Analytic Lyapunov exponents in a classical nonlinear field equation

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It is shown that the nonlinear wave equation $\partial^2 \varphi - \partial_x^2 \varphi - \mu_0 \partial_x (\partial_x \varphi)^3 = 0$, which is the continuum limit of the Fermi-Pasta-Ulam (FPU) $\beta$ model, has a positive Lyapunov exponent $\lambda_1$, whose analytic energy dependence is given. The results for a first example for field equations is achieved by evaluating the lattice-spacing dependence of $\lambda_1$ for the FPU model within the framework of a Riemannian description of Hamiltonian chaos. We also discuss a difficulty of the statistical mechanical treatment of this classical field system, which is absent in the dynamical description.

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The numerical study that E. Fermi, J. Pasta and S. Ulam made at Los Alamos, on a chain of anharmonically coupled oscillators, represents a milestone in the development of the modern theory of nonlinear dynamics. The surprising outcomes of this first computer experiment in the history of physics have been very seminal. Among the other attempts to explain the apparent lack of thermalization of the energy initially stored in one of the linear modes of the chain, Zabusky and Kruskal [2,3] remarked that a continuum limit version of the Fermi-Pasta-Ulam (FPU) model leads to the Korteweg-de-Vries (KdV) equation, when the $\alpha$ model is considered, and to a modified KdV equation when the $\beta$ model is considered. These are nonlinear, integrable partial differential equations where a special class of solitary waves exists. Zabusky and Kruskal called solitons - exists and can to some extent explain the FPU recurrences [4].

In the present work we tackle the FPU-$\beta$ model, described by the Hamiltonian

$$H(p, q) = \sum_{i=1}^{N} \frac{1}{2} p_i^2 + \frac{1}{2} (q_{i+1} - q_i)^2 + \frac{\mu_0}{4} (q_{i+1} - q_i)^4,$$

and we consider another legitimate continuum limit [6] of this system, described by the Hamiltonian

$$H(\pi, \phi) = \int_0^L dx \left[ \frac{1}{2} \pi(x)^2 + \frac{\eta}{2} (\nabla \phi)^2 + \frac{\mu_0}{4} (\nabla \phi)^4 \right],$$

and leading to the field equation (setting $\eta = \nu = 1$)

$$\partial^2 \phi \partial x^2 - \partial^2 \phi \partial t^2 + \mu_0 \frac{\partial}{\partial x} \left( \partial \phi \partial x \right)^3 = 0.$$  \hspace{1cm} (3)

Also this continuum limit of the FPU model might appear integrable on the basis of the following reasoning [6]. Let us consider the Legendre transform: $\chi = \partial_x \phi, \tau = \partial_x \psi$ and $x = \partial_x \psi, t = \partial_x \tau$ with the relation $\psi = x \chi + \tau \tau$, whence $\partial^2 \phi = D \partial^2 \psi, \partial^2 \phi = D \partial^2 \psi$, where $1/D = \partial^2 \psi \partial^2 \chi - (\partial^2 \chi \psi)^2$. Substituting into Eq.(3) we can linearize it to

$$\frac{\partial^2 \psi}{\partial \chi^2} = (1 + 3 \mu_0 \chi^2) \frac{\partial^2 \psi}{\partial \tau^2},$$

which can be solved by variable separation by setting $\psi = F(\chi)G(\tau)$, where $G'' \pm c^2 G = 0$, and $F'' \pm c^2 (1 + 3 \mu_0 \chi^2) F = 0$. In principle, by inverting this Legendre transform, Eq.(3) could be analytically solved. However, as we shall discuss, the method sketched above can only lead at most to local and not to global invertibility, both in time and space. Actually we are going to show that the field equation (3) for the FPU $\beta$ model in the continuum limit is chaotic (the Lyapunov characteristic exponent of the solutions is positive). The pattern of the Lyapunov exponent that we shall derive is shown in Fig.1. The cross-over in the energy dependence of the largest Lyapunov exponent has been attributed in Refs. [7] to a (smooth) transition between weak and strong chaos [8]. The persistence of such a cross-over also in the continuum limit is a remarkable fact. Loosely speaking, at high energy, in the strongly chaotic regime, the spatio-temporal behavior of the field $\phi(x,t)$ should look like a fully developed “turbulent” field, whereas this should not be the case at low energy, where a weakly “turbulent” dynamics would set in. Our calculation shows that, no matter whether weak or strong, chaos is present in the system at any energy, and since the system is Hamiltonian, we can believe that a standard statistical mechanical description is allowed. This raises an important problem that we now discuss.

For the lattice system corresponding to [6] the standard canonical partition function $Z = \int \prod_{i=1}^N d\pi_i d\phi_i \exp [-\beta H(\pi_i, \phi_i)]$ in the limit of lattice spacing $a \to 0$ becomes

$$Z = \int D\pi(x) D\phi(x) e^{-\beta \int_0^L dx [\frac{1}{2} \pi^2 + \frac{\eta}{2} (\nabla \phi)^2 + \frac{\mu_0}{4} (\nabla \phi)^4]}.$$

It is interesting at this point to raise a problem that comes out when some expected dynamical properties of
the field $\phi(x,t)$ are compared to their statistical counterparts worked out by means of $\mathcal{Z}$. By means of an orthogonal change of coordinates, the Hamiltonian \[ H(P_k, Q_k) = \sum_k E_k = \sum_k \left[ \frac{1}{2} (P_k^2 + \omega_k^2 Q_k^2) + \mu \sum_{k_1,j_k,j_3} C(k,j_1,k_3) Q_k Q_{k_1} Q_{k_3} \right] \] where the summations run from $k = 1$ to $k = k_{\text{max}}$ for a lattice, and from $k_0$ to $k_{\text{max}} = \infty$ in the continuum limit. In the new variables the partition function becomes \[ \mathcal{Z} = \int \prod_{k=0}^{k_{\text{max}}} dp_d dq \exp \left[ -\beta H \{ \{ P_k \}, \{ Q_k \} \} \right] \] which, in the limit $k_{\text{max}} \to \infty$, gives \[ \mathcal{Z} = \int DP(k) DQ(k) \exp \left[ -\beta \int_{k_0}^{\infty} dk H(P(k), Q(k)) \right] , \] where $k_0 = \frac{2\pi}{\omega}$ > 0 for a finite support. The generalized equipartition theorem \[ \text{(3)} \] states that \[ \langle Q_k \partial H/\partial Q_k \rangle = \text{const} \] independently of $k$, and from Ref. [11] we know that for the FPU $\beta$ model such an average is \[ \langle Q_k \partial H/\partial Q_k \rangle \approx k^2 Q_k^2 (1 + \alpha) , \] where $\alpha$ is a constant, and therefore \[ Q_k^2 \approx k^{-2} (1 + \alpha)^{-1} \] which, being independent of $k_0$, still holds true in the continuum limit, i.e. \[ \hat{\phi}(k)^2 \approx k^{-2} (1 + \alpha)^{-1} \] Whence an ultraviolet catastrophe, i.e. the divergence of average total energy when $k_{\text{max}} \to \infty$ also on a finite support $[0, L]$. However such a difficulty is absent in the dynamical equation \[ \text{(3)} \] which, being derived from a Hamiltonian, must keep the energy constant, therefore finite if it is finite at time $t = 0$.

The point is that statistical mechanics and dynamics yield very different large-$k$ spectral properties. In fact, already on the basis of the purely dimensional analysis discussed in Refs. [1], we can easily find that in order to bound the total energy (on a finite support $[0, L]$) to a finite value, the ultraviolet asymptotic power spectrum of $\phi(x)$ must be bounded above by \[ |\hat{\phi}(k)|^2 \sim k^{-3} , \] which means that the high spatial-frequency modes cannot have the same energy of the low spatial-frequency modes.

The rough estimate of the ultraviolet spectrum of the continuum model can be improved as follows. Any smooth initial condition $\phi(x,0) \in C^\infty(\mathbb{R})$ of the equation of motion \[ \text{(3)} \] has to remain smooth at any further time $t$, i.e. $\phi(x,t) \in C^\infty(\mathbb{R})$. Now, the analytic continuation $\Phi(z,t) \neq 0$ will be of class $C^\infty$ on a strip whose width $\delta$ will be determined at any given time $t$ by the distance of the closest singularity to the real axis. If $z_n^* = x_n^* + iy_n^*$ are the locations of the singularities of $\Phi(z,t)$, to the leading order one finds \[ \Phi(k) \sim k^{-\alpha} \sum_n c_n e^{ikz_n^*} \] for $k \to \infty$, where, apart from the power-law prefactor $k^{-\alpha}$, the sum is carried over the $Im z > 0$ half plane and $c_n$ are suitable coefficients. The factors $e^{ikz_n^*} = e^{ikx_n^*} e^{-ky_n^*}$ efficiently single out the closest singularity to the real axis to give \[ |\hat{\phi}(k)|^2 \leq A e^{-\delta k} \] at $k \to \infty$ which provides a better ultraviolet estimate of $|\hat{\phi}(k)|^2$ stemming from the constraint of differentiability of $\phi(x)$. Needless to say, this ultraviolet exponential fall off of $|\hat{\phi}(k)|^2$ guarantees the finiteness of the total energy for any finite support $[0, L]$. It is not unreasonable to think that a relationship might exist between the minimum width of the spatio-temporal cell where the Legendre transform of Eq.\[ \text{(3)} \] - sketched at the beginning of this paper - is invertible, that is where Eq.\[ \text{(3)} \] is locally integrable, and the width of $(k, \omega(k))$ cell where the power spectrum $|\hat{\phi}(k)|^2$ exponentially falls off. There is apparently no way of reproducing the ultraviolet exponential decay of $|\hat{\phi}(k)|^2$ - which is naturally brought about by the dynamical equation \[ \text{(3)} \] - within the statistical mechanical framework. The field $\phi(x,t)$ can be chaotic in space and time only down to some small scale which naturally provides a cutoff that, inserted into $\mathcal{Z}$, would remove the mentioned divergences. Let us mention that the physical meaning of a rigorous treatment of another classical non-linear field equation (complex Ginzburg-Landau) \[ \text{(4)} \] is coherent with the theoretical scenario depicted above.

To come now to our main result, chaotocity in the continuum limit, we calculate the Lyapunov exponent by extending to such a limit a method to tackle Hamiltonian chaos that has already given excellent analytic predictions of the largest Lyapunov exponent in the thermodynamic limit of the FPU $\beta$-model \[ \text{(4)} \] on a lattice. This method exploits the mathematical identification of an Hamiltonian flow with the geodesic flow on a suitable Riemannian “mechanical manifold” consisting of an enlarged configuration spacetime \[ \{ q^0 = t, q_1, \ldots, q_N \} \] plus one real coordinate $q^{N+1}$, whose arc-length $ds^2 = -2V(q)(dq^0)^2 + a_{ij} dq^i dq^j + 2 dq^i dq^{N+1}$ defines the so-called Eisenhart metric $g_E$ \[ \text{(4)} \]. $V$ is the potential. In the geometrical framework, the (in)stability of the trajectories is the (in)stability of the geodesics, and it is completely determined by the curvature properties of the underlying manifold according to the Jacobi equation \[ \text{(4)} \] for the geodesic deviation. This equation, written for Eisenhart metric, entails the usual tangent dynamical equation $\xi^i + \partial^2 V/\partial q^i \partial q^0 \xi^0 = 0$, which is used to measure Lyapunov exponents in standard Hamiltonian systems. Having recognized its geometric origin, it can be transformed, under certain hypotheses \[ \text{(4)} \] into an effective scalar stability equation that, independently of the knowledge of dynamical trajectories, provides a measure of their average degree of instability. This effective stability equation is in the form of a stochastic oscillator equation $\dot{\psi} + [\kappa_0 + \sigma_n \eta(t)] \psi = 0 \ [5]$, where $\kappa_0 = \langle K_R \rangle / N$, $\sigma_n = \langle (K_R - \langle K_R \rangle)^2 \rangle / N$ and $K_R = \Delta V = \sum^N_{n=1} \partial^2 V/\partial q^2$, is the Ricci curvature of the mechanical manifold, computed with $g_E$; $\eta(t)$ is a gaussian $\delta$-correlated random process of unit variance. The exponential growth rate $\lambda$ of $\langle \dot{\psi}^2 + \psi^2 \rangle$ is computed exactly to provide the following estimate of the largest Lyapunov exponent:

\[ \lambda = \frac{\Lambda}{2} = \frac{2 \kappa_0}{3 \Lambda} \Lambda = \left[ 2 \sigma_n^2 \tau + \sqrt{4 \kappa_0^3 / 3 + 4 \sigma_n^2 \tau^2} \right]^{1/2} \] \[ \text{(6)} \]

where $\tau = \pi \sqrt{\kappa_0 / (2 \kappa_0 \kappa_0 + \sigma_n^2)}$ is a characteristic time scale worked out on the basis of geometrical arguments. In the limit $\sigma_n / \kappa_0 \ll 1$ one finds $\lambda \propto \sigma_n^2 \ [5]$. 


In this geometric picture chaos is mainly originated by the parametric instability activated by the fluctuating curvature “felt” by the geodesics. The quantities $\kappa_0$ and $\sigma_\kappa^2$ can be exactly computed for the FPU-$\beta$ model as microcanonical averages by taking advantage of the analytically known canonical partition function and by using the conversion formulas relating canonical and microcanonical averages. The final analytic expressions are given in Ref. [13], and among them we report those needed here

\begin{align}
\frac{1}{N} (K_R)'^{(\theta)} &= 2 + \frac{3}{\theta} \Delta(\theta) \\
\frac{1}{N} (\delta^2 K_R)^{(\theta)} &= \frac{1}{N} \frac{9}{\theta^2} \left[ 2 - 2\theta \cdot \Delta(\theta) - \Delta^2(\theta) \right] \\
\epsilon(\theta) &= \frac{1}{8\mu} \left[ \frac{3}{\theta^2} + \frac{1}{\theta} \Delta(\theta) \right],
\end{align}

where $\Delta(\theta) = \frac{D_{-3/2}(\theta)}{D_{-1/2}(\theta)}$, with $D_{-3/2}$ and $D_{-1/2}$ parabolic cylinder functions, the parameter $\theta$ is a function of the inverse temperature $\beta$ through $\theta = (\beta/2\mu)^{1/2}$, and $\epsilon(\theta)$ is the energy per degree of freedom of the system. The microcanonical average of curvature fluctuations involves a correction term to their canonical average which involves the specific heat $c_v(\theta)$ computed, as usual, as the second derivative of the free energy. These quantities enter the formula (6) to give the analytic values of Lyapunov exponents at different energies. In order to obtain them, notice that from Eq.(9) one gets $\epsilon(\theta)$ is a function of the $\theta$ and $\kappa_0$, that is

\begin{align}
\lambda_1(\epsilon) &= \frac{\sigma_\kappa^2}{2\kappa_0} + \ldots = 9\mu^2\epsilon^2 + O(\epsilon^3) \\
\lambda_1(\epsilon) &= \frac{9}{4\sqrt{2}} \epsilon^2 + O(\epsilon^3)
\end{align}

which is in strikingly good agreement with the low energy “experimental” results for $\lambda_1$. Similar developments can be worked out in the limit $\epsilon \to \infty$ (and so $\theta \ll 1$) giving

\begin{align}
\kappa_0 &\approx \frac{4\pi}{\Gamma^2} \sqrt{2\mu\epsilon} \\
\sigma_\kappa^2 &\simeq 16\mu \left( 3 - \frac{32\pi^2}{\Gamma^4} \right)
\end{align}

by computing again $\tau(\epsilon)$ we find $\tau(\epsilon) \simeq c(\mu\epsilon)^{-1/4}$ yielding

\begin{align}
\lambda_1(\epsilon) &\approx c'(\mu\epsilon)^{1/4}
\end{align}

where $c$ and $c'$ are constants. Also this scaling law is in perfect agreement with numerical results. The comparison between the full analytic prediction of $\lambda_1(\epsilon)$, obtained by substituting Eqs.(13) and (14) into Eqs.(12), shows a perfect agreement with the outcomes of a standard numerical computation of the largest Lyapunov exponent at different values of $\epsilon$. Let us remark that the analytic prediction of $\lambda_1(\epsilon)$ is obtained in the $N \to \infty$ limit, which is implicit in the computation of the microcanonical averages of the Ricci curvature and of its fluctuations. Now, as the analytic expression in (1) is in excellent agreement with the numerical data obtained for discrete (particle) systems at different values of $N$, there is no reason to doubt that such an agreement will hold true also when $N$ is varied while keeping the total length $L$ of the system fixed, i.e. in the continuum limit. The non-trivial difference between this limit and thermodynamic limit in Ref. [13] is that $N \to \infty$ while the energy remains finite in the former case, whereas both $N$ and energy diverge in the latter case. Thus let us now consider the Hamiltonian $\{\phi_i\}$ discretized on a lattice of length $L$ and spacing $a$ (with $L = Na$)

\begin{equation}
H(\{\pi_i\}, \{\phi_i\}) = \sum_{i=1}^{N} a \left[ \frac{\pi_i^2}{2\mu} + \frac{n}{2} \left( \phi_{i+1} - \phi_i \right)^2 + \frac{\kappa_0}{4} \left( \phi_{i+1} - \phi_i \right)^4 \right],
\end{equation}

where the dimensional constants $\mu$, $\eta$, and $\kappa_0$ have been introduced. We have thus obtained a discrete (lattice) system, similar to that described by the Hamiltonian $\{\theta_i\}$ in order to make a direct comparison between the two Hamiltonians of Eqs.(10) and (11), we must now absorb the dimensional parameter $a$ into the constants of the Hamiltonian. By means of the following rescaling of the coordinates $\phi_i$ and of the time $t$: $\xi_i = \phi_i/a$, with $a = \sqrt{\mu/\eta}$, $t' = t/\gamma$ and $\gamma = \sqrt{\mu/\nu}$, and denoting by $\{\xi_i\}$ the momenta conjugated to $\{\phi_i\}$, $H$ of Eq.(16) is put in the form

\begin{equation}
H_a(\{\xi_i\}, \{\phi_i\}) = \sum_{i=1}^{N} \left[ \frac{\pi_i^2}{2} + \frac{1}{2} (\xi_{i+1} - \xi_i)^2 + \frac{\mu_0}{4a} (\xi_{i+1} - \xi_i)^4 \right],
\end{equation}

which, with the explicit computation of $\tau$ gives

\begin{equation}
\lambda_1(\epsilon) = \frac{9}{4\sqrt{2}} \epsilon^2 + O(\epsilon^3)
\end{equation}
which is just the form of $H$ in Eq.[1], so that we can apply the geometric treatment of dynamical chaos also to
the systems described by this family of Hamiltonians $H_a$. The precise meaning of this comparison is the following. The continuum Hamiltonian (2) has $H$ of Eq. (18) as its discretized version, where the parameters $\eta$, $\nu$, $\mu_0$ are equal to the values of the continuum model. After the recasting of Eq. (18) into the form (17) we can derive the value of the coupling constant $\mu$ of the discrete FPU model (1) so that a correspondence can be made between the discrete model and the lattice version (17) of the continuum model for any value of the lattice spacing $a$. Evidently the relation between the coupling constants is $\mu = \mu_0/\eta a^2$, and this tells that in order to represent the solutions of a set of systems (18) by means of those of a set of discrete systems (1) with a finer and finer sampling of the spatial support of length $L$, i.e. letting $a \to 0$, the coupling constant $\mu$ must be larger and larger. To the lattice-discretized system (17) we can now apply all the above equations for the geometric description of chaos, provided that we replace $\mu$ with $\mu_0/\eta a^2$. In passing to the continuum limit we have to let $a \to 0$ while the total energy of the system $E_{tot}$ is kept fixed. Hence the energy density $\epsilon$ has to diminish as $E_{tot}/N$, but $N = L/a$ and then $\epsilon = E_{tot} \cdot a/L$. Hence we obtain

$$\mu \cdot \epsilon = \frac{\mu_0 E_{tot}}{\eta a^2 L} = \text{cost}. \quad (18)$$

From Eq. (18) it then follows that the equations for $\kappa_0$ and $\sigma^2_0$ (3)-(4) are stable with respect to the limit to the continuum and so is the largest La
ing exponent. Therefore the field equation (3) is chaotic and its Lyapunov exponent has the pattern shown by Fig.1. This constitutes a first example of analytic calculation of $\lambda_1(\epsilon)$ for a field equation. Implicit in our computation is the possibility of approximating, as accurately as needed, a partial differential equation by means of a finite (truncated) system of ordinary differential equations, for which Lyapunov exponents are well defined. In conclusion we have shown that the continuum limit of the Fermi-Pasta-Ulam $\beta$ model is chaotic. We have discussed the interesting problematics raised by this result on the statistical description of classical field theory models that might be relevant also to the Wick-rotated quantum field theories.

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FIG. 1. Analytic Lyapunov exponent for the continuum limit as a function of the physical parameters.
Figure 1
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\[ \lambda_1 \]

\[ \mu_0 \quad E_{\text{tot}} / a \eta^2 N \]