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Editorial

Hamiltonian Lattice Dynamics

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Abstract: Hamiltonian Lattice Dynamics is a very active and relevant field of research. In this Special Issue, by means of some recent results by leading experts in the field, we tried to illustrate how broad and rich it can be, and how it can be seen as excellent playground for Mathematics in Engineering.

Keywords: Hamiltonian lattices

1. Motivations and general description

The present Special Issue is devoted to the mathematical and numerical investigation of the dynamics of a class of Hamiltonian systems with many (even infinite) degrees of freedom, often known in the literature as Hamiltonian Lattices (HL in the following). These systems often appear both in applications as well as in basic/pure science. For example, they are of relevance in physics, e.g. in the microscopic description of matter (to study crystals or Bose-Einstein condensates), or in biology, e.g. in the description of macro-molecules (like proteins or in particular the DNA double strand). These (toy) models are used in a diverse host of applications including micro-mechanics, microelectronics, nonlinear optics, granular matter, cantilever arrays, Josephson junctions, or acoustic wave guides, to just name a few. A first common trait of the above mentioned models is their discrete nature. We consider particularly relevant to highlight the existence of many discrete models and to present the corresponding Mathematics, especially for a journal devoted to the use of Mathematics in Engineering, where continuous systems and thus PDEs are more often used.

A second common point in the considered systems, beyond several specific features due to the different fields of applications, is the Hamiltonian structure: the dynamics is always described by a

canonical system of first order differential equation

$$\begin{cases} \dot{x}_j = \frac{\partial H}{\partial y_j} \\ \dot{y}_j = -\frac{\partial H}{\partial x_j} \end{cases} \quad (1)$$

where H is the Hamiltonian function and (x, y) are canonical coordinates which identify the configurations and the momenta of the system. Among the most known and used one-dimensional models we recall the Fermi-Pasta-Ulam (FPU) chains, the discrete Klein-Gordon (KG) model and the discrete Nonlinear Schrödinger (dNLS) in their classical form*:

FPU

$$H(x, y) = \sum_{j \in \mathcal{J}} \frac{y_j^2}{2} + V(x_j - x_{j-1}), \quad V(r) = \frac{r^2}{2} + \alpha \frac{r^3}{3} + \beta \frac{r^4}{4}. \quad (2)$$

KG

$$H(x, y) = \sum_{j \in \mathcal{J}} \frac{y_j^2}{2} + V(x_j - x_{j-1}) + W(x_j), \quad V(r) = \gamma \frac{r^2}{2}, \quad W(r) = \frac{r^2}{2} + \alpha \frac{r^3}{3} + \beta \frac{r^4}{4}. \quad (3)$$

dNLS

$$H(\psi, \bar{\psi}) = \sum_{j \in \mathcal{J}} \frac{|\psi_j|^2}{2} + \frac{\gamma}{2} |\psi_{j+1} - \psi_j|^2 + \frac{\beta}{2} |\psi_j|^4. \quad (4)$$

with $\mathcal{J} \subset \mathbb{Z}$ either finite (with periodic or fixed boundary conditions) or infinite (with some proper assumption on the decays of the sequences x_j and y_j , typically being in ℓ^2), and ψ complex valued. Of course there exist also several versions of these models in more than one spatial dimensions. In these cases, and making reference to the simplified description of a crystal given e.g. by the FPU system, the *lattice* structure can be related to the natural equilibrium configuration, besides being associated with a set of indices of the degrees of freedom.

The above mentioned models are the easiest and most representative HL, and their investigation has spanned several decades. Nevertheless, many other models have been subjects of a wide and fruitful study during the past and most recent times, in one or higher dimensions, either motivated by the description of old and new physical phenomena in Theoretical Physics or in order to deepen and reveal the mathematical structure and the properties of the models themselves. Among others, we can mention:

- the Frenkel-Kontorova model, already formulated in the late 1930s to describe dislocations within crystal lattices;
- the Toda model, which represents one of the rare and most celebrated integrable HL, whose dynamics has been shown to exhibit strong connections with the FPU model on the one hand, and with the Kortweg-de Vries partial differential equation on the other;

*with different choices of the interaction potential V or of the on-site potential W it is possible to include in those families other cases, e.g. granular crystals or sine-Gordon models.

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- the discrete Ablowitz-Ladik model (AL model), which is a dNLS-type integrable model, and the intermediate Salerno models, which provide a homotopic connection between the dNLS and the AL models;
 - diatomic FPU models, which provide an easy description of ionic crystals and have been successfully exploited to study experimental properties of the crystal and ergodic/mixing properties in the thermodynamical limit;
 - oscillator chains with Hertzian contact forces, which have been recently introduced to model granular crystals (whose interest is also due to practical applications, like shock absorbers), and the related discrete Schrödinger equation with the discrete p-Laplacian (known as DpS);
 - models with interactions beyond the nearest neighbours, starting from adding only the next-to-nearest neighbours interaction (as in the so-called zigzag models), up to the long range interactions (which is a all-to-all interactions model with some prescribed decay of the strength depending on the distance among sites/oscillators);
 - models with different nonlinearities, from competing cubic-quintic or saturable nonlinearities in the dNLS models, up to mixed FPU-KG models, where the nonlinear forces acting on the oscillators are due both to local and coupling nonlinearities.

We have just sketched some of the many models that have emerged in the field of HL. However, this short overview should be enough, in our opinion, to underscore the interest and the relevance of this field, both historically and prospectively. The importance of HL is confirmed even considering non-Hamiltonian extensions, like for example in lattice models where the Hamiltonian structure holds only approximately, due to a small dissipative force, or where it is completely lacking, as in discrete reaction-diffusion models. Indeed, under a more general perspective, HL can be seen as part of the wider field of Lattice Differential Equations (LDEs), which naturally emerge from the spatial discretization of PDEs. Such a connection between LDEs and PDEs manifests itself also in the common aspects of the dynamics which are explored, both in the discrete and in the continuous models; although the discrete models often preserve some of the dynamical features of the corresponding continuous one, also discrepancies have been highlighted, in order to discuss and to better understand the role of discreteness in LDEs. It is also worth to be noted that some of the mathematical methodologies of the analysis developed for the PDEs have been successfully extended to LDE: variational methods, dispersive estimates, spectral results, to mention only some of them. At the same time, these ones are combined with other techniques borrowed from the framework of ODEs, and sometimes specifically developed for classical Hamiltonian systems, e.g., perturbation theory and (resonant/non resonant) normal forms, multiscale expansions and modulation equations, as well as bifurcation theory.

Concerning the range of questions and the focus of the investigation in HL, one immediately realizes from the scientific production that a large part of the literature deals with *local aspects* of the dynamics, e.g. existence and stability of special solutions: periodic/quasi-periodic solutions (such as Discrete Solitons, Breathers and Multibreathers and their quasi-periodic extensions); travelling and stationary wave solutions; modulational instability as well as dispersive behaviours.

But very relevant is also the investigation of *global aspects* of the dynamics, of great interest for the foundations of Theoretical and Statistical Physics; e.g., ergodic and statistical properties of the system, existence of adiabatic invariants and metastable phenomena. Among the several techniques used, we might stress the use of ideas borrowed from Probability, even combined with perturbative approaches.

As in all the contemporary history of Mathematical Physics, also in the field of HL the mathemat-

ical analysis of the models have been fruitfully combined with the accurate numerical exploration, due to the hard-to-surmount barriers often encountered in a rigorous mathematical approach; it is not surprising that the numerical simulations have often provided clear evidence of new phenomena well before the latter have been mathematically proven or justified. For such a reason, the developments of effective and reliable numerical methods have played a crucial role in the field of HL, as confirmed by the rich area of symplectic integrators and chaotic indicators.

In this Special Issue we aimed at providing a reasonably balanced mix of the above described models, methods and approaches. We have indeed envisioned the Issue as an opportunity to bring together contributions showing both the more applied side of the field of Hamiltonian Lattices (possibly even at a close to "engineering" level) and papers exploring the more theoretical, let us say analytical, aspects, thus pointing the fundamental role of rigorous Mathematics. In the following Section we briefly describe the contribution of the selected papers, collecting them in groups based on their contents, independently of the order of publication.

2. A guided tour of the Special Issue

2.1. First part

We collect here the group of papers more related either to the investigation of special classes of solutions in nonlinear chains, or to the analysis of energy transfer/localization in those models, often motivated by problems related to the foundations of physics in general, or by the dynamical foundations of Statistical Mechanics in particular.

Let us start with a couple of works that share both the model, a diatomic FPU chain, and the argument of investigation, i.e. the class of solution given by travelling waves.

In "*Asymptotic approximations to travelling waves in the diatomic Fermi-Pasta-Ulam lattice*", by Jonathan A. D. Wattis [11], the author discusses approximations of travelling waves, using the continuum limit with expansions in small amplitudes, but with arbitrary ratios between the two different masses. The first order approximation of the profile is given by the usual sech(-type) functions, the second order simply represents a phase shift, while in the third order appear the first changes to the shape. From a technical point of view, the solution of the equations at each order is performed with the application of the Fredholm alternative.

In "*Metastability of solitary waves in diatomic FPUT lattices*", by Nickolas Giardetti, Amy Shapiro, Stephen Windle and J. Douglas Wright [5] a similar subject is considered, but from the point of view of (meta-)stability. Considering the long wave setting, where the KdV approximation is known to hold for long times, the authors investigate numerically what happens to KdV soliton solutions for times longer than those for which the KdV approximation is valid. This is an interesting question since the finite energy solution considered cannot converge to the infinite energy nanopteron, which is the natural generalization of the solitary wave solution of monoatomic chains for the problem at hand. As a result, the typical behaviour is that of a solitary wave plus an oscillatory wake of small amplitude, but frequency which appear to be fixed by the mass ratio; the wake is finite, always trailing the solitary profile, and continuously albeit slowly growing in space at the expense of the solitary component.

We come now to consider three works whose common interest can be seen in the dynamical proper-

ties relevant for some physical features of the corresponding models. In particular they can be inserted in the long and fruitful series of papers originating from the pioneering work by Fermi and collaborators [4] about energy equipartition in nonlinear chains, with a clear motivation in the dynamical foundations of Statistical Mechanics.

In “*Stages of dynamics in the Fermi-Pasta-Ulam system as probed by the first Toda integral*”, by Helen Christodoulidi and Christos Efthymiopoulos [2], the original type of investigation of [4] is revisited by using the first non trivial Toda integral. With several classes of initial conditions, both in and far from equipartition, the authors explore the different stages of dynamics. For non equilibrium initial data they consider the different timescales corresponding to the initial almost integrable behaviour as well as the subsequent relaxation towards thermalization, detecting a dependence on the number of degrees of freedom for the specific energy threshold below which the two timescales are exponentially long; for equilibrium initial conditions they observe always a small diffusion transversal to the Toda surfaces, suggesting a persistence of regularity within the final equilibrium state.

In “*Universal route to thermalization in weakly-nonlinear one-dimensional chains*”, by Lorenzo Pistone, Sergio Chibbaro, Miguel D. Bustamante, Yuri V. L’vov and Miguel Onorato [9], a similar problem is investigated, considering both a KG lattice and the FPU model studied in the previous paper. In this work, assuming the applicability of the Wave Turbulence theory, the authors analyse the corresponding consequences in terms of time scales to energy equipartition. The claim is that the equipartition time scales as a power law of the specific energy, both in the thermodynamic limit and in the discrete regime, for all the models considered, at least in a range of parameters. Extensive numerical simulations are shown to support the theory, with the discussion of some discrepancies observed. Another interesting outcome of their approach is the possible universality of the route to thermalization once this is ruled by exact resonances.

In “*Energy transmission in Hamiltonian systems of globally interacting particles with Klein-Gordon on-site potentials*”, by Jorge E. Macías-Díaz, Anastasios Bountis and Helen Christodoulidi [8], a relevant variation on the classical models is considered, i.e. the presence of long range interactions, well beyond the nearest neighbour case. In such a setting, driving the chain in one end and adding a damping at the other end, the authors investigate the energy transmission along the chain, detecting a threshold in the “length” of interaction above which nonlinear supra-transmission is present. The results are specifically obtained for a KG model, but their validity is conjectured also for other variants.

2.2. Second part

We consider here some works more related to applications.

The first two papers of this group are among those providing a nice balance between a topic with direct relations with application and the use of high level analytical tools.

In “*Solitary waves in atomic chains and peridynamical media*”, by Michael Herrmann and Karsten Matthies [6], in the context of peridynamics[†] — a branch of solid mechanics where nonlocal integro-differential equations are used instead of PDEs — the authors consider travelling waves through a variational characterization. They prove the existence of solitary profiles and their approximation with

[†]We point the attention of the interested reader to a Special Issue of the journal Materials Science devoted to Peridynamics: <https://www.aimspress.com/newsinfo/895.html>

periodic travelling waves. They also investigate various asymptotic regimes, and complement their presentation with numerical simulations of the profiles.

In “*Wannier functions and discrete NLS equations for nematicons*”, by José Antonio Vélez-Pérez and Panayotis Panayotaros [10], optical beams in a nematic liquid crystal are considered. To this end they study the derivation of a nonlocal dNLS system which generalizes previous models. Starting from a system of PDEs of NLS-elliptic type, and using a periodic Schroedinger operator, a Wannier basis is considered, in order to pair the original system with the evolution of the Wannier coefficients. Numerical evaluations of some integrals are required during the analysis of the problem.

The next two papers share a slight detour from the main theme of the Issue by exploring the non Hamiltonian side of the world; indeed they both consider damping in their models.

In “*Breathers and other time-periodic solutions in an array of cantilevers decorated with magnets*”, by Christopher Chong, Andre Foehr, Efstathios G. Charalampidis, Panayotis G. Kevrekidis and Chiara Daraio [1], the authors really touch upon the engineering side by considering and implementing a real physical system, besides studying its mathematical model. They build a micro-mechanical oscillator array made of cantilevers coupled with the addition of magnets. The corresponding model is a mixed FPU-KG chain, with damping to take into account friction effects, and forcing to consider particular experimental conditions. Focusing on time periodic solutions of breathers type, they observe experimentally the dynamics and compare it with the corresponding solutions of the mathematical model, with good agreement; bi-stability and hysteresis are also explored and discussed.

The second “non conservative” paper is “*Instabilities via negative Krein signature in a weakly non-Hamiltonian DNLS model*”, by Panayotis G. Kevrekidis [7]. The author considers a discrete counterpart of the dissipative Gross-Pitaevskii, to describe thermal fluctuations in Bose-Einstein condensates. Thus a weakly non Hamiltonian dNLS is considered, in the anti-continuous limit; by means of spectral arguments, the stability of some solitary wave solutions is investigated, with particular emphasis on the role of the non Hamiltonian perturbing term. Besides the analytical arguments, some numerical explorations complete the picture of the system at hand.

We conclude this tour of our Special Issue with the paper “*Computational efficiency of numerical integration methods for the tangent dynamics of many-body Hamiltonian systems in one and two spatial dimension*”, by Carlo Danieli, Bertin Many Manda, Thudiyangal Mithun and Charalampos Skokos [3]. It might be considered as an ancillary (not to be confused with minor or irrelevant) work with respect to many other papers of the Issue; indeed many results presented here have also a strong numerical component and the paper by Danieli et al. deals with the numerical methods used to integrate the systems of ODEs involved in lattice dynamics. They concentrate their attention in particular on the problem of efficiency, with a deep analysis of several numerical schemes, and special emphasis on symplectic integrators. They also take into account the integration of the tangent dynamics, which is necessary for the computation of the Lyapunov exponents. We are convinced that such an effort will prove useful for the community of people working on lattice dynamics with numerical methods.

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