Supersonic Discrete Kink-Solitons and Sinusoidal Patterns with “Magic” Wavenumber in Anharmonic Lattices

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Abstract. – The sharp pulse method is applied to Fermi-Pasta-Ulam (FPU) and Lennard-Jones (LJ) anharmonic lattices. Numerical simulations reveal the presence of high energy strongly localized “discrete” kink-solitons (DK), which move with supersonic velocities that are proportional to kink amplitudes. For small amplitudes, the DK’s of the FPU lattice reduce to the well-known “continuous” kink-soliton solutions of the modified Korteweg-de Vries equation. For high amplitudes, we obtain a consistent description of these DK’s in terms of approximate solutions of the lattice equations that are obtained by restricting to a bounded support in space exact solutions with sinusoidal pattern characterized by the “magic” wavenumber $k = 2\pi/3$. Relative displacement patterns, velocity versus amplitude, dispersion relation and exponential tails found in numerical simulations are shown to agree very well with analytical predictions, for both FPU and LJ lattices.

Introduction. – The interest in studying moving nonlinear localized excitations (solitons, kink-solitons, etc.) is mainly motivated by the fact that they can be related to transport properties. In this respect, one dimensional lattices of anharmonic oscillators can serve as a testing ground for nonlinear transport. In this Letter we present numerical and analytical studies of the dynamical properties of strongly localized excitations of anharmonic lattices with two-body interparticle potentials \cite{1}. Invariance under the symmetry transformation that shifts the positions of all the oscillators by the same amount relates anharmonic lattices with interparticle couplings to a wide class of systems which share such continuous symmetry, e.g. quasi-one dimensional easy plane ferromagnets and antiferromagnets, ferrimagnetic systems with spiral structures and even quantum Hall double layer pseudo-ferromagnets \cite{2}. The spontaneous breakdown of this translational symmetry leads to the apperance of gapless Goldstone modes, which itself generates kink-soliton solutions in the presence of nonlinearity. Anomalous transport properties \cite{3} could appear for all systems in this class. It is extremely important to assess whether such properties could be related to the existence of moving localized excitations. In the weakly nonlinear continuum limit and for gapless dispersion relations
one can prove [4] that all localized solutions can be described by the Korteweg-de Vries (KdV) or modified KdV (mKdV) equations [5, 6, 7, 8, 9]. On the lattice, small-amplitude solutions can be represented as KdV or mKdV solitons in terms of relative displacements, while they are kinks for absolute displacements. The energy of such objects is proportional to the kink amplitude and thus lattice discreteness has to be taken into account when considering high energy (i.e. strongly localized) objects. Since in this limit one cannot use the ordinary continuum approximation, Rosenau [10] has recently proposed a theoretical approach that takes explicitly into account lattice discreteness. Applying this approach to the Fermi-Pasta-Ulam (FPU) lattice [1], he derived, in the limit of strong nonlinearity, a different continuum equation, which supports a new kind of localized solution that he called compacton [11].

On the other hand, the existence of approximate kink-like solutions of the FPU lattice with characteristic sinusoidal displacement pattern with the “magic” wavenumber \( k = 2\pi/3 \) has been predicted on the basis of a direct analysis of the discrete lattice equations [12]. This ansatz relies on the existence of exact extended propagating nonlinear sinusoidal waves having this particular wavenumber [12, 13]. Such patterns are also extremely successful in modelling stationary and slowly-moving discrete breathers in the FPU lattice [12, 14, 15].

The numerical study of moving strongly localized excitations of anharmonic lattices has been so far limited to discrete breathers (DB) [16] that move with small velocity. Two types of numerical methods have been commonly used to study the time evolution of DB’s: i) exact [16, 17] or approximate [18, 19] DB’s are put initially onto the lattice and ii) modulational instability of zone-boundary and large-wavenumber modes is induced [14, 15, 20, 21, 22, 23, 24]. The first method allows one to investigate single moving localized objects, but it assumes the knowledge of exact or approximate solutions. By using the second method, a number of localized modes is produced: they move, collide and merge, and it is therefore hard to investigate each single moving object. On the other hand, no mathematical proof of existence of moving DB’s has been obtained (see [25] for a discussion of this issue and a possible way out).

In this Letter we show a new numerical method to produce strongly localized objects. This method is inspired by the one used in real experiments to generate optical solitons in fibers as well as magnetization envelope solitons in Yttrium Iron Garnet film waveguides [26]. A sharp pulse is applied at one end of an unperturbed sample. Then, the system itself chooses the stable propagating localized mode and the only thing that is left is to follow its motion. We have first performed these numerical experiments for an FPU chain with quadratic and quartic interactions between neighbors, which describes purely transverse vibrational excitations. For large amplitudes, we observe supersonic strongly localized discrete kink-solitons (DK) in which just three oscillators are excited. They show very low energy loss. We have repeated these experiments for more realistic Lennard-Jones (LJ) interparticle potentials, also revealing the existence of DK’s.

Fast moving kinks have been observed in the Frenkel-Kontorova (FK) model [27, 28]. Moving kinks appear also in translationally invariant lattices with Hertz potentials (see e.g. Ref. [29] and references therein), but in this case there is no attractive force and the localized wave dynamics is different from that of the FPU lattice.

**Sharp Pulse Method.** – The equations of motion of the FPU-\( \beta \) lattice [11] are

\[
\ddot{u}_n = u_{n+1} + u_{n-1} - 2u_n + (u_{n+1} - u_n)^3 + (u_{n-1} - u_n)^3,
\]

where \( u_n \) is the transverse displacement of the \( n \)-th oscillator from its equilibrium position in dimensionless units.

In the numerical experiment we oscillate the first particle of the chain in the following
manner:

\[ u_1 = A_0 \cdot \sin(\omega_0(t_0 - t)) \quad \text{if} \quad 0 < t \leq t_0 \quad \text{and} \]

\[ u_1 = 0 \quad \text{if} \quad t > t_0, \]

while the right end \( u_N \) is pinned. After applying the above pulse, we pin both ends of the lattice.

The numerical experiment shows the existence of kinks that propagate with large and slightly different velocities. Throughout this paper we will use two different representations of the spatial profile: either we use absolute lattice displacements \( u_n \) or we show relative displacements \( v_n = u_{n+1} - u_n \). Hence the kinks are shown as true steps in the first representation (see Fig. 1a) or as sharp peaks in the second representation (see Fig. 1b).

As time evolves, the plateaus between the DK's widen but the shape of the kinks does not change. During the collisions, the kink-solitons cross each other without any appreciable energy loss (this is not shown here for FPU lattices but later on for LJ lattices, see the right graph in Fig. 4).

The existence of these localized objects is possible because of the peculiar symmetry \( u_n \rightarrow u_n + \text{const} \) of the interparticle potential. Systems with such a symmetry have an infinitely degenerate ground state and its spontaneous breakdown leads to the appearance of gapless Goldstone modes that determine the formation of kinks.

Since the potential energy of the FPU chain is only a function of the relative displacements \( v_n = u_{n+1} - u_n \), these are the variables to be considered for the appropriate physical picture. In these new variables the equations of motion (1) can be exactly rewritten as

\[ \ddot{v}_n = v_{n+1} + v_{n-1} - 2v_n + v_{n+1}^3 + v_{n-1}^3 - 2v_n^3. \]

Eq. (3) leads, in the continuum approximation and selecting one direction for the wave motion, to the modified Korteweg-de Vries (mKdV) equation if one keeps only the first terms in the two small parameters \( 1/N \) and amplitude. The mKdV equation supports exact soliton solutions. Indeed, for small pulse amplitudes we could observe mKdV solitons. However, as

Fig. 1 – a) Absolute \( u_n \) and b) relative \( v_n = u_{n+1} - u_n \) displacements versus the lattice site \( n \) at time \( t = 20 \) in dimensionless units. In the \( u \)-space we observe a sequence of kinks with different amplitudes, while in the \( v \)-space the localized objects have solitonic form of different height. This simulation is performed with \( A_0 = 11, \omega_0 = \sqrt{2}, t_0 = 1 \) and \( N = 200 \).
the driving amplitude $A_0$ of the pulse is increased we observe the DK’s of Fig. 1. Therefore, in terms of relative displacements, the objects that we observe in our simulations can be considered as discrete extension of the solutions of the mKdV equation. The existence of fast moving objects with amplitude independent short localization length was first considered in Ref. [12]. In the remaining of this Letter, we develop a theoretical approach that, making use of this result allows us to describe the main physical properties of the DK’s we observe in our simulations.

Approximate Analytical Description. — Exact extended sinusoidal wave solutions of the FPU (and other) lattices have been recently found by several authors [12, 13, 30]. One of such solutions has the “magic” $k = 2\pi/3$ wavenumber and can be written in terms of relative displacements as $v_n = A \cos(kn - \omega t)$. It has been proposed that such exact solution can acquire a compact support and maintain its validity as approximate solution [12]. For instance, in the case of stationary and slowly-moving discrete breathers in the FPU-$\beta$ lattice, half a period truncations of the sinusoidal envelope of the displacement patterns with $k_e = \pi - k = \pi/3$ wavenumber well reproduce large amplitude localized oscillations [12, 13, 15]. Following the same strategy, we here propose a similar truncation that turns out to describe very well our supersonic DK’s:

$$v_n = \pm \frac{A}{2} [1 + \cos(\frac{2\pi}{3}n - \omega t)] \quad \text{if} \quad -\pi < \frac{2\pi}{3}n - \omega t < \pi;$$

and $v_n = 0$ otherwise. In the large amplitude limit we can neglect short exponential tails in the sinusoidal pattern (4) (see, however, Eq. (6) below). Substituting this ansatz into Eq (4) and performing the rotating wave approximation [31] for the second harmonic, we obtain the following relations for the frequency $\omega$ and velocity $V$ as the functions of the amplitude $A$ of the DK’s.

$$\omega = \sqrt{3 + (45/16)A^2}; \quad V = \omega/(2\pi/3) = 3\sqrt{3 + (45/16)A^2}/(2\pi).$$

First of all, we can observe that the analytical solution of formula (4) is consistent with the numerical observation that three lattice sites are always excited (see Fig. 1). Besides that, we have numerically checked the dependence of velocity on amplitude (see left graph in Fig. 2) and the time dependence of the relative displacement of a given oscillator (see right graph in Fig. 2). Our theoretical expression gives a very good agreement with all numerical data. Furthermore, the right graph of Fig. 2 shows that the relative displacement patterns of both the measured and the analytical solution has everywhere a smooth envelope. Therefore, we can conclude that the compacton with sharp cosine-like support and with non-smooth relative displacement envelope, described in Refs. [10, 11], doesn’t compare well with our numerical results. We’ll come back to this and related issues in a forthcoming publication [33].

In relation to this latter comment, it is important to remark that our DK’s have a localized bulk sided by exponential tails (see Fig. 3a). The decay length $\Lambda$ is a function of the velocity, as shown in Fig. 3b. This dependence can be derived analytically representing the relative displacements in the tails as $v_n \sim \exp[\pm(n - Vt)/\Lambda]$ and substituting this ansatz into equations (4). Considering the limit $n - Vt \gg \Lambda$, one gets the relation [12]:

$$V^2 = 4A^2 \sinh^2(1/2\Lambda).$$

As follows from Eq. (6), the decay length $\Lambda$ is real positive only for supersonic excitations with $V > 1$ and it diverges for $V = 1$. Again, the agreement with numerical data, shown in Fig. 3b, is very good.
To check the stability of the approximate solution \((4)\), we directly put it on the unperturbed lattice, imposing to the kink-soliton the initial velocity given by formula \((5)\). In several simulations we observe the long-living motion of a slightly modified kink-soliton. Since in our experiments the boundaries are pinned, we observe edge reflection. Both at edge reflections and during collisions, the kink-solitons do not significantly change their amplitudes and shapes.

**Realistic Potentials.** – In order to check the generality of our results we have performed a similar analytical and numerical study of the Lennard-Jones (LJ) interparticle potential

\[ V(r) = 4e \left[ \left( \frac{s}{r} \right)^{12} - \left( \frac{s}{r} \right)^6 \right], \]

where \(r\) is a distance between neighboring particles, \(e\) and \(s\) are constants. After the appropriate rescalings of space and time: \(r \rightarrow (2)^{1/6} s \cdot r\) and \(t \rightarrow t\sqrt{m/12e}\), we obtain the following equations of motion for the relative displacements:

\[
\frac{d^2 v_n}{dt^2} = \frac{2}{(1 + v_n)^{13}} - \frac{1}{(1 + v_{n-1})^{13}} - \frac{1}{(1 + v_{n+1})^{13}} - \frac{2}{(1 + v_n)^7} + \frac{1}{(1 + v_{n-1})^7} + \frac{1}{(1 + v_{n+1})^7}.
\]

(7)

The dispersion relation for linear waves can be derived by substituting the pattern \(v_n = A\cos(kn - \omega t)\) in Eq. \((7)\). In the \(A \rightarrow 0\) limit we get the value of maximal group velocity of linear waves \(v_{\text{max}} = \sqrt{6}\) (see dashed line in the left panel of Fig. 4).

Seeking for strongly localized solutions, we substitute again the “magic” wavenumber sinusoidal pattern \((4)\) into the equations of motion \((7)\). We choose the minus sign in the relative displacement pattern \((4)\), which corresponds to the conditions under which we observe supersonic kinks in LJ lattices. Then, we expand the r.h.s. of the equations of motion in powers of \((A/2) \cos(2\pi n/3 - \omega t)\), keeping terms up to fifth order. To treat the powers of cosines we again perform the rotating wave approximation \((32)\). We don’t report here the formula that we obtain for the velocity-amplitude relation to save space, but its graph is plotted in the left panel in Fig. 4 as a solid line. The agreement between analytics and numerics is quite satisfactory, confirming that the “magic” wavenumber ansatz works also for LJ potentials.
Fig. 3 – a) Logarithmic plot of the relative displacement pattern of a single DK which moves from the left to the right. We use the right exponential decay, which is not affected by radiation, to fit the decay length $\Lambda$. b) Dependence of the decay length, $\Lambda$, upon the velocity of the DK. The solid line is obtained from formula (6) and the points are results of numerical experiments. The dashed line shows the velocity, $V = 1$, at which the decay length diverges.

We have also investigated numerically the DK’s interaction process. As seen from the right panel of Fig. 4, kink-solitons retain their shapes and velocities after interaction. The effect of the interaction manifests itself only in tiny trajectory shifts, as it is expected from the weakly nonlinear continuum approximation (see e.g. [9]).

Conclusions. – Summarizing, we have used the sharp pulse method to generate large amplitude, supersonic discrete kink-solitons with amplitude independent short localization length. These objects reduce to the well known kink-soliton solutions of the mKdV equation for small amplitudes. We have shown that large amplitude kink-solitons are characterized by a sinusoidal pattern with the “magic” wavenumber $k = 2\pi/3$, and propagate with supersonic velocities increasing with the amplitude. Both the FPU and the more realistic LJ interparticle potential have been considered. The agreement between the lattice kink theory and the numerical experiments for both types of anharmonic lattices is so good that it encourages us to draw the general conclusion that strongly localized discrete kink-solitons are common for systems with two-body interparticle potentials.

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Fig. 4 – Left Graph: “Magic” wavenumber ansatz for the discrete kink-soliton velocity versus amplitude for a LJ interparticle potential. The analytical result (solid line) compares extremely well with numerics (open circles). The dashed horizontal line indicates the maximal group velocity of linear waves (equal to $\sqrt{6}$). Right graph: Interaction of the DK’s created at the opposite ends of the chain. The strongly localized DK’s retain their shapes after interaction.

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