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Numerical integration of variational equations for Hamiltonian systems with long range interactions

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A R T I C L E I N F O

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This paper is dedicated to the loving memory of our dear friend and colleague Professor Theodore Papatheodorou, in appreciation for all he taught us about how to be a dedicated scientist and a principled human being.

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A B S T R A C T

We study numerically classical 1-dimensional Hamiltonian lattices involving inter-particle long range interactions that decay with distance like $1/r^{\alpha}$, for $\alpha \geq 0$. We demonstrate that although such systems are generally characterized by strong chaos, they exhibit an unexpectedly organized behavior when the exponent $\alpha < 1$. This is shown by computing dynamical quantities such as the maximal Lyapunov exponent, which decreases as the number of degrees of freedom increases. We also discuss our numerical methods of symplectic integration implemented for the solution of the equations of motion together with their associated variational equations. The validity of our numerical simulations is estimated by showing that the total energy of the system is conserved within an accuracy of 4 digits (with integration step $\tau = 0.02$), even for as many as $N = 8000$ particles and integration times as long as 10^6 units.

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1. Introduction

Hamiltonian systems describing 1-Dimensional (1D) particle chains characterized by interactions of various ranges constitute an active area of research with increasing interest due to their applicability in many scientific fields. In particular, the relevance of long (vs. short) range interactions has been extensively studied and intensely debated in a wide variety of problems of statistical mechanics, mean field theories, active matter, dynamical networks, etc. regarding the various degrees of chaos involved in their time evolution. In statistical physics for example, the classical Boltzmann framework for the appropriate entropy functional at thermal equilibrium is not adequate for describing systems with long range interactions, as remarked already by J.W. Gibbs [14].

In the past 25 years, a great number of researchers [21,13,18,22,23,3] have shown that there exist long lasting quasi-stationary states (QSS) in a variety of physical and biological systems characterized as *non-additive*, i.e. that cannot be decomposed in entirely independent parts. In such cases, a different entropy functional (the so-called Tsallis entropy) appears to be more suitable for their thermodynamic description, while the associated probability distribution functions are of the q-Gaussian type with $q > 1$. This divergence from the classical Boltzmann–Gibbs Maxwellian distributions of $q = 1$, raises new questions regarding the statistical and dynamical behavior of such systems in the thermodynamic limit of very large N and total energy E, with E/N constant.

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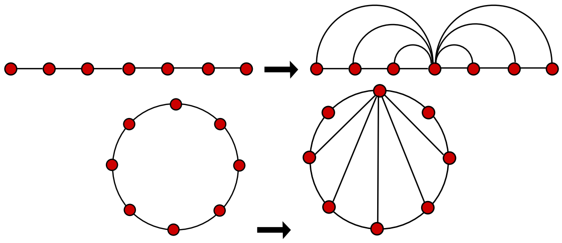

Fig. 1. Lattices with nearest neighbor interactions ($\alpha \to \infty$) on the left are converted into long range systems on the right. In our paper the strength of this interaction decays with distance as $1/r^\alpha$, for finite $\alpha \geq 0$. Upper panels correspond to fixed or open boundary conditions and lower panels to periodic boundary conditions.

As we have demonstrated in recent publications [8,9], systems with long range interactions (LRI) have significant advantages, since they often exhibit *a weaker chaos* than those with interactions only between nearest neighbors. For example, in active matter systems consisting of self-propelled particles (like birds) it has been observed that nonlocal communication acts as a counterbalance against external threats or attacks. This is the case, for instance with flocks of starlings described by the so-called topological model introduced by the STARFLAG group [4]. Their observations on groups of starlings in Rome revealed that synchronized movements are based on a fixed number of interacting neighbors, independent of the distance between them. Moreover, it was shown in [8] that the number n of interacting particles in the topological model is crucial for the coherence of the group: n needs to be large enough to overcome random perturbations as well as maintain cohesion.

On the other hand, the study of LRI in the classical framework of dynamical systems is of great interest. Spatially localized oscillations called breathers, well-known as simple periodic solutions of lattices with nearest neighbor interactions, make their appearance also in Hamiltonian systems with LRI (see [12] for more details). Another interesting type of collective behavior occurs in the form of long-living QSS of the type mentioned above, while in a system of N coupled planar rotators that interact via long-range forces critical regions were found where these states appear [15]. Moreover, in [15,1] a systematic study of the largest Lyapunov exponent showed that it decays as a power-law with N, making the system quasi-integrable in the thermodynamic limit. Such QSS were also studied in a generalized mean field system, where interactions decay with distance according to $1/r^\alpha$ [7,10].

More recently, the Fermi–Pasta–Ulam-β model (FPU-β) with LRI was studied in [9,16] and opened a new branch of research in this field. In [16] for example, the authors explore instability regimes for the low frequency modes of an FPU-β chain in relation to the long-standing question of the relaxation times required to reach energy equipartition among all modes.

In the present paper we focus on two topics: (i) First we extend recent studies of nearest-neighbor Hamiltonian lattices to analogous models involving LRI, and (ii) we employ numerical integration schemes to compute the tangent dynamics needed for the calculation of the largest Lyapunov exponent. The structure of our paper is as follows: In Section 2 we discuss in detail the transition to LRI for different boundary conditions, while in Section 3 we solve the associated variational equations for specific chaotic states. Subsection 3.1 gives the basic properties and definitions of symplectic integrators and discusses in Subsection 3.2 the so-called tangent map method. Finally, in Section 4 we apply these techniques to two different Hamiltonian systems: the mean field model of planar rotors and the FPU-β chain, both with interactions modulated by the factor $1/r^\alpha$. We end with our conclusions in Section 5.

2. Hamiltonian particle chains with long range interactions

Let us consider a 1D Hamiltonian chain with quadratic kinetic energy in the generalized momenta and a potential that depends purely on the generalized positions and contains nearest neighbor interactions together with an on-site potential. This system is described by the Hamiltonian

$$\mathcal{H} = \frac{1}{2}\sum_i p_i^2 + \sum_i W(x_i) + \sum_i V(x_{i+1} - x_i) \ , \tag{1}$$

where p_i and x_i are canonical conjugate pairs of positions and momenta and boundary conditions are chosen arbitrarily.

To convert the 1D lattice (1) to an LRI system, all nearest neighbor interacting terms[1] in the potential, i.e. the position differences $x_{i+1} - x_i$, should be replaced by the difference combinations $x_i - x_j$, $i, j = 1, \ldots, N$, so that particles can form a fully connected graph (see Fig. 1). Then, of course, one can apply interactions which depend on the topological distance and decay with distance as $1/r^\alpha$, with $\alpha \geq 0$, as in [1]. Next, (1) is converted to a Hamiltonian with LRI:

[1] Or some of them. In [9] we considered LRI on the quartic potential of FPU-β model, while the quadratic one was left unchanged.

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