Internal modes in sine-Gordon chain

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We address the issue of internal modes of a stable kink in a discrete sine-Gordon equation. The aim of the present study is to elucidate the effects due to the detachment of the frequency dependence of antisymmetric internal mode from the spectrum. We analyze the frequencies of the lowest modes as functions of both the number of sites and the discreteness parameter. Using a simplified approach we explain the origin of the spectrum peculiarity, which arises when the frequency dependence detaches from the quasicontinuous spectrum at some value of the intersite coupling.

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I. INTRODUCTION

The existence of internal modes in nonintegrable equations has been known for more than two decades [1,2]. A particular example of this phenomenon is the existence of internal (shape) modes of kinks in the well-known discrete sine-Gordon equation (DSGE). This set of differential-difference equations reads (in normalized dimensionless units)

$$\ddot{u}_n + \sin u_n + \lambda[(u_n - u_{n-1}) - (u_{n+1} - u_n)] = 0, \qquad (1)$$

where $u_n(t)$ is the field variable, which can have a multitude of physical meanings [3], and λ is a coupling parameter. The dot in Eq. (1) means the time derivative and index n numerates the 1D chain sites. The spectrum of linear waves around the ground state solution ($u_n=2\pi m$, with m being an arbitrary integer) is given by

$$\omega^2 = 1 + 4\lambda \sin^2 \frac{k}{2}, \qquad (2)$$

where ω is the frequency of linear waves and k is the wave number. The lowest (gap edge) frequency is $\omega=1$ (in the renormalized units).

The features and behavior of kink internal modes for DSGE, as well as for more general types of the so-called Frenkel-Kontorova (FK) model, have been already studied in great detail [3–7]. The spectrum of linear waves of DSGE around a discrete kink contains either one or two localized modes, depending on the value of parameter λ [3,6]. (We consider the stable kink centered between the chain sites.) The frequencies of these modes lie in the gap below the spectrum.

In general, the phenomenon of the appearance of an internal mode (the detachment from the spectrum) is quite widespread. The detachment can take place in a number of different systems and can occur from both the upper and lower edges of the spectrum [3,4]. Such effects can be often observed while considering the spectra of Floquet modes around the discrete breathers (i.e., around the dynamical nonlinear excitations). The localization of modes at the impurity has been known for a long time in the theory of crystal defects [8]: the existence or absence of the internal mode is governed by the Lifshitz criterion. Thus we can also gain the detachment of the internal mode varying the parameters of the impurity.

However, to our knowledge, notwithstanding the great quantity of results nobody so far has concentrated on the mechanism of the internal mode detachment: only the existence or absence of this mode has been the chief subject of interest [2,6,7]. In this paper we shall focus on the concomitant effects due to the detachment of the internal mode frequency from the spectrum. So, the questions addressed are the following: (i) how the splitting of internal modes, which detach from the spectrum at some nonzero value of coupling parameter (or some other effective parameter altering the system state), affects the remaining spectrum of higher modes and (ii) how the localized (for larger λ) mode behaves before the detachment.

II. STATIC KINK DISTRIBUTION AND SPECTRUM PECULIARITIES

Static kink. The approximate analytical solution for a static kink of DSGE (1) can be found in two limiting cases: the strong coupling limit (large λ), when the discrete kink acquires the form of that in the continuous SGE with small corrections due to discreteness (see, e.g. [9] and references cited therein), or in the so-called anticontinuum limit (extremely small values of λ), when the kink distribution can be found in the form of a series in powers of λ [5,6]. In this paper we shall deal with the latter case (the internal modes for the former one were studied in Refs. [2,7]). The obvious "kink" solution (equilibrium) in the uncoupled limit ($\lambda=0$) is $u_n^0=2\pi m$ for $n\leqslant 0$, $u_n^0=2\pi(m+1)$ for $n\geqslant 1$ (we settle the kink center between the sites "0" and "1"). By the implicit function theorem there exists a unique continuation $u_n^0(\lambda)$, also called a localized equilibria [6], for a nonzero λ, which is exponentially localized in space. The static distribution for the kink can be found using perturbative iterations [6] and for the DSGE it is given up to the first power in λ by

$$u_1^0 = 2\pi\lambda + O(\lambda^2),$$

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$$u_0^0 = 2\pi(1-\lambda) + O(\lambda^2). \tag{3}$$

The other sites move by at most $O(\lambda^2)$ with the exponential decay as $|n| \to \infty$.

Linear spectrum properties. Let us now summarize the results on the existence of internal modes in the DSGE containing a single kink. For small λ only the lowest symmetric Pierls-Nabarro (PN) mode, associated with the kink oscillations in the PN relief, has the frequency inside the gap: it corresponds to the translational kink mode of the continuous SGE activated due to the discreteness. This mode remains the internal mode for the whole interval of kink stability. (For a finite system with free ends the instability occurs when the characteristic spatial scale of the kink outgrows the size of the system. For a large system the PN mode softens at some critical value of $\lambda \sim L^2$, where $L \gg 1$ is the system size [10].) The properties of this mode are well understood and studied [3,5], and we shall be mainly concerned with the other internal mode. For larger (but still weak) λ there exists the "critical" point λ_d, where one more (antisymmetric) mode dependence detaches from the continuous spectrum [6]: this mode corresponds to the oscillation of the kink width. (More complicated on-site FK-type potentials may have a larger variety of localized internal eigenmodes [4] or, for the case of more than one kink in the chain, the DSGE may possess a larger number of internal modes as well [3].) The existence of the second internal mode for large λ obviously matches the criterion given by Kivshar *et al.* in Ref. [2] for nearly integrable SGE (see also Ref. [7] for details): the magnitude of the detachment is of the order of λ^{-1}.

Calculation of the spectrum. First we suppose that our system has $2N$ sites and substitute $u_n(t)=u_n^0+v_n e^{i\omega t}$ in Eq. (1). Then we linearize the obtained equations with respect to v_n noting that for the antisymmetric modes the symmetry is $v_n=-v_{-n+1}$ (recall that the kink center is settled between the sites "0" and "1"). After that one gains the following linear system: for the site "1" we have

$$(\omega^2 - 3\lambda - \cos u_1^0)v_1 + \lambda v_2 = 0, \tag{4a}$$

for other sites

$$(\omega^2 - 2\lambda - \cos u_n^0)v_n + \lambda(v_{n-1} + v_{n+1}) = 0, \tag{4b}$$

and for the free end site

$$(\omega^2 - \lambda - \cos u_N^0)v_N + \lambda v_{N-1} = 0. \tag{4c}$$

For the symmetric modes ($v_n=v_{-n+1}$) the first equation (4a) is to be replaced with

$$(\omega^2 - \lambda - \cos u_1^0)v_1 + \lambda v_2 = 0. \tag{4d}$$

Then we found numerically the static kink distribution and resolved the linear eigenvalue problem given by Eqs. (4a)–(4d). The spectrum of several lowest modes in the vicinity of the detachment point is shown in Fig. 1. In fact, the plots of the frequency dependencies for small λ (involving the detachment region) have been already presented in Refs. [3,6], where, however, a large scale was used and a big number of dependencies was plotted simultaneously. At the same time, magnifying the spectrum region close to the detachment point we can see some interesting peculiarities: as the

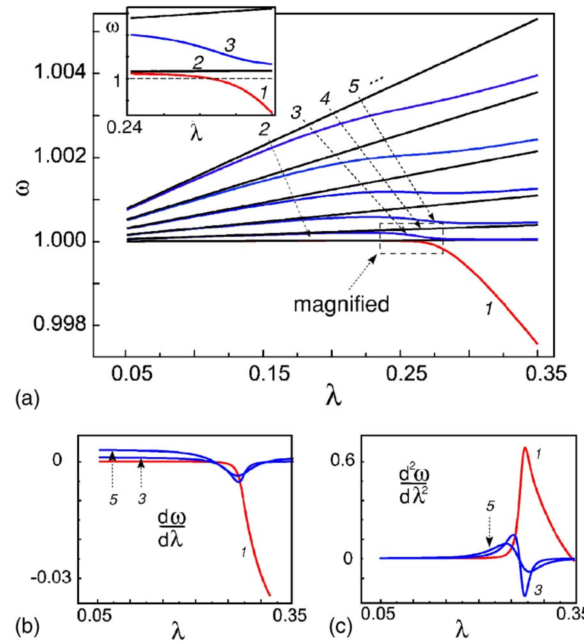

FIG. 1. (Color online) Numerical results for DSGE containing 250 sites with a kink centered in the middle of the chain between the sites. (a) The dependencies of frequencies on the value of λ for several lowest modes (the dependence for the lowest PN mode is not presented); the numbers correspond to the mode number, i.e., to the number of nodes for the corresponding eigenfunction. The inset shows the magnified region in the vicinity of the detachment value λ_d (the bandgap threshold is marked by the dashed line) . The bottom panels show the behavior of (b) $d\omega/d\lambda$ and (c) $d^2\omega/d\lambda^2$ for the three lowest antisymmetric modes (1, 3, and 5).

internal mode frequency goes back to the spectrum for small λ, it brings about a conspicuous change in the behavior of higher modes; see Fig. 1(a). However only the dependencies of odd modes (the mode number corresponds to the number of eigenfunction nodes) "feel" the return of the localized first antisymmetric mode to the spectrum. The modes with even number of eigenfunction nodes were not influenced by the detachment of this mode. So, we can infer that only those modes that have the same symmetry as the mode which detaches from the spectrum, experience a pronounced change [which can also be seen in the behavior of the derivatives, Figs. 1(b) and 1(c)]. This change becomes less and less abrupt with the increase of mode number. In addition, as can be seen in the inset of Fig. 1(a), the dependence of the first antisymmetric mode indeed enters the spectrum: it crosses the band edge frequency $\omega=1$ at the point $\lambda_d \approx 0.26$ (of course, it crosses only the band threshold but none of the frequency dependencies). For smaller λ the dependence of the former antisymmetric localized mode belongs to the spectrum of usual delocalized waves, tending to coalesce with the dependence of second (symmetric) mode.

We also note another interesting feature of the eigenfrequency dependencies. Before the detachment of the antisymmetric mode, for λ close to zero the dependencies for odd modes tend to coalesce with those of *higher* even modes, i.e., the frequencies of modes with numbers $2n+1$ come closer and closer to those for the modes with numbers $2n+2$. However, after the detachment, for large λ the dependencies for odd modes with numbers $2n+1$ tend to coalesce with the dependencies for *lower* even modes, i.e., with those having numbers $2n$. Thus the inflection of the odd modes dependencies and peculiarities of their derivatives in the vicinity of λ_d is merely a manifestation of this change in the tendency for coalescence, i.e., of the spectrum renormalization due to the detachment of one mode.

It is interesting to note that the features observed can be found in other physical situations: the spectrum of Floquet eigenmodes around a discrete breather in the nonlinear Klein-Gordon chain may involve the detachments of frequency dependencies. The spectrum renormalization described above can be seen in the magnified region of the spectrum near the detachment point; see Fig. 1(b) of Ref. [11].

It is also worth mentioning that the typical peculiarities of the DSGE spectrum persist in the case of small number of coupled DSGEs. We checked the systems of two, four, etc. coupled DSGEs with the stable kink in the middle and found that the lowest antisymmetric mode dependence initially went up but then dropped down in the "gap." However the detachment point value λ_d was changing in these cases gradually tending to its saturation value $\lambda_d \approx 0.26$ with the increase of the number of sites. The changes of the behavior of the higher mode dependencies due to the detachment were less pronounced for a small number of sites.

From our analysis it became evident that the spectrum renormalization property and frequency peculiarities, which occur in the computer studies where finite systems are used, are size- and symmetry-dependent. Thus it is interesting what changes in this typical frequency behavior we should expect when the system size is varied. In the next section with the use of the simplified model (an idealized two-site kink) we shall examine how these observed spectrum peculiarities relate to the size of the system.

III. STUDY OF SPECTRUM WITH THE USE OF TWO-IMPURITY MODEL

For small λ we can use the approximate expressions for u_n^0 Eq. (3), and in the leading approximation substitute in Eqs. (4a): $\cos u_1^0 \approx 1 - 2\pi^2\lambda^2$, $\cos u_n^0 \approx 1$ for $n>1$. This means that we effectively replaced the kink with two isotopic impurities located at sites "1" and "0," and the "strength" of these impurities changes as λ is varied. Evidently, in the limit $\lambda \to 0$ this approach has to give the asymptotically correct results. Of course, the usage of the two-impurity model is less justified in the vicinity of λ_d. Therefore this model would only do as an example system possessing the spectrum features similar to those of DSGE and having the same spectrum asymptotics in the weak coupling limit. The results given by such a simplified approach in the vicinity of λ_d can be taken for the qualitative explanations and then have to be compared with the numerical data for the DSGE.

Seeking the solution of Eq. (4) in the form $v_n = Ae^{\kappa n} + Be^{-\kappa n}$, with constant A and B, from Eq. (4b) one obtains a spectral dependence for $\omega(\kappa)$ in the form (2), where $\kappa = ik$. Then using the consistency condition for two remaining equations, Eqs. (4a) and (4c), after some straightforward algebra we arrive at the relation which defines the allowed values of κ for antisymmetric modes:

$$(1-2\pi^2\lambda)\sinh[\kappa(N-1)] + 2\pi^2\lambda \sinh[\kappa N] - \sinh[\kappa(1+N)] = 0. \tag{5}$$

Expanding this relation in the vicinity of $\kappa=0$ ($\kappa N \ll 1$) up to κ^5 we determine the allowed values of κ for the frequency of first antisymmetric mode, ω_1, and for the next, third mode, ω_3, from the biquadratic equation: $a\kappa^4 + b\kappa^2 + c = 0$. The expressions for the coefficients are

$$a = \frac{(\lambda-\lambda_d) + 5(2N^2+N^4)(\lambda-\lambda_d) - 5\lambda(2N^3+N)}{60},$$

$$b = (\lambda-\lambda_d)/3 + N^2(\lambda-\lambda_d) - N\lambda,$$

$$c = 2(\lambda-\lambda_d),$$

and the detachment point is $\lambda_d = 1/\pi^2$. The notable fact, which can be extracted from Eq. (5), is the following: if λ is close to zero, $\lambda \ll N^{-1}$, we have $\kappa^2 = -k^2 \sim N^{-2}$, and for this value of coupling parameter one finds the expressions for frequency dependencies as

$$\omega_1^2 \approx 1 + 2\lambda(3-\sqrt{3})N^{-2}, \tag{6a}$$

$$\omega_3^2 \approx 1 + 2\lambda(3+\sqrt{3})N^{-2}. \tag{6b}$$

So, initially, for small λ, the lowest antisymmetric mode, Eq. (6a), goes up being inside the spectrum. The next antisymmetric mode, Eq. (6b), goes up as well. However quite a different situation occurs if one moves inside the region where the inequality $|\lambda-\lambda_d| \ll N^{-1}$ holds, i.e., in the close vicinity of λ_d. In this region one obtains $\kappa^2 \sim N^{-1}$ (here the inequality $\kappa N \ll 1$ is true because of the additional smallness provided by the factor $[\lambda-\lambda_d]$). Then for the frequency dependencies we have

$$\omega_1^2 \approx 1 - 2(\lambda-\lambda_d)N^{-1}, \tag{7a}$$

$$\omega_3^2 \approx 1 - 4(\lambda-\lambda_d)N^{-1} + 6\lambda_d N^{-2}. \tag{7b}$$

The second derivative of ω_1 at the point $\lambda=\lambda_d$ involves the term independent on N: $d^2\omega_1/d\lambda^2 = -4\lambda_d^{-1}$. Therefore we can conclude that in the limit $N\to\infty$ the splitting of this dependence from the lower boundary of the spectrum must have a parabolic form. From the expressions (6a), (6b), (7a), and (7b) it becomes evident what brings about the peculiarity as λ approaches λ_d, i.e., as the first antisymmetric mode detaches from the spectrum. For λ close to zero we have $d\omega_{1,3}/d\lambda \sim N^{-2}$, whereas in the vicinity of λ_d the different dependence takes place: $d\omega_{1,3}/d\lambda \sim N^{-1}$. (Note that the sign of the first derivative also changes.) Because of this the initial weak ($\sim N^{-2}$) growth for small values of λ changes to more rapid ($\sim N^{-1}$) decrease in the close vicinity of λ_d. The dependencies for the absolute value of first derivatives at $\lambda = \lambda_d$ on the number of sites are shown in Fig. 2. For $N' = 2N \gtrsim 30$ they are in a good agreement with analytical results (7a) and (7b). With the increase of N this agreement becomes better inasmuch as we omitted the higher (with respect to N^{-1}) terms in Eqs. (7a) and (7b). In the region $\lambda < \lambda_d$ there must be an extremum point λ_{ext}, $d\omega_i/d\lambda|_{\lambda_{\mathrm{ext}}} = 0$,

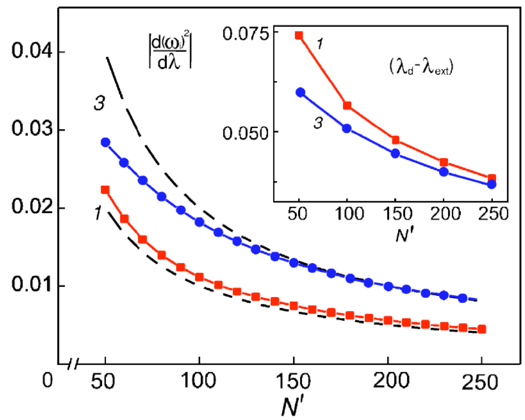

FIG. 2. (Color online) The dependencies for the absolute values of the derivative at the point $\lambda=\lambda_d$ on the number of sites for the first (antisymmetric) mode and for the next, third mode. The digits correspond to the mode number. Dashed curves for each mode show the analytical prediction obtained by virtue of Eqs. (7a) and (7b). The inset shows the dependence of deviation $\lambda_d-\lambda_{ext}$ of the extremal point from the detachment point as a function of the number of sites $N'=2N$.

for both dependencies $\omega_{1,3}(\lambda)$, at which the monotonic growth changes to decreasing. These extremum points, λ_{ext}, tend to λ_d as N gets bigger: $(\lambda_d-\lambda_{ext})\sim N^{-1}$. The dependencies of the value of difference, $(\lambda_d-\lambda_{ext})$, on the number of sites N are presented in the inset panel of Fig. 2. For $\lambda>\lambda_d$ the first antisymmetric mode gets into the spectrum gap and becomes an internal mode. However the dependence for the next, third antisymmetric mode, in spite of its tendency to drop down, cannot cross the dependence of the preceding second (symmetric) mode and therefore these two dependencies get closer and closer to each other.

Now consider an infinite system. We seek the solution in the form of localized wave, $v_n\sim e^{-\kappa n}$, $\kappa>0$. Whereupon the only condition defining the allowed values of κ for antisymmetric modes becomes as follows:

$$e^{-\kappa}+2\pi^2\lambda-3-4\lambda\sinh^2\frac{\kappa}{2}=0. \tag{8}$$

Expanding this relation we arrive at the dependence: $\kappa_1=2\lambda_d^{-1}(\lambda-\lambda_d)$, and then one finds the expression for the frequency of the antisymmetric localized mode as

$$\begin{cases}\omega_1^2=1\,, & \text{for } \lambda<\lambda_d\,,\\ \omega_1^2\approx 1-4\lambda_d^{-1}(\lambda-\lambda_d)^2, & \text{for } \lambda>\lambda_d,\end{cases} \tag{9}$$

in agreement with this dependence given in Ref. [12] and in consistency with the result for the finite system. The characteristic spatial scale for the eigenfunction of this internal mode is $l_1=\kappa_1^{-1}$. Obviously, the smaller l_1, the better the eigenfunction is localized. We see that at the outset, as this mode detaches, $l_1\sim(\lambda-\lambda_d)^{-1}$.

Let us proceed to studying the symmetric modes. The relation which defines the allowed values of κ for those reads

$$(1+2\pi^2\lambda)\sinh[\kappa(N-1)]-2(1+\pi^2\lambda)\sinh[\kappa N] + \sinh[\kappa(1+N)]=0. \tag{10}$$

Then we again expand this relation for $\kappa N\ll 1$ up to the fifth power and determine κ from the biquadratic equation: $d\kappa^4+g\kappa^2+f=0$, where

$$d=\frac{5N(\lambda+\lambda_d)+10N^3(\lambda+\lambda_d)-\lambda(5N^4+10N^2+1)}{60},$$

$$f=N(\lambda+\lambda_d)-(N^2+1/3)\lambda,$$

$$g=-2\lambda.$$

In the region $\lambda\ll N^{-1}$ one obtains

$$\omega_0^2\approx 1-2\lambda_d^{-1}\lambda N^{-1}, \quad \omega_2^2\approx 1+6\lambda N^{-2}. \tag{11}$$

The dependencies for symmetric modes have neither an inflection point nor any peculiarity at $\lambda=\lambda_d$.

For the infinite system the relation for κ is written as follows:

$$e^{-\kappa}+2\pi^2\lambda-1-4\lambda\sinh^2\frac{\kappa}{2}=0. \tag{12}$$

Then we arrive at the dependence for PN mode for weak coupling in the form

$$\omega_0^2\approx 1-4\lambda_d^{-2}\lambda^3, \tag{13}$$

which is in agreement with this dependence given in Refs. [5,12]. The localization distance now is: $l_0=\kappa_0^{-1}\sim\lambda^{-3/2}$. Thus we can infer that the localization for PN mode with the growth of coupling value λ develops faster than for the antisymmetric internal mode.

The results for the frequency dependencies (9) and (13) could also be obtained with the use of the Green function (Lifshitz) technique for a linear chain with impurities (see the monograph [8]), which was employed in Refs. [4,5].

IV. CONCLUSION

To sum up, we investigated the features of spectrum and kink internal modes of DSGE. The detachment of the antisymmetric internal mode brought about the renormalization of the linear spectrum and caused the inflections of the dependencies of the odd modes in the vicinity of λ_d. The observed effects are size and symmetry dependent. We gave an analytical explanation of this fact using the two-impurity model (i.e., regarding an idealized two-site kink). The analysis within the framework of such a simplified approach is not asymptotically correct in the vicinity of λ_d and can in general give only qualitative results. However, we found a good quantitative correspondence of our analysis with the numerical data for large N. For the infinite system the dependence of first antisymmetric mode detaches smoothly (with zero first derivative) from the band edge, but for the finite system it does cross the bandgap threshold. For extremely small values of λ the first antisymmetric mode belongs to the spectrum of delocalized waves. The initial weak growth ($\sim N^{-2}$) of lowest antisymmetric modes frequencies with the increase of the value of coupling then changes to more rapid ($\sim N^{-1}$) decrease in the vicinity of the detachment point. The extremum points of these lowest odd-modes dependencies, $\lambda_{\rm ext}$, approach the detachment point λ_d as the number of sites gets bigger: $(\lambda_d - \lambda_{\rm ext}) \sim N^{-1}$. At $\lambda = \lambda_d$ the first antisymmetric mode drops into the spectrum gap. The higher antisymmetric modes come closer and closer to the preceding symmetric modes with the increase of coupling but the renormalization is less pronounced and develops slower for higher modes. The symmetric modes do not reveal any peculiarity at λ_d. The spectrum renormalization due to the detachment of one mode seems to be quite a typical property and can be observed in other systems as well (independently on the boundary conditions).

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