ENERGY CASCADE IN FERMI-PASTA-ULAM MODELS

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We show that, for long–wavelength initial conditions, the FPU dynamics is described, up to a certain time, by two KdV-like equations, which represent the resonant Hamiltonian normal form of the system. The energy cascade taking place in the system is then quantitatively characterized by arguments of dimensional analysis based on such equations.

1. Introduction

The problem posed by Fermi, Pasta and Ulam (FPU) [1] concerns "in large" the dynamical characterization of the approach to equilibrium of nearly-integrable Hamiltonian systems with many degrees of freedom, which is obviously relevant to build up a meaningful statistical mechanics. FPU considered weakly nonlinear oscillator chains, for initial conditions with energy in the lowest Fourier mode (the longest wavelength mode) and numerically integrated the equations of motion paying special attention to the evolution in time of the modal energies. As is well known, the expected fast trend to energy equipartition among the Fourier modes was not observed, which is what is known since then as the FPU paradox. For references on history, consequencies and relevant results in the field see [2, 3, 4].

The aim of the present contribution is to look at the FPU problem from a somehow new point of view, which allows us to give some quantitative estimate of physically relevant quantities characterizing the transfer of energy from large spatial scales, where it is put initially, to small ones or, in other words, from low Fourier modes (large wavelength) to high (short wavelength) Fourier modes. We will refer to such a process as to the *energy cascade*, or simply the cascade. The term is borrowed from the theory of hydrodynamic turbulence, which actually displays a phenomenology similar to that of the FPU problem.

In the present paper, in order to avoid technical difficulties of minor importance, in place of considering the FPU model itself, we study the simpler problem of a class of PDEs which are naturally related to it.

The structure of the paper is the following. First of all it is recalled how certain PDEs arise in the study of the FPU problem. Then we endow such PDEs with a proper Hamiltonian structure and suitably simplify them by performing one step of averaging. Finally, through dimensional analysis we give an estimate of the effective number n_{eff} of degrees of freedom sharing the energy and thus actually involved in the dynamics. We also estimate the time τ needed to reach this state of partial equipartition. As will be shown, such estimates turn out to be in agreement with some recent numerical results available in the literature.

The presentation is quite informal; the material consists essentially of "snapshots" taken from a quite longer work in progress by the present authors.

2. Boussinesq equations modeling FPU chains

The equations of motion of a weakly nonlinear oscillator chain are

$$\ddot{r}_n = [\Delta(r + g r^{p-1})]_n \quad , \quad n = 0, \ldots, L \; . \tag{1}$$

Here $r_n = q_{n+1} - q_n$, where q_n is the displacement of the n-th particle from its equilibrium position on the chain; Δ is the usual discrete laplacian ($[\Delta f]_n \equiv f_{n+1} + f_{n-1} - 2f_n$), while $g > 0$ is the coupling constant and the integer $p \geq 3$ is the degree of nonlinearity (in the potential). We will suppose the chain to be periodic of period L, i.e. $r_0(t) = r_L(t)$, for any $t \geq 0$.

Now, for long–wavelength initial excitations, which is the problem of interest in the present work, finite differences, such as $r_{n+1} - r_n$, are small; one can then formally expand the operator $\Delta = 4 \sinh^2(\partial_n/2)$ appearing in (1) in powers of ∂_n and retain the first few terms in the r.h.s. of the equation. Renaming the spatial independent variable n as x, we get a PDE for the continuous field $r(x,t)$, namely

$$r_{tt} = \left[r + (1/12) r_{xx} + g r^{p-1} \right]_{xx} \quad , \quad r(0,t) = r(L,t) \quad . \tag{2}$$

Such a PDE is a generalized Boussinesq (gB) equation, and was considered as a starting point in approaching the FPU problem e.g. in [5] and [6].

In introducing a PDE, we pass from a system with a finite number (precisely L) of degrees of freedom to a system possessing infinitely many

degrees of freedom. But of course the gB system is meaningful, i.e. it represents a good approximation of the original system, only if finite differences remain small, that is to say only if long–wavelength Fourier modes take part in the evolution in a significant way. The consistency of the approximation breaks down when modes of wavelength of order one (the size of the lattice step of the original chain model) receive a significant amount of energy or, in other words, when a number of degrees of freedom of order L is excited. From now on, we will focus on the gB equation (2).

3. Hamiltonian structure of the gB equation

To our knowledge, the Hamiltonian structure of the gB equation (2) was pointed out first by Zakharov [6], in a famous paper where he showed that the (properly said) Boussinesq equation, corresponding to the case $p = 3$ is in fact integrable (in the Lax and in the Hamiltonian sense). Zakharov introduced an auxiliary field Φ (periodic on $[0, L]$) thought of as the coordinate, while r was thought of as the corresponding conjugate momentum. Then, if one defines the Hamiltonian

$$H[r, \Phi] = \int_0^L \left(\frac{\Phi_x^2 + r^2}{2} - \frac{r_x^2}{24} + g \frac{r^p}{p} \right) \, dx \quad , \tag{3}$$

the corresponding pair of Hamilton equations associated to H, namely

$$\begin{cases} \Phi_t = \delta H / \delta r = r + (1/12) r_{xx} + g r^{p-1} \\ \\ r_t = -\delta H / \delta \Phi = \Phi_{xx} \end{cases} , \tag{4}$$

turns out to be equivalent to the second order gB equation. Notice that the flow of equations (4) preserves $\int_0^L r \, dx$, which has to be set to zero, since in the original periodic lattice one always has $\sum_{n=0}^{L-1} r_n \equiv 0$.

Now, for our purposes, it is quite convenient to perform a noncanonical change of variables which is analogous to that used e.g. by Craig and Groves [7] in approaching the water wave problem. Let us introduce the change of variables $(r, \Phi) \mapsto (\xi, \eta)$, where

$$\xi = \frac{r + \Phi_x}{\sqrt{2}} \quad , \quad \eta = \frac{r - \Phi_x}{\sqrt{2}} \quad . \tag{5}$$

Then, after substitution, the Hamiltonian (3) reads

$$H[\xi, \eta] = \int_0^L \left[\frac{\xi^2 + \eta^2}{2} - \frac{(\xi_x + \eta_x)^2}{48} + g \, \frac{(\xi + \eta)^p}{2^{p/2} p} \right] \, dx \ , \tag{6}$$

while the equations of motion (4) transform into

$$\begin{cases} \xi_t = [\xi + (1/24)(\xi+\eta)_{xx} + (g/2^{p/2})(\xi+\eta)^{p-1}]_x \\ \eta_t = -[\eta + (1/24)(\xi+\eta)_{xx} + (g/2^{p/2})(\xi+\eta)^{p-1}]_x \end{cases} . \tag{7}$$

The latter equations can be quite conveniently rewritten in Hamiltonian form, namely

$$\begin{pmatrix} \xi \\ \eta \end{pmatrix}_t = \widehat{\sigma}\partial_x \begin{pmatrix} \delta H/\delta\xi \\ \delta H/\delta\eta \end{pmatrix} \quad , \tag{8}$$

where $\widehat{\sigma}$ denotes the diagonal Pauli matrix $\mathrm{diag}(1,-1)$. It can be easily checked that $\widehat{\sigma}\partial_x$ is a degenerate Poisson operator. The corresponding Casimir invariants of the system are the linear functionals of the form $\int_0^L (c_1\xi + c_2\eta)\, dx$, with arbitrary constants c_1 and c_2. By the definition of the variables ξ and η given in (5) and by the geometric condition $\int_0^L r\ dx = 0$ one deduces that the physically meaningful Casimir leaf is the one defined by $\int_0^L \xi\ dx = \int_0^L \eta\ dx = 0$.

4. Averaging

One has to keep in mind that a typical long–wavelength initial datum for equations (7) is

$$\xi_0(x) = \eta_0(x) = \sqrt{\varepsilon}\cos(2\pi x/L) \quad , \tag{9}$$

where ε plays the role of the specific energy (energy per degree of freedom) in the original FPU system. Indeed, substituting (9) in the expression of the Hamiltonian (6) yields $H[\xi_0,\eta_0] \equiv E = \varepsilon L + o(\varepsilon L)$, the leading contribution εL coming from the first two terms of the Hamiltonian. Moreover, if one evaluates the r.h.s. of equations (7) on the initial datum (9), one realizes that the leading terms in the evolution equations for ξ and η are ξ_x and $-\eta_x$, respectively. The other terms turn out to be small because both ε and $1/L$ are supposed to be small quantities. As a consequence, one can regard the Hamiltonian (6) as being a perturbation of

$$H_0 = \int_0^L \frac{\xi^2+\eta^2}{2}\ dx \quad . \tag{10}$$

According to a standard technique in perturbation theory [8], one can then average the whole Hamiltonian (6) over the flow generated by the unperturbed Hamiltonian H_0 (10), and thus simplify the dynamics. Such a flow,

acting on vector–valued fucntions periodic on $[0, L]$, is given by

$$\mathbf{\Phi}^t = e^{t\widehat{\sigma}\partial_x} \quad (\mathbf{\Phi}^L = \mathbf{\Phi}^0 = I) \ , \tag{11}$$

and the averaged Hamiltonian $\overline{H} \equiv \int_0^L H[\mathbf{\Phi}^s(\xi, \eta)]ds/L$ turns out to be

$$\overline{H}[\xi, \eta] = \int_0^L \left[\frac{\xi^2 + \eta^2}{2} - \frac{(\xi_x)^2 + (\eta_x)^2}{48} \right] + \frac{Lg}{2^{p/2}p} \sum_{n=0}^{p} C_n^p \langle \xi^n \rangle \langle \eta^{p-n} \rangle \ . \tag{12}$$

In the above expression, $C_n^p \equiv p!/(n!(p-n)!)$ while $\langle f^j \rangle \equiv \int_0^L f^j \, dx/L$; we will refer to the latter as to the moment of f of order j, or simply the j-th moment of f. The equations of motion associated to $\overline{H}$ are

$$\begin{cases} \xi_t = \xi_x + (1/24)\xi_{xxx} + (g/2^{p/2}) \sum_{n=1}^{p-1} C_n^{p-1} \langle \eta^{p-n-1} \rangle (\xi^n)_x \\ \\ \eta_t = -\eta_x - (1/24)\eta_{xxx} - (g/2^{p/2}) \sum_{n=1}^{p-1} C_n^{p-1} \langle \xi^{p-n-1} \rangle (\eta^n)_x \end{cases} . \tag{13}$$

These are generalized Korteweg-de Vries (gKdV) equations. One can easily check that for $p = 3$ and $p = 4$ they yield, respectively, the KdV and the modified KdV equation, which are both integrable.

Notice that now, as a consequence of averaging, the two moments of second order of ξ and η are constants of motion for system (13). Moments of order greater than two will be time–dependent, and as a consequence the above equations are actually coupled and of integro-differential type for $p \geq 6$.

Up to this point we have shown that, for long–wavelength initial data, the gKdV equations constitute the resonant hamiltonian normal form of the FPU system (actually represented by the gB equation). We recall that in the case of short–wavelength initial conditions the resonant normal form has been shown to be constituted by nonlinear Schroedinger equations [9].

5. Dimensional analysis

The fundamental role played by the KdV equation in the FPU problem (in the case $p = 3$) was pointed out first by Zabusky and Kruskal [10]. In such a work they pointed out that the flow of such an equation displays two distinct regimes, which we recall here. Keeping in mind once again that initial data for the problem in study have the form (9), at very short times the derivatives will be small, and the dispersive terms ξ_{xxx} and η_{xxx} can be neglected in the equations of motion (7); as a consequence one gets two generalized Hopf (or inviscid Burgers) equations whose flow would display singularities in a finite time. Anyway, in going towards the singularity

the derivatives increase and at a certain time the terms ξ_{xxx} and η_{xxx} can no longer be neglected. Then dispersion becomes important and a sort of balance between dispersion and nonlinearity prevents the shock formation, thus giving rise to solitons (for a recent aprroach to the FPU problem strongly based on solitons see [11]). At this stage one expects a state of partial equilibrium to have been reached. So, there remains only to translate in quantitative terms what has been just said, and this is easily achieved through dimensional analysis. An enlightening treatment of the mathematical foundations of dimensional analysis can be found in the book of Gallavotti [12].

If one denotes by M the typical value of the fields ξ and η at time t and by ℓ the typical length–scale of variation of the same fields, one then estimates e.g. $\xi_x \sim M/\ell$. Analogously, if τ denotes the typical time–scale of variation of the fields, then one has e.g. $\xi_t \sim M/\tau$.

Now, in the equations of motion (7), following what pointed out by Kruskal, one can neglect the dispersive term if the ratio of the dispersive terms to the nonlinear ones appearing on the r.h.s. of the equations is less than 1, namely if

$$\frac{\xi_{xxx}}{g(\xi^{p-1})_x} \sim \frac{1}{g\ell^2 M^{p-2}} < 1 \quad . \tag{14}$$

One the other hand, if such an inequality holds, the dynamics is ruled by the a generalized Hopf equation, and this has the property that the maximum of its solution is a constant of motion. Thus, recalling (9), one can set $M = \sqrt{\varepsilon}$, which inserted in (14) yields

$$\ell > \ell_{min} \equiv g^{-1/2}\ \varepsilon^{-(p-2)/4} \quad . \tag{15}$$

The latter inequality must be interpreted as follows: ℓ_{min} gives the order of magnitude of the smallest spatial scale to which energy flows; at smaller spatial scales the dynamics is essentially dispersive and the corresponding Fourier modes of the system are almost frozen. The relaxation time τ_{rel} needed for the energy to flow up to the spatial scale ℓ_{min} is the one for which dispersion becomes important and $\xi_t \sim \xi_{xxx}$, namely

$$\tau_{rel} \sim \ell_{min}^3 = g^{-3/2}\ \varepsilon^{-3(p-2)/4} \quad . \tag{16}$$

It must also be stressed that if the minimal wavelength to which energy is transfered is $\lambda \sim \ell_{min}$, then the highest Fourier mode involved in the dynamics is the one corresponding to $k_{max}/L \sim 1/\ell_{min}$. Such a value of k_{max}/L of coincides with the fraction n_{eff} of degrees of freedom of the system actually sharing the energy.

6. Comments

First of all it has to be pointed out that from the estimates (15) and (16) one realizes that the quantities characterizing the cascade are intensive: they depend only on the specific energy $\varepsilon = E/L$. Thus, at least at a formal level, such estimates hold in the thermodynamic limit $E \to \infty$, $L \to \infty$ at E/L fixed. Of particular significance is the fact that $n_{eff} \sim \varepsilon^{3(p-2)/2}$, which is a small number if ε is small, so that the system does not reach equipartition at least on time scales of order τ_{rel}.

The numerical results available in the literature are mostly concerned with the case $p = 3$. In such a case, the scaling $k_{max} \sim \varepsilon^{1/4}$ was observed both by Berchialla et al. [13] and by Biello et al. [14], while in reference [14] the scaling law $\tau_{rel} \sim \varepsilon^{-3/4}$ too was measured. The agreement with the simple predictions given in the present paper seems thus to be promising.

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References

1. E. Fermi, J. Pasta and S. Ulam, in E. Fermi "Collected Papers", University of Chicago Press (1965).
2. G. Benettin, in "Molecular dynamics simulation in classical statistical mechanical systems", Proceedings of the E. Fermi Summer School of Varenna (1986); ed. by G. Ciccotti and W. G. Hoover.
3. J. Ford, *Phys. Rep.* **213**, 271-310 (1992).
4. A. Carati, L. Galgani, A. Ponno and A. Giorgilli *Il Nuovo Cimento B* **117**, 1017-1026 (2002).
5. N. J. Zabusky, in "Nonlinear Partial Differential Equations", Academic Press, New York (1967); ed. by W. F. Ames.
6. V. E. Zakharov, *Sov. Phys. JETP* **38**, 108-110 (1974).
7. W. Craig and M. D. Groves, *Wave Motion* **19**, 367-389 (1994).
8. J. A. Sanders and F. Verhulst, "Averaging Methods in Nonlinear Dynamical Systems", Springer-Verlag, New York (1985).
9. D. Bambusi, A. Carati and A. Ponno, *Discrete and Continuous Dynamical Systems-Series B* **2**, 109-128 (2002).
10. N. J. Zabusky and M. D. Kruskal, *Phys. Rev. Lett.* **15**, 240-243 (1965).
11. A. Ponno, *Europhysics Letters* **64**, 606-612 (2003).
12. G. Gallavotti, "Foundations of Fluid Dynamics", Springer-Verlag, Berlin (2001).

13. L. Berchialla, L. Galgani and A. Giorgilli, *Discrete and Continuous Dynamical Systems-Series B*, (2004) in print; available on the web pages of L. Galgani and A. Giorgilli.
14. J. A. Biello, P. R. Kramer and Y. V. Lvov, in "Proceedings of the fourth international conference on dynamical systems and differential equations, Wilmington, NC, USA (2002)"; available on the web: `arXiv:nlin.CD/0210007 v1` and `arXiv:nlin.CD/0210008 v1`.