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Analyzing chaos in higher order disordered quartic-sextic Klein-Gordon lattices using q-statistics

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ABSTRACT

In the study of subdiffusive wave-packet spreading in disordered Klein–Gordon (KG) nonlinear lattices, a central open question is whether the motion continues to be chaotic despite decreasing densities, or tends to become quasi-periodic as nonlinear terms become negligible. In a recent study of such KG particle chains with quartic (4th order) anharmonicity in the on-site potential it was shown that $q-$Gaussian probability distribution functions of sums of position observables with $q > 1$ always approach pure Gaussians ($q = 1$) in the long time limit and hence the motion of the full system is ultimately "strongly chaotic". In the present paper, we show that these results continue to hold even when a sextic (6th order) term is gradually added to the potential and ultimately prevails over the 4th order anharmonicity, despite expectations that the dynamics is more "regular", at least in the regime of small oscillations. Analyzing this system in the subdiffusive energy domain using q-statistics, we demonstrate that groups of oscillators centered around the initially excited one (as well as the full chain) possess strongly chaotic dynamics and are thus far from any quasi-periodic torus, for times as long as $t = 10^9$.

1. Introduction

Anderson localization [1], i.e. the absence of wave diffusion in disordered media, is a phenomenon affecting many physical processes, such as for example the conductivity of materials, the behavior of granular matter, the dynamics of Bose–Einstein condensates, etc. The effect of nonlinearity on the localization properties of wave packets in disordered systems has attracted the attention of many researchers, both experimentally [2–4] and theoretically [5–28,31]. Recent studies of nonlinear disordered variants of two typical one-dimensional Hamiltonian lattice models, namely the Klein–Gordon (KG) oscillator chain and the discrete nonlinear Schrödinger equation, revealed the statistical characteristics of energy spreading and showed that nonlinearity destroys localization [7,8,11,13,18,19]. In these papers, the existence of different dynamical behaviors in different energy density regimes was established, their particular dynamical characteristics were determined and their appearance was theoretically explained.

However, important questions regarding the asymptotic behavior of wave-packet spreading, and the persistence of chaos in such systems, still remain unanswered. Some researchers have conjectured [29,30] that wave packets will eventually approach torus-like structures in phase space, exhibiting at the same time less chaotic behavior which eventually leads to the halt of energy spreading in the chain. Although most numerical investigations on nonlinear disordered lattices show that wave packets continue spreading chaotically, at least up to times accessible to computer simulations, some numerical indications of a possible slowing down of spreading for particular models have been reported in the literature [17,24]. The diversity of the models studied so far includes systems with different numbers N_{IoM} of integrals of motion or conserved quantities, and the degree of anharmonicity σ which is related to a corresponding n-body interaction or equally to the number of interacting normal modes mediated by the anharmonicity. $N_{\mathrm{IoM}} = 1$ for the mentioned case of KG lattices, while $N_{\mathrm{IoM}} = 2$ for the DNLS case. In most studied cases $\sigma = 2$ which corresponds to quartic anharmonicity and two-body interactions. Here we will also study $\sigma = 4$ which corresponds to sextic anharmonicity and three-body interactions.

To investigate the potential asymptotic approach to regular (or irregular) dynamics, the properties of the motion in the subdif-

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fusive regime of the KG model with $\sigma = 2$ were recently studied [25,31]. In [25], the computation of the maximum Lyapunov exponent (MLE) showed that although chaotic dynamics slows down as expected from a subdiffusive process, it does not cross-over to a regime of regular behavior. In [31] the dynamics of a disordered quartic (termed KG4) lattice was studied using q-statistics [32] by analyzing probability distribution functions (pdfs) of position observables describing the evolution of wave packets initiated by exciting the central lattice particle. In that work it was shown that the overall motion displays strongly chaotic behavior for long times, again with no signs of the dynamics relaxing on quasi-periodic tori.

In this paper, we apply the above methodology followed in [25,31] to a KG model which includes a gradually increasing sextic anharmonicity which is assumed to show an asymptotic slowing down of the wave packet spreading - if existing - at earlier times, since the impact of this anharmonicity is weaker than the quartic one, as long as small densities are considered. In line with what we discovered in the KG4 model [31], both the full lattice, as well as groups of particles around the initially excited one at the center remain strongly chaotic and show no signs of approaching quasi-periodicity, even after very long integration times (at least up to $t = 10^9$, with time scales dictated by the linear equations being of order one). On the other hand, individual particles far from the center, after interacting with the wave-packet behave at first weakly chaotically, but later also tend to strong chaos for times as long as $t = 10^9$. We find that the closer the particles are to the center of the lattice, the more strongly chaotic their behavior is (with pdfs closer to the Gaussian $q = 1$ case), and that the dynamics of the whole lattice is always strongly chaotic, with pdfs obeying Boltzmann–Gibbs thermostatistics. Thus, all our results indicate that the wave packet spreading is a truly chaotic process which does not show any tendency to become more regular. Our results are also supported by the computation of the time dependence of the largest Lyapunov exponent which again show no cross-over into a regime of regular behavior, similar to the KG4 case [25].

The paper is structured as follows: In Section 2 we present the KG model and outline the used statistical methods in the spirit of the Central Limit Theorem (CLT). In Section 3 we examine the mixed case of both quartic and sextic anharmonicities in the potential and consider the statistical properties of the dynamics as the sextic terms become increasingly more important. In Section 4, we focus on the purely sextic anharmonicity model and describe the results obtained when we excite only the central particle of a 500 particle chain and monitor the chaotic evolution of individual particles, groups of particles about the central one, as well as the whole system. Our conclusions and a discussion follow in Section 5.

2. Model and numerical methods

The Hamiltonian of the disordered one-dimensional KG lattice studied in [11] is

$$H = \sum_{l=1}^{N} \frac{p_l^2}{2} + \frac{\tilde{\epsilon}_l}{2} x_l^2 + \frac{|x_l|^{\sigma+2}}{\sigma+2} + \frac{1}{2W}(x_{l+1} - x_l)^2, \quad (1)$$

where l is the lattice site index, x_l and p_l are respectively the generalized canonically conjugated coordinates and momenta (with $x_{N+1} = 0$), σ measures the degree of anharmonicity and $W = 4$ controls the nearest neighbour interaction strength and thus the effective strength of disorder. Disorder enters through the on-site harmonic squared frequencies $\tilde{\epsilon}_l$ which are random uncorrelated numbers chosen uniformly from the interval $\left[\frac{1}{2}, \frac{3}{2}\right]$. The total energy $E \equiv H \geq 0$ of the system serves as a control parameter of the nonlinearity for fixed disorder strength W. The case $\sigma = 2$ corresponds to the typical quartic disordered KG4 model. Wave packet spreading in the KG4 case was studied in several papers [7,8,13,18,19,25,31]. The equations of motion follow as $\dot{x}_l = \partial H/\partial p_l$ and $\dot{p}_l = -\partial H/\partial x_l$.

The dynamics of wave packet spreading in the Hamiltonian (1) was analyzed in detail in [11] for several anharmonicity values σ, following the evolution of the normalized energy density

$$z_l = \frac{E_l}{\sum_{i=1}^{N} E_i} \quad (2)$$

of the site-energies $E_l = \frac{p_l^2}{2} + \frac{\tilde{\epsilon}_l}{2} x_l^2 + \frac{|x_l|^{\sigma+2}}{\sigma+2} + \frac{1}{4W}[(x_{l+1} - x_l)^2 + (x_{l-1} - x_l)^2]$. The main goal was to monitor the evolution of the second moment m_2

$$m_2 = \sum_{l=1}^{N} (l - \bar{l})^2 z_l \,, \quad \bar{l} = \sum_{l=1}^{N} l z_l \quad (3)$$

which quantifies the wave packet degree of spreading, and the participation number

$$P = \frac{1}{\sum_{l=1}^{N} z_l^2}, \quad (4)$$

which measures the number of the most strongly excited sites in the system. In [11] it was found that the wave packet spreads incoherently and subdiffusively with $m_2 \propto t^{\alpha}$ and $P \propto t^{\alpha/2}$ with the exponent

$$\alpha = \frac{1}{\sigma + 1} \quad (5)$$

up to the largest computed times, indicating no loss of incoherent (chaotic) dynamics and no cross-over to coherent (regular) dynamics.

In the present paper we consider a hybrid model (termed KG46 here) which interpolates between the quartic $\sigma = 2$ and sextic $\sigma = 4$ cases by including sextic terms in (1). We expect that sextic terms are generating weaker nonlinear terms in the equations of motion, and could amplify a crossover to regular dynamics, if present. In all our models we follow the evolution of single-site excitations of the central particle in the subdiffusive regime defined in [11] (see Fig. 1 in [11]), by considering $N = 500$ sites and setting the total energy of our lattice to some constant energy E. In particular, for a given set of $\tilde{\epsilon}$ values, we choose $x_l = 0$ and $p_l = \sqrt{2E}\delta_{l,N/2}$, where $\delta_{i,j}$ is the Kronecker delta, thus exciting precisely one oscillator in the center of the system which has N sites.

To study the resulting trajectories, we integrate numerically the equations of motion of Hamiltonian (1) by the 4th order Yoshida's symplectic integrator [33]. In our simulations, we set the integration time step to $\tau = 0.05$, which typically keeps the relative energy error at about 10^{-6}. Furthermore, to obtain reliable statistical results that are independent of the particular realizations, we consider an ensemble of 64 disorder realizations, i.e. 64 random sequences of $\tilde{\epsilon}_l$ values in (1). Apart from the computation of m_2 and P, we also evaluate the MLE λ_1. For this purpose, we use the same symplectic integration scheme for the integration of the variational equations of system (1) according to the *tangent map method* [34–36]. The variational equations govern the evolution of small deviation vectors from the studied trajectory and are used for the evaluation of the MLE according to the so-called standard method [37–39].

We use the solutions of the equations of motion of Hamiltonian (1) to construct pdfs of suitably rescaled sums of M values of a generic observable $\eta(t_i)$, $i = 1, \ldots, M$, which depends linearly on the position coordinates of the solution. Viewing these as independent and identically distributed (iid) random variables (in the limit of $M \to \infty$), we evaluate their sum

$$S_M^{(j)} = \sum_{i=1}^{M} \eta(t_i)^{(j)}, \; j = 1, \ldots, N_{\text{ic}}, \quad (6)$$