this point, it was noted that even a completely integrable system of linearly coupled oscillators shows a kind of thermalization for generic initial conditions. Specifically, after initially exciting one particular mass in the linear chain, one can observe an effective energy sharing among all particles. Having this analogy in mind, the authors of Ref.[23] performed an analytical study of energy sharing between linear modes in the α -model (1) with 2,3,5 and 15 oscillators. One of the results of this analysis was a modification of the resonance condition obtained previously in Ref.[18] required for strong energy sharing, $\sum m_k \omega_k \lesssim \alpha$, where m_k are nonzero integers which depend on the particular coupling used. It was also found that, apart from this condition, strong energy sharing occurs for only certain initial conditions, not for all conditions. As a result, it was concluded that the dynamics of the FPU model may be consistent with the existence of additional integrals of motion; however, one can still speak about thermalization. To check this, the distribution of linear mode energies $E_k = \dot{Q}^2 + \omega_k^2 Q^2$ was obtained numerically for $n = 5$ by examining the time dependence of $E_k(t)$. A very good correspondence to the exponential dependence was found, in accordance with the predictions of statistical mechanics.

Thus, a new approach to thermal equilibrium problem was suggested: instead of the search of the ergodicity, one should study the conditions for strong energy sharing between normal modes. Moreover, it was suggested that in addition to the total energy, other integrals of motion may exist. At least one integral of motion was indicated to exist [23], due to a peculiarity of the model (the unperturbed part is purely linear, unlike many other examples for which in the absence of perturbation the unperturbed motion is nonlinear, see the discussion below).

A new viewpoint according to which typical nonlinear systems are non-ergodic, has found rigorous confirmation based on the extensive mathematical studies of A. Kolmogorov, V. Arnold and J. Moser (KAM theory, [24, 25, 26], see, also, in [27]). In 1954 Kolmogorov formulated the theorem that states that a weak nonlinear perturbation of an integrable system destroys the constants of motion only locally in the regions of resonances. In other regions of phase space, a set of points of positive measure remains for which quasi-periodic motion persists. This effect occurs for quite generic conditions on both the unperturbed motion and the type of perturbation. Loosely speaking, these conditions are: the unperturbed system has to be nonlinear and the perturbation has to be weak enough and with a

sufficient number of continuous derivatives. In the first proof of V. Arnold of Kolmogorov's theorem [25], for technical reasons, the number M of derivatives was assumed to be vary large. However, in subsequent studies by J. Moser [26], the minimal value of M was significantly reduced (see, also, [16, 17] where corresponding estimates of this number were discussed and improved). Although a direct application of KAM theory to the FPU model is questionable (see discussion below), the main result according to which one should not expect the ergodicity for a weak nonlinear perturbation, was essential for the acceptance of a non-ergodic dynamics in nonlinear lattices.

Another perturbative approach has been suggested in Ref.[28]. It is based on the concept of Birkhoff-Gustavson normal forms as approximations to the Hamiltonians of the FPU lattices. Using these forms, one can show that for weak nonlinearity the motion of the FPU model is near-integrable. Further developments of this approach are reported in Refs.[29, 30] where the role of discrete symmetries and resonances was examined in great detail. In was also claimed that with the use of normal forms, the KAM theorem can be verified.

In view of the KAM theory, it is important to mention the paper [31] in which energy sharing and equilibrium were numerically studied for a chain of particles with elastic collisions. Specifically, in addition to linear forces between particles, elastic collisions were assumed caused by the finite diameters of particles. In contrast to the recurrence dynamics in the FPU model, in Ref.[31] behavior that can reasonably be described as ergodic was found for $N = 3$ up to $N = 32$ particles. This ergodicity was observed both in the equipartition of the energy among all linear modes, in the time average, and by a rapid relaxation to equilibrium with the predicted values of temperature and pressure. This result was extremely important for the understanding that the type of interaction between particles plays essential role. As was understood later, the numerical data of Ref.[31] are in agreement with a rigorous proof by Y. Sinai [32] of ergodicity for a system of hard spheres with elastic collisions contained in a box. Moreover, apart from ergodicity, *mixing* was proved in Ref.[32] which currently is considered as the most important property of dynamical chaos. Note that mixing automatically implies ergodicity.

IV. INTEGRABILITY

Inspired by the FPU paradox, in 1962 N. Zabusky analytically studied the continuous limit (8) of the α -model (1). He found an exact analytical solution for fixed initial conditions which turns out to break down at time $t_c \sim 1/\bar{\epsilon}$. At this time, the first derivative x_z develops a discontinuity, therefore, x_{zz} becomes singular. This means that the long-time dynamics of the FPU can not be approximated by the differential equations (8). On the other hand, for time scales less than the breakdown time t_c the comparison of the analytical solution with numerical data of [1] was reasonable. As was found in [22, 33], this critical time t_c corresponds approximately to the time at which the energy in the second mode reaches its first maximum (if only the mode with $k = 1$ is initially excited).

Further analysis [33] showed that to study analytically what happens in the related continuous model, one must include the higher spatial derivatives that were omitted in taking the lowest continuum limit (8-9). To do this, one should use the following Taylor expansion of spatial and temporal differences,

$$x_{n\pm 1} - x_n = \left[\pm ax_z + \frac{a^2}{2}x_{zz} \pm \frac{a^3}{6}x_{zzz} + \frac{a^4}{24}x_{zzz\cdots} \right]_{z=z_n} \quad (10)$$

where $a = L/N$ and $x(z) = x_n$, $z = na$. Therefore, the corresponding equation for the *beta*-model takes the form,

$$\frac{\partial^2 x}{\partial t^2} = \left[1 + \bar{\beta} \left(\frac{\partial x}{\partial z} \right)^2 \right] \frac{\partial^2 x}{\partial z^2} + \frac{a^2}{12} \frac{\partial^4 x}{\partial x^4} \quad (11)$$

which describes shallow water waves in classical hydrodynamics (see the discussion in [34]).

For traveling waves in one direction only (e.g., to the right), one can approximately derive the equation

$$\frac{\partial u}{\partial \tau} + u \frac{\partial u}{\partial \xi} + \delta^2 \frac{\partial^3 u}{\partial \xi^3} = 0 \quad (12)$$

which is known as the Korteweg-de Vries (KdV) equation [35]. Here $u = \partial x / \partial \xi$, $\xi = z - c_0 t$, $\tau = \bar{\epsilon}^* t$, $\bar{\epsilon}^* = \frac{1}{2} \bar{\epsilon} c_0$, and the velocity c_0 in our units is 1. The parameter $\delta^2 = a/24\bar{\beta}$ is the dispersion which plays essential role in discrete lattices.

Apart from shallow water waves, the KdV equation is used to describe hydromagnetic waves in cold plasmas, ion-acoustic waves, and long waves in anharmonic crystals (for references see [34]). Numerical study [4] of this equation in 1965 (see, also, [36]) has led to the discovery of solitary waves (or solitons), nonlinear waves that propagate through the media

without changing their form. Specifically, it was observed that starting with the simplest initial condition ($x(z, 0) = C \sin \pi z$ with $\dot{x}(z, 0) = 0$), solitons appear and strongly interact with each other, however, after interaction they preserve their identities. This remarkable property of stability of solitons (see, also, [37]) was treated as an indication of the existence of a large number of integrals of motion. Due to the direct relevance of the KdV to the FPU model, the authors of Ref.[4] proposed that the recurrent dynamics in FPU lattices may be explained in terms of solitons as well.

The numerical discovery of solitons [4] has attracted much attention to the KdV equation and triggered extensive analytical studies. In particular, in Ref.[38] it was rigorously shown that two solitons keep their shape after interacting, and specific methods were proposed to prove the stability for the general case of any large finite number of solitons. Further heuristic methods were developed in Ref.[39] to predict the number and speed of solitons emerging from arbitrary initial conditions. Later, a nonlinear transformation between the KdV equation and another nonlinear equation (namely, by changing the term uu_z by u^2u_z in Eq.(12)) was found in Ref.[40]. After this, a rigorous method for solving the KdV equation was developed in Refs.[41, 42], by reducing the original nonlinear problem to a linear one. As a result, complete integrability of the KdV equation was proved for fixed boundary conditions. Similar properties of the KdV equation with periodic boundary conditions have been found numerically in direct numerical simulations [36].

This remarkable integrability of the KdV equation was used to propose that similar properties may occur in nonlinear lattices. Thus, in Ref.[43] a nonlinear model (Toda-lattice) was introduced (see, also, [44]) with nearest neighbors interacting through the following potential,

$$U(z) = \frac{a}{b}e^{-bz} + az \quad (13)$$

where a and b satisfy $ab > 0$. The corresponding equations of motion have the form,

$$\ddot{x}_n = a \left[e^{-b(x_n - x_{n-1})} - e^{-b(x_{n+1} - x_n)} \right]. \quad (14)$$

Formally, this lattice reduces to a harmonic lattice with the spring constant $\kappa = ab$ in the limit $b \rightarrow 0$, keeping $ab = \text{const}$. One can also see that this corresponds to the α -model (1) when $\alpha = -b/2$. Moreover, in the limit as $b \rightarrow \infty$, the Toda lattice reduces to a hard sphere systems. Therefore, the model (14) covers two extreme limits of the interaction, from harmonic to hard-sphere.

The first indication of the integrability of the Toda lattice appeared in numerical data of Ref.[45]. It was shown that for $N = 3$ the trajectories cross the Poincarè section in a way that the corresponding points lie on smooth curves. No evidence was found of regions with scattered points that is typical of integrable systems. Moreover, when studying the divergence of neighboring phase trajectories, linear separations of the trajectories were always observed. This fact is indicative of stability of motion, unlike the opposite case of unstable motion for which the separation of trajectories increases exponentially with time. Similar behavior was found for $N = 6$ particles. Later, it was rigorously proved [46] that this lattice with periodic boundary conditions has N integrals of motion. Even the initial value problem can be solved for an infinite Toda-lattice by using the inverse scattering method, if the motion is restricted to a finite region of phase space, see details in [34]. It is important to stress that the integrability of motion in the Toda lattice does not prevent energy sharing among the linear modes (defined in the absence of nonlinearity). As was shown in Ref.[45], energy sharing increases with an increase of nonlinearity. Therefore, good statistical properties can appear in completely integrable systems, provided the number of degrees of freedom is large, but not for all quantities.

As a result of the very impressive discovery of integrability of the KdV and Toda lattices, it was often assumed (and this opinion still persists in some publications) that the FPU paradox was fully resolved by the concepts of integrability and solitons. However, the reality turned out to be even more exciting because of the direct relevance of the FPU problem to the dynamical chaos.

V. STRONG CHAOS

Analytical treatment

Another approach to the FPU problem is based on the concept of dynamical chaos. For about ten years after 1955, an understanding of the fact that dynamical systems with few degrees of freedom may manifest quite strong irregular motion, turned into systematic studies of “stochasticity”. This term was used to relate the irregular motion of completely deterministic systems to that known for physical systems which are governed by stochastic forces. Currently, two other terms are widely accepted, *dynamical chaos*, and *deterministic*

chaos. These terms more correctly emphasize the purely deterministic nature of chaos. This is in contrast to conventional statistical mechanics which assumes, *ad hoc*, a probabilistic description of systems due to their underlying “randomness”. For a long time, the problem of establishing the conditions under which statistical mechanics is valid, was one of the central problems in theoretical physics. The concept of dynamical chaos solves this problem, a fact which is still not well accepted by physicists although, is quite familiar to mathematicians. According to the modern viewpoint, classical statistical mechanics can be considered as a *particular case* of classical mechanics which describes *both* regular and chaotic dynamics. Thus, a statistical description, being useful and important, is an approximate one, and can be deduced from dynamical equations of motion under the conditions of dynamical chaos.

One of the important studies of the problem of foundation of classical statistical mechanics is the work by N.Krylov [47]. In his book, he analyzed the mechanism responsible for statistical behavior of dynamical systems, which is the exponential instability. By this term one means that the separation $\Delta(t)$ between two neighboring trajectories (in phase space) for generic initial conditions increases in time exponentially, $\Delta(t) \sim \Delta(0) \exp(ht)$. Here, the rate of the instability, h , is called the “dynamical entropy”. Later, this quantity was rigorously studied by Kolmogorov and Sinai and it then assumed the name “Krylov-Kolmogorov-Sinai entropy” (*KS-entropy*). The positiveness of this quantity, $h > 0$, currently is used as the definition of dynamical chaos. Due to this instability, the dynamics of a system is extremely sensitive to its initial conditions, thus leading to mixing and other statistical properties (for details see, for example, [17, 48]).

Numerical and analytical studies of dynamical chaos were strongly influenced by accelerator physics. As is known, the motion of charged particles in circular accelerators is affected by forces due to external magnetic fields that are required for the focusing of particles in a stable orbit. On the other hand, since the particles perform many revolutions ($10^7 - 10^{12}$) around a ring, nonlinear forces, although weak, are important for a long-term stability of particle motion. Early studies of nonlinear resonances in accelerators in 1956-1959 have led to the understanding that they can result in a kind of irregularity of motion. To the best of our knowledge, the first observation of this effect refers to the report [49], in which the authors numerically studied the motion of electrons in a periodic electromagnetic field. Similar problems of stability have emerged when studying the motion of electrons in magnetic traps (see the references and discussions in [16, 17]).

The analysis of the stability of motion of particles in the presence of nonlinear perturbations has led B. Chirikov in 1959 to the concept of the *overlap of nonlinear resonances* [5]. This term refers to the situation when nonlinear resonances strongly interact with each other. Specifically, it was found that when the nonlinearity is weak, one can consider any particular resonance separately, making use of perturbation theories. However for a strong nonlinearity, the resonances can not be treated separately because in the frequency space (or correspondingly, in action space) they are very close to each other. Thus, the overlap of resonances gives rise to the onset of a specific instability which leads to irregular (chaotic) motion. The analytic estimate for this overlap, known as the Chirikov criterion, turned out to be very effective for determining the conditions under which the dynamical chaos occurs in nonlinear systems [17]. Results of first experimental studies of the nonlinear resonances, their interaction and the onset of stochastic motion in electron-positron storage rings were reported in Refs.[50, 51].

Application of the overlap criterion to the FPU model (2) has been reported in Ref.[6]. According to Eq.(7), there are two kinds of nonlinear terms. The term with $i = j = l$ on the right-hand side plays a specific role and can be written separately,

$$\ddot{Q}_k + \omega_k^2 Q_k \left[1 - \frac{3\beta}{4N} \omega_k^2 (2 - \omega_k^2) Q_k^2 \right] = \frac{\beta}{8N} \sum_m F_{km} \cos \theta_{km}, \quad \dot{\theta}_{km} = \bar{\omega}_{km}. \quad (15)$$

Here $\bar{\omega}_{km}$ are the exact frequencies (including perturbation terms) of oscillations of normal modes that slowly depend on time. One can see that the selected term determines the nonlinear correction

$$(\delta\omega)_k = -\frac{3\beta}{8N} \omega_k^2 (2 - \omega_k^2) \langle Q_k^2 \rangle \quad (16)$$

to the linear frequency ω_k . Even when small, this correction can not be neglected since it depends on the energy of the k -th normal model. Note, that $(\delta\omega)_k$ can be obtained in first order perturbation theory, by averaging $\langle Q^2(t) \rangle$ over the period of the unperturbed motion.

The equations (15) describe the motion of nonlinear oscillators under the influence of external forces with amplitudes $\beta F_{km}/8N$. The spectrum of the perturbation due to these forces is given by the resonance frequencies $\omega_{km} = 2 \sin \frac{\pi(k+2m)}{2N}$ with integers $\pm m = 0, 1, 2, \dots$ [6]. For small values of $k \ll N$ (low modes corresponding to acoustic waves) the separation between resonances in frequency space is $\omega_{k+1} - \omega_k \approx 2\pi/N$. Therefore, if nonlinear oscillations of a particular normal mode such as the maximal shift of frequency is much less

than Δ_ω , then one can neglect the influence of neighboring resonances. In this case one can obtain the width, $\Delta\Omega$, of a nonlinear resonance by keeping one resonance term only. The resonance criterion states that if $\Delta\Omega$ is of the order or larger than the separation

$$\Delta_\omega = \omega_{k+1} - \omega_k \quad (17)$$

between neighboring resonances, then trajectories can no longer be associated with a particular k -resonance and can wander between these two resonances. This transition from one to another resonance occurs in a quite irregular way, thus resulting in a kind of diffusion in frequency (or in action) space. In this case strong energy sharing between resonances is expected.

For acoustic waves with $\Delta_\omega \approx 2\pi/N$ the critical perturbation for the resonance overlap is defined as [6],

$$3\beta_{cr} \frac{E}{N} \sim 3 \frac{\sqrt{\Delta k}}{k} \quad (18)$$

where E is the total energy of the lattice, therefore, E/N is the energy per normal mode, and Δk is the number of initially excited modes around the central k -mode. Here, units in which the distance between particles is fixed, $a = 1$, are used, therefore, the length of the chain is $L = N$.

For the case in which high (optical) modes are initially excited, $N - k \ll N$, the critical perturbation is given by the estimate [6],

$$3\beta_{cr} \frac{E}{N} \sim \frac{3\pi^2 \Delta k}{N^2} \left(\frac{k}{N} \right)^2. \quad (19)$$

Note that in this case the mean frequency spacing between nearest resonances is much less than that for low normal modes, $\Delta_\omega \approx \pi^2/2N^2$, see Eq.(17). For both acoustic and optical cases, the quantity $3\beta_{cr} \frac{E}{N} \approx 3\beta_{cr} \left(\frac{\partial x}{\partial z} \right)_m^2$ is the nonlinear term in the corresponding continuous model, which serves as a control parameter of perturbation.

The above estimates determine the ‘‘stochasticity border’’ for the β -model. From the condition (18) one can see that for the lowest value $k = 1$ (the most studied case in the FPU model [1]), one must have a very strong perturbation in order to observe the non-recurrent behavior. Indeed, the nonlinear term in energy units in numerical studies of FPU has never exceeded 10%, therefore, the system was well below the stochasticity border. This explains the FPU paradox. On the other hand, from the estimate (19) for high modes with k close

to N , the critical value of the nonlinear parameter β is relatively small and one can easily observe irregular motion with strong energy sharing among a large number of high modes. In fact, in a few runs of FPU with higher modes, one can see a more complex dynamics, and according to the expression (19), the parameters used in [1] approximately correspond to the border of stochasticity. It was stressed in Ref.[6] that the border of stochasticity between quasi-periodic and stochastic motion is not sharp. Rather, it is relatively wide and has a very complicated structure. For this reason, strong dependence on initial conditions is expected in the transition zone.

The analytical estimates obtained above refer to the overlap of two nearest resonances with k and $k + 1$. Therefore, they give the conditions for the onset of *local* stochasticity, and should not be treated as the threshold of widespread sharing of energy between *all* linear modes. The analysis [6] shows that when only a particular k -mode is excited, the stochastic exchange of energy occurs to higher modes as well, at least for some group of initial linear modes. Indeed, with the flow of excitation in k -space from low to higher k , the border of stochasticity decreases with increasing k , see Eq.(18). It is interesting to note that, unlike the case of acoustic waves with $k \ll N$, if high optic modes are initially excited, strong sharing between acoustic and optical modes occurs provided that low modes initially have a small amount of energy.

Based on the resonance overlap approach, a specific study has been performed in Ref.[52] for the α -model (1). The analytical treatment has shown that this model appears to be much more stable than the β - model. This is due to the fact that the nonlinear correction for linear frequencies in the first order of perturbation theory vanishes for the α -model (see Eq.(6)) and one needs to consider the second order approximation. Also, it was found that the most favorable conditions for the onset of stochasticity in this model occur when initially the modes with $k \sim N/2$ are excited. To compare with, both the limits of $k \ll N$ and $k \sim N$ turn out to be more stable. In general, the analysis of Ref.[52] indicated that the α -model may be quite close to being integrable and further numerical studies have confirmed this.

Numerical data

Extensive numerical studies of the α - model have been performed in Refs.[7, 53, 54] exploring the above analytical predictions. As was discussed in Ref.[6], the most important

property of stochastic motion is the exponential instability of trajectories with respect to a small change of initial conditions. To measure this instability, it was proposed to use the existence of the additional integral of motion in the FPU-model, namely, parity. As is clear from equations of motion, for fixed boundary conditions, $x_0 = x_{N+1} = 0$, there is no interaction between the even, $k = 2, 4, 6, \dots$, and the odd, $k = 1, 3, 5, \dots$, modes. Therefore, when only odd modes are initially excited, the energy of the even modes has to be zero. However, in numerical experiments [7] it was unexpectedly observed that when exciting the first mode with $k = 1$, the energy of even modes is not exactly zero, and moreover, this energy increases with time. Above the border of stochasticity the rate of this increase was found to be exponential, until the energy of the even modes approaches the energy of the odd modes. The mechanism of this phenomena is due to round-off errors (of the order of 10^{-19}) which can not be avoided in numerical studies. One should note that these errors are not random since they are determined by a particular fixed algorithm. Therefore, they should be treated as a kind of dynamical perturbation which is not included in the original equations of motion. As a result, the energy of the even modes can be considered as a distance (in energy space) between two close trajectories. This concept was found to be very useful for determining the degree of instability.

Given, after some initial time, a small amount of energy in the even modes ($\sim 10^{-14}$ of the total energy), the rate of instability for the β -model (2) has been numerically computed as a function of the model parameters. Three regions of initial conditions have been examined: small modes with $k = 1$ or $k \ll N$, high modes with $k \lesssim N$, and the intermediate region with $k \approx N/2$. In all of these cases quite good correspondence with the analytical estimates of Ref.[6] has been found. Specifically, for perturbations below the critical value, the rate of instability was approximately zero. This was in significant contrast to perturbations above the border, for which strong exponential instability was easily observed. In order to be sure that the numerical method used in determining the border is not an artifact, an additional check was done for two trajectories belonging to the same parity. The results were found to be analogous to those obtained from the energy increase of the even parity modes.

In order to study quasi-periodic oscillations for normal modes involved in the dynamics, in Ref.[55] the possibility of describing a recurrence using truncated equations of motion was analyzed. It was found that for typical FPU conditions the dynamics of the model can be essentially described by a few equations for the modes close to the initially excited one.

Namely, when exciting the mode with $k = 15$ for $N = 32$, three (with $k = 14 - 16$) and five (with $k = 13 - 17$) coupled equations have been examined numerically.

The important question studied numerically in Ref.[7] is the dependence of the rate h of instability on the perturbation parameter β . As expected from the predictions of Ref.[56], for large values of β the dependence

$$h \approx \Delta_\omega \ln \frac{\beta}{\beta_{cr}} \quad (20)$$

has been found to correspond to numerical data, with Δ_ω as the mean distance between the unperturbed frequencies, see Eq.(17). On the other hand, when the perturbation was not very strong, the dependence turned out to be very different and it can be fitted as $h \approx \Delta_\omega (\beta/\beta_{cr})^{4/3}$. It was proposed that for a weak enough perturbation, the instability, being exponential, is due to high order resonances. Although these resonances are more dense, the diffusion among these resonance is much slower. Therefore, apart from the strong stochasticity (chaos) determined by the overlap of main resonances (due to the first order of perturbation theory), one can speak about *weak chaos* which can also lead (on much larger time scales) to strong energy sharing between normal modes (see Sect. VII).

In addition to the instability of motion, in Ref.[7] other statistical characteristics of the dynamics have been studied as well: energy sharing among modes, the time dependence of the energies of each mode, time correlations $\langle x_n(t)x_n(t+\tau) \rangle$ and $\langle E_k(t)E_k(t+\tau) \rangle$ for displacements and energies, as well as correlations between energies of different modes. The results strongly support the onset of strong chaos above the border as analytically predicted in Ref.[6].

Additional numerical study has been reported in Ref.[53] (see, also, [54]) with higher accuracy and a larger number of particles (up to $N = 500$). These new data confirmed the main findings of Ref.[7] concerning the border of stochasticity. Moreover, the exponential dependence (20) for the rate of exponential instability was also supported by these data. One of new observations was the existence of an initial time scale on which a non-chaotic excitation of modes different from the initially excited one occurs. After this initial time, a stochastic exchange of energy begins. Therefore, it was proposed to modify expression (18) for the stochasticity border by using larger values of k due to this effect. This effect seems to be relevant to the emergence of solitons that occurs in the Toda lattice. Therefore, the following picture seems to be more correct: first, an initial regular dynamics occurs in the

model, with the excitation of higher modes. After some initial period of time, a stochastic exchange between the modes comes into play, with a practical irreversibility of motion and onset of thermalization. Note that this thermalization can be restricted to a finite number of modes, much less than the total number N of degrees of freedom.

To compare with the KdV equation (12), one should recall that this equation is an approximation to the FPU model. The main difference lies in the assumption that the waves traveling in different directions can be considered independently. This fact may be crucial in the analysis of the application of the KdV to the FPU model. In order to check how important the above approximation is, in Refs.[53, 54] a specific study of the FPU model with periodic boundary conditions $x_0 = x_N$ was carried out. The quantity of interest was the emergence of waves traveling in a direction opposite to that of the initial wave. Specifically, the percentage of energy of standing waves in comparison with the total energy for the k -th mode was calculated as a function of the perturbation β at some (large) fixed time. It was found that for small perturbations, opposite moving waves practically do not appear. However, for $\beta \sim \beta_{cr}$ the amount of energy in the waves in the opposite direction is of the order of total energy. This fact demonstrates that for large perturbations the FPU model is very different from the KdV model.

VI. FURTHER RESULTS

Energy sharing and equipartition

The existence of an initial period of time (“induction period”) for which the motion does not reveal strong energy sharing, was studied in detail in Ref.[57] for the β -model with zero boundary conditions (see, also, the study [58] of the 2D model). After this period, strong energy sharing between a large number of modes was clearly seen, thus corresponding to the predictions of Refs.[6] of the onset of strong stochasticity. It was also found that this period increases as the nonlinear coupling decreases. As the criterion for the establishment of thermal equilibrium, in Ref.[57] velocity-velocity correlations between close in the chain particles were used. It was shown that below a critical value of the nonlinear coupling these correlations are very small; this was used as an indication of thermal equilibrium. These results were compared with those obtained for the model with linear coupling only [59] for

which the correlations were found to be stronger due to the absence of ergodicity.

However, the approach of Ref.[57] based on the examination of correlation functions has been criticized in Ref.[60] (see, also, [61]). It was argued that this method does not give global information about the phase space of the system, and strongly depends on the choice of correlation functions. Analyzing other methods for determining the chaotic transition, the authors of Ref.[60] proposed to study the distribution of energy modes after a relatively short period of time. Their analytical analysis showed that at short times this distribution has an exponential dependence, $W(k, t) \sim \exp[-B(t)k]$, on the function $B(t)$ that depends on the model parameters. Numerical data have shown that with a high accuracy the distribution of energies corresponds to the analytical expression for $B(t)$. At later times for large enough nonlinearity the distribution $W(k, t)$ was found to be of the expected form $W(k, t) \sim 1/k^2$, corresponding to the Boltzmann distribution of mode energies. These results also confirm the existence of the stochasticity threshold in its dependence on the nonlinearity parameter β .

An interesting quantity to measure the energy sharing has been proposed in Ref.[62]. This quantity was found to be quite useful in the study of relaxation properties of nonlinear lattices. In order to characterize the energy spread in the mode representation, the spectral (Shannon) entropy $S(t)$ is used,

$$S(t) = \sum_{k=1}^N w_k(t) \ln w_k(t) \tag{21}$$

where $w_k = E_k / \sum_i E_i$ is the normalized energy of a particular mode. The spectral energy is zero when only one normal mode is excited, and reaches its maximal value $S_{max} = \ln(N/2)$ for complete equipartition of total energy among all modes. To avoid clear dependence on the number of oscillators, the normalized quantity

$$\eta = \frac{S_{max} - S_{\infty}}{S_{max} - S(0)} \tag{22}$$

was introduced. Here S_{∞} is the maximum value reached by $S(t)$ in the time evolution, associated with the “asymptotic” value of $S(t)$. This quantity η is bounded between zero (which corresponds to complete “localization” in one mode), and one (which corresponds to perfect equipartition).

Computing the normalized spectral entropy η , in Ref.[62, 63] strong evidence in favor of the existence of an equipartition threshold was given. In numerical simulations, periodic

conditions were used for the β -model, with initial excitation of a group of modes $\bar{k} \pm \Delta\bar{k}/2$ with small values of $\bar{k} \ll N$. The integration period was chosen large enough to ensure a practical independence of η on time. These numerical data revealed the remarkable result of a universal form of dependence of η on the energy density $\epsilon = E/N$ for many values of N from 64 to 512. It is interesting to note that this effect is insensitive to randomization of the FPU model, for which linear forces were assumed to be different for different particles (see details in [62]). According to these results, the threshold of equipartition does not disappear in the large N -limit.

Since in numerical computations [62, 63] the mean value of \bar{k} for initially excited modes was taken to be proportional to N (as well as $\Delta\bar{k} \sim N$), it was claimed, that the obtained results are in formal contradiction to the condition (18) of a strong chaos, where the threshold disappears with $\Delta k \sim k \sim N \rightarrow \infty$. The explanation of this contradiction lies in understanding the meaning of the stochasticity threshold (18). Indeed, according to its derivation, this condition refers to the overlap of nearest resonances only, and there is no direct relation to energy sharing among all modes. Although the numerical data show that a large number of modes appears to share their energy above this threshold, the question about complete equipartition remains open.

An important comparison of the FPU model with the Toda lattice is given in Ref.[64]. As was already discussed (see, e.g. Refs.[45, 65]), quite strong energy sharing may be observed in the FPU model in the regime of strong recurrence, below the border of strong stochasticity. For this reason, the dynamics of the Toda lattice and FPU models were analyzed from the viewpoint of equipartition. As was pointed out, one should distinguish between “energy sharing” and “equipartition”. It was shown that strong energy sharing can be observed in both models. However, equipartition occurs in the FPU model only, which is understood to be non-integrable. The numerical data which demonstrate this difference are based on the form of the normalized spectral entropy η for large times. Namely, for the Toda lattice the spectral entropy $S(t)$ never reaches its maximum value, in contrast to the FPU model for which it does reach the maximum. Therefore, for the Toda-lattice the dependence of η on the energy density $\epsilon = E/N$ does not show a transition to zero.

Stability conditions

In order to characterize the difference between integrable and non-integrable lattices, in Ref.[64] it was proposed to study these models from the viewpoint of stability. Specifically, it was observed that the time dependence of the trajectory in the artificial phase space $\dot{\eta}(t)$, $\eta(t)$ is clearly different for these two cases. Were the FPU trajectories appear irregular and unstable to an external perturbation, for the Toda lattice the trajectories reveal clear quasi-periodicity and stability to this perturbation. Thus, in order to distinguish between integrable and non-integrable chains, a study of the stability of motion is needed.

The first analytical study of the stability of motion in the FPU model is reported in Ref.[55]. It was found that the recurrence dynamics in the β -model with fixed boundary conditions may be correctly described by keeping a small number of equations for those modes that are essentially involved in the dynamics. For these equations, one can write the condition of a linear stability which stems from the corresponding Mathieu equation. According to this condition, a critical value of perturbation exists above which the motion is unstable. However, the relevance of this instability to the overlap of nonlinear resonances remains unclear.

Another approach to instability of motion has been developed in Ref.[66] in application to the KdV equation. It was analytically observed that certain KdV solutions are unstable. Using this fact, an attempt was made to relate this instability to that observed in the FPU lattice. The analytical predictions obtained for the KdV model have been claimed to explain the instability of motion in the FPU model. In this study specific initial conditions in the form of a cnoidal wave were used, for which numerical data manifested a good correspondence to analytical predictions.

The above analytical studies have suffered from the absence of reliable expressions that would predict the dependence on the nonlinear parameter and the number of particles. The first attempt to shed light to this problem was made in Ref.[67] where the stability condition was obtained for the specific case of the highest linear frequency, which is initially excited. Note that for periodic boundary conditions the linear spectrum is doubly degenerate. Therefore, the highest frequency corresponds to the middle of the spectrum, $k = N/2$. Using a variational equation for this mode, a simple approximate formula for the β -model (in the

large N -limit) was derived,

$$3\beta_s \frac{E}{N} \approx \frac{9.7}{N^2}. \quad (23)$$

Applying this estimate in Ref.[57] to numerical data obtained for $N = 15$ and zero boundary conditions, some discrepancy was found. In this respect the authors claimed that their critical value is, in essence, an upper estimate for the threshold of the chaotic transition, and can not be compared with the condition of wide spread energy sharing. Another uncertainty is due to the different boundary conditions used in the analytical evaluation. Later, the stability condition (23) was obtained [68] (with almost the same constant) in the more general context of bifurcations of periodic orbits in nonlinear Hamiltonian lattices, and with some relation to symmetry breaking and vibrational localization (breathers).

Similar analysis has been done [67] for the α -model. The corresponding stability condition turned out to have the same form,

$$\alpha_s \frac{E}{N} \approx \frac{0.84}{N^2}. \quad (24)$$

This result is quite unexpected since the α -model is assumed to be closer to being integrable than the β -model. Additional study of the stability of the α and β -models with attractive potentials, $\alpha < 0$ and $\beta < 0$ was performed in Ref.[67].

The important results are reported in Ref.[69]. Using the so-called *narrow packet approximation*, the following stability condition was derived for the β -model,

$$3\beta_g \frac{E}{N} \approx \frac{\pi^2}{N^2}. \quad (25)$$

It was found that for $\beta > \beta_g$ a parametric instability of motion emerges for wave packets that populate a number of linear modes for k within the interval $|k - k_0| = \Delta k \ll k_0$ in a region of the optical phonon spectrum around $k_0 \approx N/2$. Note that for the periodic boundary conditions used in Ref.[69], the value $k_0 = N/2$ corresponds to the mode with highest frequency, due to the double degeneracy of unperturbed frequencies ω_k . The point is that for such initial conditions the FPU model reduces to the nonlinear Schrödinger equation, which is known to be completely integrable (see details and discussion below). This fact establishes a link between nonlinear lattices of the FPU type and models which are now widely used in application to the Bose-Einstein condensation.

According to the condition (25), if the amplitude of the initially excited modes exceeds some critical value, the parametric instability results in a rapid spread of the wave packet

over many linear modes. Even though this packet spreads rapidly, the narrow packet approximation remains valid for some time. One can see that formally Eq.(25) coincides with the condition for the onset of stochasticity due to overlap of two close nonlinear resonances, see Eq.(19). It should be stressed that strictly speaking, both conditions correspond to the low boundary for the emergence of chaos and may be different from those for strong energy sharing among all modes. Note also that the result of Ref.[69] practically coincides with Eq.(23), which also refers to the instability of the highest mode.

It is also very instructive that the condition of the validity of the narrow packet approximation obtained in Ref.[69] reads as

$$3\beta_p \frac{E}{N} \approx \frac{\pi^2}{N}. \quad (26)$$

This condition may be treated as the critical value above which strong equipartition among *all* modes arises in the lattice. The important point is that the additional factor N stands in the denominator of Eq.(26) in comparison with the stability condition (25). Therefore, one can propose that the difference between the critical value of perturbation for *local* (chaotic) energy exchange between nearest modes in the k -space, and *global* equipartition of energy in the lattice, is mainly due to this additional N -dependence. Note, however, that what we discuss here refers to the initial excitation of the high frequencies only. The problem of stability for small values of k (acoustic waves) seems to be very different.

The problem of stability of solutions in the β -model with periodic boundary conditions has been studied in a generalized approach in Ref.[70]. A complete rigorous analysis has been done for the π -mode considered in Ref.[67], resulting in an additional correction term which depends on number of particles. It was shown that other exact solutions exist below some critical value of nonlinear parameter β . Moreover, the presence of multi-mode invariant manifolds was shown. It was also pointed out that the relevance of the instability of these solutions to widespread stochasticity is not clear, although numerical data generally manifest such a connection (compare Eq.(23) and Eq.(25) with Eq.(19) where $k \approx N$). The general case of a nonlinear lattice with both α and β terms has been under careful study in Ref.[71] where, in particular, the relevance of the instability of the highest frequency mode to stable localized solutions (breathers) has been discussed (see, also, [72, 73]). The role of periodicity of boundary conditions can be examined with the use of Birkhoff normal forms, see details in Ref.[74].

Lyapunov exponents

As is discussed in Ref.[6], the important quantity that characterizes dynamical chaos, is the local instability for which two close trajectories in phase space diverge, in time, exponentially fast. For this reason, many modern numerical studies are based on the calculation of the rate of this instability (KS-entropy). A detailed analytical and numerical analysis of the method of calculating the KS-entropy in many-dimensional dynamical systems has been performed in Ref.[75]. The approach developed by these authors was found to be extremely useful in the study of dynamical chaos in various physical systems. Extensive numerical analysis of KS-entropy in application to anharmonic chains with a Lennard-Jones interaction is reported in Ref.[76]. This lattice is known to exhibit the stochasticity transition in a more clear way, compared with the FPU model (see, e.g. Ref.[77]). These data show that the standard procedure of computing the dynamical entropy due to the average $h \sim \langle \ln |d(t)/d(0)| \rangle$ along the trajectories is quite stable with respect to different kinds of computational errors, and gives reliable results. However, it should be noticed that in this method the quantity h is not exactly the Kolmogorov entropy, although it often is close to it. The exact expression for the KS-entropy is a sum of all positive Lyapunov exponents (LE) (for details and references, see, e.g. Ref.[48]). Actually, the above method determines the largest Lyapunov exponent, and this is sufficient to distinguish between chaotic motion, $h > 0$, and (quasi)-periodic, $h = 0$, motion. On the other hand, it was argued in Ref.[60] that the largest Lyapunov exponent may not show a correct picture since it does not experience different ergodic regions. However, in Ref.[78] an opposite conclusion was drawn from numerical data, according to which different non-connected regions of chaos can also be detected, by searching the fluctuations of the largest Lyapunov exponent.

Since the largest Lyapunov exponent $\lambda_1 \approx h$ can be used as a measure of chaoticity in a system, analytical estimates of λ_1 and its scaling properties are extremely important. In Ref.[79] it was argued that the spectrum of Lyapunov exponents for long chains may be well approximated by the Lyapunov exponents of products of independent random matrices, provided the energy per mode, ϵ , is sufficiently large. This point has been used in Ref.[80] where an analytical estimate for λ_1 was derived in the large N -limit. Specifically, a Gaussian model with noise was used as an approximation of the dynamical FPU model, and the analytical results were compared with numerical calculations. An amazingly good

correspondence was found between analytical predictions and numerical data, and two scaling dependencies were discovered, $\lambda_1(\epsilon) \sim \epsilon^2$ for $\epsilon \rightarrow 0$, and $\lambda_1(\epsilon) \sim \epsilon^{1/4}$ for $\epsilon \rightarrow \infty$. In comparison with the previously obtained numerical data in Ref.[81], the first scaling was confirmed. As for the second one, for large ϵ , their result $\lambda_1 \sim \epsilon^{2/3}$ of [81] was different. Later theoretical study in Ref.[82] confirmed the dependence $\lambda_1(\epsilon) \sim \epsilon^{1/4}$ by making use of a different approach. An important point of the studies in Refs.[80, 81, 82] is that there is a clear transition from one scaling to another. According to Ref.[82], this transition occurs at $E \approx \pi^2/3N\beta$ which corresponds to the onset of strong chaos, see (19). This very important fact confirms previous findings that below the border of strong chaos, found from the Chirikov criterion, weak chaos persists. Thus, one may expect energy equipartition for any weak nonlinearity, however, after much longer times (see discussion below).

Much more information can be drawn from the knowledge of *all* Lyapunov exponents, not only from the largest one. A numerical method of computing all LE in many-dimensional systems has been developed in Ref.[83, 84]. Currently, this method is widely used in many applications, both classical and quantum. Of particular interest is the distribution of LE as a function of the index j according to which the Lyapunov exponents are ordered in an increasing way. Spectrum of the LE has been numerically studied for the β -model in Ref.[85] where it was found that already for 40 to 60 particles the limiting distribution emerges. Thus, these results demonstrate the existence of a thermodynamical limit for the spectrum of LE. The obtained distribution was discussed in Ref.[85] with a view towards its relevance to random matrix approaches.

A very interesting study was reported in Ref.[86]. As was already mentioned above, the α -model seems to be more stable than the β -model. For the first time this point was noted in Ref.[52] where the resonance overlap criterion was obtained for the α -model. The same conclusion can be drawn from the analysis of nonlinear differential equations of the KdV types, from the viewpoint of their integrability [87]. In order to quantify the difference between the integrable Toda lattice and non-integrable α -model, in Ref. [86] the largest LE, λ_1 , was computed for both models as a function of time. It was found that at large time scales which are inversely proportional to the energy density $\epsilon = E/N$, the time dependence of $\lambda_1(t)$ is practically indistinguishable for both models. However, starting from some critical time, a drastic difference is clearly seen: for the α -model λ_1 tends to a positive value, in contrast to the Toda-lattice where λ_1 continues to vanish with an increase of time. As a

possible explanation of this remarkable effect, the authors conjectured the coexistence of tiny chaotic regions and relatively large regions of stable motion in the phase space of the β -model. It was argued that the trajectory might be trapped for a long time in a relatively large stable regions. Then after some time, the trajectory “finds” a way to leave the stable region and enter a stochastic region. Apart from this suggestion, there is no satisfactory explanation of the observed effect. Note that the computation performed in Ref.[86] was in exact correspondence with the old computations of FPU, however, with the highest accuracy and for the longest time ever achieved. Specifically, the lowest frequency mode with $k = 1$ was initially excited.

The observed effect is interesting from many viewpoints. First, it again confirms the point that the practical difference between integrable and non-integrable models may be very small, and this difference can be detected only on very large time scales. Second, it gives direct evidence of the existence of the threshold of *weak* chaos, although indirect indications for the β -model have been reported before (see, e.g. [88]). Third, it shows that the largest Lyapunov exponent λ_1 seems to be the only quantity which can give reliable results concerning weak chaos. By searching other initial conditions, the authors of Ref.[86] claim that the existence of the stochasticity threshold ϵ_c can be clearly seen by examining λ_1 .

Another important result of Ref.[86] is the N -dependence of the stochasticity threshold for the case when all modes are initially excited. With an increasing number of particles, it was found that the scaling dependence $\epsilon_c \sim 1/N^2$ is well supported by the numerical data. Thus, in the limit $N \rightarrow \infty$ the threshold in the FPU model vanishes. So far, there is no satisfactory explanation of this result. Note that most studies have been done for the β -model, and it is questionable whether there are quantitative properties shared by these two models.

VII. WEAK CHAOS

As was shown analytically in Ref.[89], nonlinear lattices of the FPU type have an important peculiarity. Specifically, the unperturbed motion is linear, therefore, the KAM theory [24, 25, 26] formally can not be applied. Indeed, one of the conditions for applicability of the KAM theory is that the unperturbed frequency of oscillations has to be dependent

on energy. For this reason, there is no rigorous ground to expect that under a very weak perturbation the motion of the FPU model remains stable. Indeed, the analysis of Ref.[89] has shown that the resonance overlap can occur for arbitrarily small but nonzero values of the parameters α and β . Therefore, stochastic motion does not disappear in the limit of vanishing perturbation, although the degree of stochasticity may be very small. This situation, known as “nearly linear oscillations” arises in many practical applications and requires specific methods of study [90].

Another effect which is important in view of discussion about the behavior of the FPU models for a weak perturbation, is the influence of nonlinear resonances that appear in high orders of perturbation theory. Indeed, the overlap criterion [6] is based on consideration of the first-order resonances only. On the other hand, second-order resonances may create a wide resonance net and lead to strong equipartition which can occur at much larger time scales. This problem was briefly discussed in [6, 7], and further numerical studies have confirmed the point that apart from *strong* chaos (with a fast equipartition and large values of the Lyapunov exponents), one can speak about *weak chaos*. This weak chaos is characterized by a much weaker equipartition of energy, smaller values of LE, and a different kind of scaling of the LE. Recently, the role of these high order resonances was examined in Ref.[91], together with a detailed analysis of peculiarities related to the nearly-linear character of the oscillations. The α -model was examined and the stochasticity threshold has been found for both strong and weak interactions.

The concept of weak chaos poses an important question of whether the threshold of stability for an infinite time scale vanishes in the thermodynamical limit, $N \rightarrow \infty$. To shed some light in this problem, in Ref.[92] numerical simulations have been made for the β -model (with periodic boundary conditions) paying main attention to the long-time behavior. Measuring the spectral entropy (22), it was found that the result strongly depends on whether initially one mode, $\Delta k = 1$ or a group of modes with $\Delta k \gg 1$ is excited (with both k and Δk proportional to N). In the first case, the data indicate the existence of a threshold $\beta E/N \sim const.$ In the second case the threshold vanishes as $\beta E/N \sim 1/N^\gamma$ with $\gamma \approx 1$. As one can see, these results are in contradiction with the estimate (18) obtained for resonance overlap. The existence of finite times of relaxation to the equipartition has been also confirmed in Ref.[93] where the strong influence of initial transient times has been detected, after which generic behavior emerges with no dependence on initial conditions.

One specific question widely discussed in the literature is how fast is the relaxation to a steady-state distribution of energy among normal modes. Extensive study of this problem was performed in Ref.[81] (see, also, [94]). The authors made an attempt to relate the data for time dependence of the spectral entropy $\eta(t)$, to the estimates of Refs.[95, 96, 97] for the rate of the Arnold diffusion. In 1964 V. Arnold has proved [98] that many-dimensional nonlinear systems are, in general, globally unstable due to a very peculiar diffusion (*Arnold diffusion*), for details see, e.g. [17, 48]). Loosely speaking, this diffusion occurs (below the border of resonance overlap) for initial conditions *inside* the narrow stochastic layers which surround any nonlinear resonance. Due to an everywhere dense set of resonances (of different orders), starting from a point inside this *Arnold web*, the trajectory diffuses over the web *along* these resonances. Although Arnold diffusion is extremely weak (exponentially small in the perturbation parameter), the motion is unbounded in phase space of the system. There is a widespread belief (although still there are no reliable numerical results) that Arnold diffusion is responsible for a weak instability in FPU lattices. By fitting data to Nekhoroshev's expressions, in Ref.[81] the following empirical dependence has been obtained,

$$\eta(t) = \exp[-(t/\tau)^\nu] \tag{27}$$

for $t < \tau_R$, and

$$\eta(t) = \eta_\infty \equiv \exp[-(\tau_R/\tau)^\nu] \tag{28}$$

for $t \geq \tau_R$, with the numerical estimate of $0.3 \leq \nu \leq 0.5$. As for the relaxation time τ_R , it is argued that it is proportional to the energy density, $\tau_R \sim \epsilon$, and therefore, to the number of particles N for fixed total energy. The nonzero value of τ_∞ is discussed in Ref.[99]. Among others, the most realistic explanation of this result is that it is due to fluctuations of the energies E_k , which are not taken into account in the normalization factor for η . One of the important conclusions drawn in Refs.[81, 99] is that the equipartition of energy is always reached. This supports the expectation of non-existence of a minimal critical value of nonlinearity for the stochasticity. Another conclusion is that the critical value of perturbation ϵ_c which marks the transition from weak to strong stochasticity, corresponds to the overlap condition (18).

The region of weak stochasticity was closely examined in Ref.[100]. For initial conditions the low modes were excited in the β -model with zero boundary conditions. As was shown numerically, for low initial energy the distribution of mode energies after large time follows

an exponential decrease with increasing the mode number. This exponential dependence was explained theoretically, by finding an approximate solution of equations of motion written in a form similar to that of nonlinear Schrödinger equation. It was also shown numerically that a single nonlinearity parameter,

$$R = 6\pi^{-2}\beta E_\gamma(N + 1), \quad (29)$$

governs the local interactions between the low $k \ll N$ modes. For $R \gg 1$ there is a critical energy $E_c \approx 2.8$ (for $\beta = 0.1$) for which strong diffusion in k -space leads to equipartition. Below this border the diffusion leads to an exponential distribution of mode energies. It is noted that R being sufficiently large corresponds to the overlap criterion of the onset of widespread stochasticity. In further studies [101] the energy transitions and different time scale have been classified and discussed, as a function of energy. These results have been generalized in Ref.[102] to FPU-type lattices with two types of masses randomly distributed along the chain.

The dependence on initial conditions is another important question. One can classify the following cases: (i) single mode excitation with small k ; (ii) a group of low frequency modes with Δk and k proportional to N (thermodynamic limit); (iii) single mode excitation with $k \approx N/2$ (narrow packet approximation), and (iiii) high frequency excitation with $k \approx N$. As one can see, other important cases are missed in this picture, thus showing how difficult, in general, the problem is of statistical relaxation in nonlinear lattices. Comparison of cases (i) and (ii) was done in Ref.[101]. It was found that transient times to equipartition in case (ii) are proportional to \sqrt{N} , in comparison with single mode excitations (i) where this time does not exist or is not important. The transient times are characterized by non-universal dynamical characteristics, in contrast with larger times for which one can find a good scaling dependence on the energy density E/N . Concerning the case (iiii), one can refer to Ref.[103] where the energy equipartition for initially excited high frequency modes was studied. As for the case (iii), the important findings are analytical ones, with much attention given to the instability conditions.

VIII. NSE AND BEC

As was found in Ref.[69], one of remarkable properties of the β -model (2) is its direct relevance to the nonlinear Schrödinger equation (NSE). Indeed, let us write the Hamiltonian corresponding to the equations of motion (2),

$$H = \sum_{n=1}^N \left[\frac{p_n^2}{2} + \frac{1}{2} (x_{n+1} - x_n)^2 + \frac{\beta}{4} (x_{n+1} - x_n)^4 \right]. \quad (30)$$

In the following, we consider periodic boundary conditions, $x_0 = x_N$. In analogy with the quantum mechanics, we use the canonical variables a_k and a_k^* ,

$$a_k = \frac{1}{\sqrt{2\omega_k}} (\mathcal{P}_k - i\omega_k \mathcal{Q}_k^*) \quad (31)$$

where

$$\mathcal{P}_k = \frac{1}{\sqrt{N}} \sum_{n=1}^N p_n e^{-i\frac{2\pi kn}{N}}; \quad \mathcal{Q}_k = \frac{1}{\sqrt{N}} \sum_{n=1}^N x_n e^{i\frac{2\pi kn}{N}} \quad (32)$$

with $\omega_k = 2 \sin \frac{\pi k}{N}$ as the frequency of the k -th linear mode, $k = 1, 2, \dots, N$. Assuming that the initial packet in k -space is narrow and centered at $k_0 \approx N/2$, it can be shown [69] that the Hamiltonian takes the form,

$$H = \sum_{k=1}^N \omega_k a_k^* a_k + \frac{1}{2} \sum_{k_1 k_2 k_3 k_4} V_{k_1 k_2 k_3 k_4} a_{k_1}^* a_{k_2}^* a_{k_3} a_{k_4} \delta_{k_1 + k_2 - k_3 - k_4} + \mathcal{O}(1). \quad (33)$$

Here the term $V_{k_1 k_2 k_3 k_4} = V_0 + W_0(q_1 + q_2 + q_3 + q_4)$ with $V_0 = \frac{3\beta}{N} \left(\sin \pi \frac{k_0}{N} \right)^2$ and $W_0 = \frac{3\pi\beta}{4N^2} \sin \frac{2\pi k_0}{N} \ll V_0$ describes the (*resonant*) four-wave interaction [104](with $q = k - k_0 \ll k_0$). All other (*non-resonant*) terms of $\mathcal{O}(1)$ can be neglected in this approximation. By expanding ω_k at the point k_0 , one can obtain, $\omega_k \approx \omega_{k_0} + \Lambda q - \Omega q^2$. The parameters Λ and Ω are $\Lambda = \frac{2\pi}{N} \cos \frac{\pi k_0}{N} \approx (\pi/N)^3$ and $\Omega = \left(\frac{\pi}{N} \right)^2 \sin \frac{\pi k_0}{N} \approx (\pi/N)^2$. As a result, the equations of motion $i\dot{a}_k = \partial H / \partial a_k^*$ can be written as

$$i\dot{A}_q = -\Omega q^2 A_q + V_0 \sum_{q_1, q_2, q_3} A_{q_1}^* A_{q_2} A_{q_3} \delta_{q + j_1 - j_2 - j_3} \quad (34)$$

where $A_q = \exp(i(\omega_{k_0} + \Lambda q)t) a_{q+k_0}$. As one can see, these equations describe a nonlinear chain of interacting oscillators. Using the transformation $\Phi(\theta, t) = \sum_q A_q(t) \exp(iq\theta) = \Phi(\theta + 2\pi, t)$, we obtain the NLS equation,

$$i\frac{\partial \Phi}{\partial t} = \Omega \frac{\partial^2 \Phi}{\partial \theta^2} + V_0 |\Phi|^2 \Phi. \quad (35)$$

This *classical* equation is well known in the physics of interacting particles and widely discussed in many applications. It is a particular case of the Gross-Pitaevskii (GP) equation [105, 106] which attracts much attention in connection with Bose-Einstein condensation (BEC). Using the mean-field approximation, this equation describes the evolution of the condensate wave function, and, in essence, is of semi-classical nature. The important peculiarity of the GP-equation is its complete integrability (see, e.g., [107]). This is of special interest from the point of view of the statistical properties of the condensate. As was confirmed numerically [69], in the FPU β -model good conservation of first three integrals of motion, analytically derived for the GP-equation, can be observed provided the initial packet is centered at $k_0 = N/2$.

The model of type (33) was recently examined using close numerical investigations [108]. Specifically, the dynamics of the condensate in one-dimensional geometry was assumed to be governed by the following Hamiltonian in the action-angle representation, $A_n = \sqrt{I_n} \exp(i\theta_n)$,

$$H = \sum_n \omega_n I_n + \frac{g}{2} \sum_{n_1 n_2 n_3 n_4} V_{n_1 n_2 n_3 n_4} (I_{n_1} I_{n_2} I_{n_3} I_{n_4})^{1/2} e^{-i(\theta_{n_1} + \theta_{n_2} - \theta_{n_3} - \theta_{n_4})}. \quad (36)$$

Here $\hbar\omega_n = n^2\pi^2\hbar^2/2mL^2$ labels the single-particle energy levels, m is the mass of particles, L is the length of the one-dimensional box, and $V_{n_1 n_2 n_3 n_4}$ corresponds to the matrix elements $\int_0^L \phi_{n_1} \phi_{n_2} \phi_{n_3} \phi_{n_4} dz$ of the interaction, with ϕ_n as the normalized modes of the box (see details in Ref.[108]).

In the study of the model (36), methods developed for classical nonlinear lattices have been extensively used. Of particular interest was the time-dependence of the normalized spectral entropy (22) since it can be used to distinguish between regular and irregular dynamics of the condensate. Note that due to the zero boundary conditions used in Ref.[108], the dynamics may be non-integrable in contrast to the GP-equation. For a weak interaction the dynamics was numerically found to be quasi-periodic for generic initial conditions, which may be compared with the recurrent motion in the FPU models. On the other hand, with increased interaction strength, the dynamics appears to reveal chaotic properties. This effect was accompanied by a strong decrease of the spectral entropy $\eta(t)$, and by irreversible dynamics. The main result is that starting from conditions in which the low modes were initially excited, the energy diffusively spreads over modes with higher frequencies. The stochasticity was found to be stronger for low excited modes, in contrast to the FPU model.

This fact may be explained by the different kinds of the unperturbed frequency spectrum in these two models.

The above results show that many of properties of classical nonlinear lattices, especially, non-integrable models of the FPU type, can be discussed in a more general context, namely, in the context of the physics of interacting quantum particles. Although the latter subject is not new, the problem of the onset of *many-body chaos* in quantum systems of interacting Fermi and Bose - particles has recently attracted much attention due to its important physical applications (see, e.g. [109]). In this respect, an interesting study was reported in Ref.[110, 111] where the quantum analog of Eq.(34) was introduced,

$$i\dot{A}_j = -j^2(1+q)\Omega A_j + \hbar V_0 \sum_{j^2, j^3, j^4} A_{j^2}^\dagger A_{j^3} A_{j^4} \delta_{j+j^2-j^3-j^4} \quad (37)$$

Here $[A_j, A_k^\dagger] = \delta_{jk}$ and $q = \hbar\beta \cot(\pi/2N)/32N$, with ω and V_0 defined as in the classical model.

Analytical studies [110, 111] of the dynamical instability of motion gave quite unexpected results. As was already discussed in Section VI, in the narrow packet approximation the classical dynamics of the FPU model displays an instability above the critical value given by Eq.(25). In contrast to this result supported by other studies, in the quantum model the instability occurs for any weak perturbation. On the other hand, the rate of this instability turns out to be slower than for the classical model. If the latter effect could be explained by quantum suppression of classical instability (as in the Kicked Rotor model [112, 113, 114]), the absence of the instability threshold is a somewhat new effect. One can suggest that this effect is due to quantum tunneling in the effective potential, and further studies appear to be very important.

The above approach has been recently developed and applied in Ref. [115] to the problem of collapse in the Bose-Einstein condensation with an attractive potential. As is known, the collapse dynamics can not be described by the Gross-Pitaevskii equation, therefore, new ideas are important. As was shown in Ref.[115], near the instability threshold quantum effects turn out to play an important role and have to be taken into account. Specifically, when comparing the GP and quantum dynamical growth of the unstable modes, the absence of the instability threshold was confirmed for the quantum model, in contrast with the GP equation. This means that the quantum solution is always unstable, and eventually collapses in a finite time. The difference between the GP and the quantum model is important when

approaching the classical (GP) critical limit of the instability. This effect may be compared with an exponentially fast spread of wave packets in quantum systems which are chaotic in the classical limit. As was shown in Ref.[116, 117], for classically chaotic systems quantum effects are extremely strong and reveal themselves on a very short (logarithmic) time scale. Recent rigorous results [118] on the quantum instability of averages near stationary points seem to have a direct relevance to the more general problem of quantum corrections in the region of chaos.

It would be interesting to study the influence of terms, neglected in the narrow packet approximation, when obtaining the NLS equation (35). It is easy to show that by keeping the next terms in the expansion of ω_k and V_{k_1, k_2, k_3, k_4} about the point k_0 , one can derive the following equation,

$$i\frac{\partial\Phi}{\partial t} = \Omega\frac{\partial^2\Phi}{\partial\theta^2} + V_0|\Phi|^2\Phi + i\chi\frac{\partial^3\Phi}{\partial\theta^3} - 4iW_0|\Phi|^2\frac{\partial\Phi}{\partial\theta}, \quad (38)$$

which describes the dynamics of the FPU model more correctly than the Gross-Pitaevskii equation (with $\chi = \frac{1}{6}\partial^3\omega_k/\partial k^3$ at $k = k_0$). The additional terms in the above equation may be important for describing the evolution of wave packets for large time scales, and for the breakdown of integrability.

One recent attempt to consider the dynamics of the Bose-Einstein condensate by making use of an approach developed in the field of *quantum chaos*, was performed in Ref.[119]. Using numerical simulations, the authors focus on the dynamics of the Bose-Einstein condensate on a ring, which is described by the quantum Hamiltonian,

$$\hat{H} = \sum_k \epsilon_k \hat{n}_k + \frac{g}{2L} \sum_{k, q, p, r} \hat{a}_k^\dagger \hat{a}_q^\dagger \hat{a}_p \hat{a}_r \delta_{k+q-p-r}. \quad (39)$$

Here $\hat{n}_k = \hat{a}_k^\dagger \hat{a}_k$ is the occupation number operator, \hat{a}_s^\dagger and \hat{a}_s are the creation-annihilation operators, and $\epsilon_k = 4\pi^2 k^2 / L^2$. As one can see, this Hamiltonian can be considered to be the quantum version of the classical Hamiltonian (33) describing the evolution of the FPU model in the narrow packet approximation. The behavior of this system is governed by only one parameter n/g , where n is the particle density on a ring of length L , and g is the strength of the interaction between bosons, determined by the interatomic scattering length.

As is known, for weakly interacting particles, $n/g \rightarrow \infty$, the mean-field approximation gives the correct description of the dynamics. In the other limit of strongly interacting particles, known as the Tonks-Girardeau regime, $n/g \rightarrow 0$, the density of interacting bosons

becomes identical to that of non-interacting fermions. The transition between these two regimes is known to correspond, approximately, to $n/g \approx 1$.

The main interest in Ref.[119] was to observe and quantify the degree of irregularity in the dynamics of the condensate. Specifically, the situation in which all bosons initially occupy the single-particle level with the angular momentum $k = 0$ has been explored, with further analysis of the evolution of the condensate in time. The main result of the study in Ref.[119] was that with an increase of the interaction strength g , regular (quasi-periodic) dynamics alternates with irregular behavior of the observable quantities. This transition was found numerically to occur at the transition from the mean-field to the Tonks-Girardeau regimes. Given the clear evidence of the efficiency of the proposed approach, these results open the door for further studies of the condensate dynamics from the viewpoint of many-body chaos.

IX. CONCLUDING REMARKS

Due to space limitations, many recent studies are not discussed here, although they are relevant to the FPU model. In the first line, one should mention an increasing interest in the existence of localized nonlinear oscillations (breathers) emerging in nonlinear lattices (for a review, see, e.g. [120]). For some time, their existence in the FPU model was questionable, mainly do to the fact that the main interest initially was related to low-frequency excitations. As was shown in the early paper [121], localized optical excitations (high frequency modes) can be observed in the FPU model with alternative masses. This was the first indication that by exciting the highest modes in the FPU lattice, a new kind of solution with special structure emerges (the most recent results on the diatomic FPU model are reported in Ref.[122]). Although self-localized solitons in anharmonic lattices without impurities were predicted quite long ago Refs.[123, 124], only recently the existence of breathers in FPU lattices has been proved rigorously (see, e.g. Refs.[125]). In connection with the FPU problem one should mention the results of Refs.[126, 127] where it was shown that breathers can be responsible for the slow relaxation of initially thermalized nonlinear lattices. This effect seems to be relevant to the long-term regular dynamics in the FPU models, which is alternated by a strong energy sharing between linear modes. To date, many studies of breathers (including *chaotic breathers*, see in Ref.[128]) in the FPU model have been carried out, and we hope that the reader can find in this issue more information on the subject.

Coming back to the original question about the ergodicity and thermalization in the FPU model, one should conclude that some of problems still remain open. In particular, the existence of the threshold for weak chaos in the thermodynamical limit $N \rightarrow \infty$ is still under study by many researchers. As is clear from the above discussions, the main difficulty, apart from the numerical one, is the strong dependence of the results on the model parameters. The behavior of the model depends strongly on whether low or high frequency modes are initially excited. Also, the number of excited modes seems to be important for the dynamics, as is indicated in previous studies. Last, but not least, is the fact of a difference between the *alpha* and *beta*-models. Therefore, future studies are desirable, both analytical and numerical.

One should mention the direct relevance of the FPU model to the models of the Bose-Einstein condensation. As was shown in Ref.[69], the narrow packet approximation in the β -model leads to the Gross-Pitaevskii equation with an attractive potential. Thus, the instability of highest modes in periodic FPU lattices corresponds to that of the Bose-Einstein condensate. This fact is important for further studies of instabilities both in the nonlinear classical lattices and in quantum models of the Bose-Einstein condensate. Note that now it is possible to control experimentally the sign of the interaction between bosons, and to observe the collapse of the condensate (see, for example, [129]).

Another new direction is the study of dynamics of quantum models of interacting Bose particles. In particular, direct quantization of classical nonlinear chains related to the Gross-Pitaevskii equation shows a close analogy for the dynamics in classical and quantum models. Recent numerical data [119] for the transition between the mean field and Tonks-Girardeau regimes have revealed the onset of irregular motion of the condensate. This type of transition is known to occur in quantum models of interacting particles which are chaotic in the classical limit. Therefore, one can expect that methods well developed in the theory of quantum chaos, may give a new insight on the dynamics of interacting bosons in the condensates.

The above practical problems are part of the more general problem of quantum-classical correspondence for systems with irregular behavior. From this point of view, the FPU model is of particular interest and can be considered as an important example. As discussed in Ref.[130], there are two mechanisms which are responsible for the appearance of statistical behavior of dynamical (deterministic) systems. The first mechanism is the thermodynamic limit with $N \rightarrow \infty$, which is well known since the early days of statistical mechanics. The

important point here is that this limit has nothing to do with chaos, it is based on the ergodicity of motion only, which is known to be the weakest statistical property. As we already discussed, perfect statistical and thermodynamical properties are known to emerge even in completely integrable systems such as the Toda-lattice. Although there are initial conditions which correspond to solitons, the measure of these specific conditions is extremely small, and surely can be neglected practically. Therefore, the role of additional terms that break the integrability, becomes important when the number N is finite. The expectation of FPU was based on their belief that $N = 32,64$ is large enough in order to observe the equipartition in the presence of small nonlinearity.

The second mechanism for the onset of statistical properties in dynamical systems is, in principle, different. It is based on a local instability of motion for generic initial conditions in the phase space of the system. With this mechanism the ergodicity is not important provided the total measure of initial conditions with regular motion is very small, although it can be finite. Due to this local instability (with reflecting boundaries in phase space), this motion reveals clear mixing properties, leading to strong sensitivity of the motion to initial conditions. As a result, an apparent irreversibility of motion emerges since any weak external perturbation gives rise to non-recurrence of the initial conditions. The important point for this scenario is that the dynamical chaos can emerge in systems with few degrees of freedom, in contrast to the first (thermodynamic) mechanism. It is important to stress that, although these two mechanisms are different, the common feature is that in both cases the time dependence of the observables can be described by infinite number of statistically independent frequencies (see details in Ref.[130]).

Turning to quantum systems, the origin of “quantum chaos” in dynamical systems is based on the first mechanism, with no relevance to local instability of trajectories. Specifically, irregular behavior of a system emerges when an initial wave packet consists of many exact *chaotic* eigenstates with statistically independent frequencies (see, e.g. [131]). This concept is very important for establishing the conditions for the onset of chaos in quantum systems and in quantifying their irregular properties. Therefore, the understanding of physical effects found in the FPU model, as well the use of tools developed for identifying these effects, may be useful for the study of quantum systems with complex behavior.

As a consequence of their research on the FPU model, in this brief review the authors made an attempt to comment on the main ideas, tools and results related to the FPU

paradox, after 50 years of the celebrated paper. For one of the authors (FMI), the FPU problem was his initial scientific PhD research. For GPB, the relation discovered between the FPU model and nonlinear Schrödinger equation has contributed to his interests in Bose-Einstein condensation problems. And for both of us, the preparation of this manuscript provided a welcome opportunity to learn much more about new trends in the physics of nonlinear phenomena.

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