On the internal modes in sine-Gordon chain

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We address the issue of internal modes of a kink of a discrete sine-Gordon equation. The main point of the present study is to elucidate how the antisymmetric internal mode frequency dependence enters the quasicontinuum spectrum of nonlocalized waves. We analyze the internal frequency dependencies as functions of both the number of cites and discreteness parameter and explain the origin of spectrum peculiarity which arises after the frequency dependence of antisymmetric mode returns back to the continuous spectrum at some nonzero value of the intersite coupling.

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The existence of internal modes is a well known peculiarity of nonintegrable systems [1]: If one linearizes a nonintegrable equation above the static nonlinear solution, then the effective potential of the linear equation obtained appears to be not reflectionless in contrast to the integrable case. The particular example 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 as (in normalized dimensionless units):

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

where \( u_n(t) \) is the field variable, which can have a multitude of physical meanings [2], \( \lambda \) is a coupling parameter, \( \dot{\cdot} \) means the time derivative and index \( n \) numerates the 1D chain sites. The features and behaviour 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 very details [2, 3, 4, 5].

The spectrum of linear waves of DSGE around a kink contains either two or one localized mode, depending on the value of parameter \( \lambda \). (We consider the stable kink centered between the chain sites.) The frequencies of these modes lie inside the spectrum gap; the linear spectrum itself is given by

\[ \omega^2 = 1 + 4\lambda \sin^2 \frac{k}{2}, \]  

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

However, up to our knowledge, notwithstanding the great quantity of results none so far has concentrated on the way an internal modes ceases to exist: Only the fact of existence or nonexistence of that mode has been the subject of interest [1, 2, 3, 4, 5]. In this paper we focus on the effect entailed by the detachment of the internal mode frequency from the spectrum. So, the question arises: How the internal modes, which split off from the spectrum at some nonzero value of coupling parameter (or some other effective parameter altering the system state), affect the spectrum itself and how they behave while still being inside the spectrum.

To begin with, we note that the analytical approximate solution for a static kink of DSGE [1] can be found either in the so-called anticontinuum limit (extremely small values of \( \lambda \)) as a series in powers of \( \lambda [4] \), or in the opposite case of strong coupling (large \( \lambda \), when the discrete kink solution acquires the form of that in the continuous SGE with small corrections due to discreteness (see e.g. [6]).

Let us now summarize the results on the existence of internal modes in the DSGE containing a single kink. For small \( \lambda \) 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 continuous SGE, activated due to discreteness. This mode remains the internal mode for the whole interval of kink stability. The properties of this mode are well understood and studied [2, 4], and we shall be mainly concerned with the other internal mode. For larger (but still weak) \( \lambda \) there exists the "critical" point \( \lambda_{\text{d}} \), where one more mode dependence detaches from the continuous spectrum: this mode corresponds to the oscillation of kink width. (More complicated on-site FK-type potentials may have a larger variety of localized internal eigenmodes [2] or, for the case of more than one kink in the chain, the DSGE possesses a larger number of internal modes as well [2].) The existence of the second internal mode for large \( \lambda \) obviously matches the criterium given by Kivshar et al. in Ref. [1] for nearly integrable SGE (see also Ref. [5] for details).

The effects we shall discuss can be readily seen in Fig. 1. As the internal mode frequency goes back for small \( \lambda \) to the quasicontinuous spectrum, it brings about a conspicuous change in the behaviour of higher modes. 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 the even number of eigenfunction nodes do not react to this return. So, we can infer that only the modes having the same symmetry as the

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any of the frequency dependencies). For smaller mode, which detaches from the spectrum, experience pronounced change (which can be also seen in the behaviour of the derivatives, Fig. 1a-c). This change "propagates" inwards the spectrum becoming less and less abrupt with the increase of mode number. In addition, as can be seen in the inset of Fig. 1a, the dependence of the first antisymmetric mode indeed enters the spectrum: it crosses the band edge frequency \( \omega_c \) at the point \( \lambda_c \approx 0.26 \) (of course, it crosses only the band threshold but not any of the frequency dependencies). For smaller \( \lambda \) the dependence of former antisymmetric localized mode tends to coalesce with the spectrum of usual delocalized waves, tending to coalesce with the dependence of second (symmetric) mode. Also we note another interesting feature of eigenfunctions at the critical point: for weak coupling parameter values and stays inside the gap below. The value of \( \omega_c \) for which this dependence crosses the band threshold can be roughly estimated as \( \lambda_c \approx 1/\pi^2 \). One also notes that the frequency of PN-mode, \( \omega_0 \), drops to zero for \( u^0 = \pi/2 \). This manifests the well known fact that for the finite size chain there occurs an instability when the characteristic spatial scale of a kink overgrows the size of a system (see e.g. Ref. 7, 8). For a large system the PN-mode softens at some critical value \( \lambda \sim L^2 \), where \( L \gg 1 \) is the system size. For two pendulums, setting \( u_1^0 = \pi/2 - U \), \( u_2^0 = 3\pi/2 + U \), \( U \ll 1 \), one finds the frequency dependencies near the critical point: \( \omega_1^0 \approx (\lambda - \lambda_c)/2\lambda_c^2 \), with \( \lambda_c = 1/\pi \), and \( \omega_1^2 = \omega_0^2 + 2\lambda \). We see that at the critical point \( \omega_1^2(\lambda_c) = 2/\pi \ll 1 \), i.e. the frequency remains inside the gap. Thus we expect that this internal mode dependence for a big system does not return back to the

\[
\ddot{u}_{1,2} + \lambda (u_{1,2} - u_{1,2,1}) + \sin u_{1,2} = 0. \tag{3}
\]

Linearizing Eqs. 3 around the ground state solution, \( u_1 = u_2 = 0 \), we arrive at the eigenfrequency dependencies: \( \omega_0^2 = 1 \), \( \omega_1^2 = 1 + 2\lambda \). The higher frequency corresponds to the antiphase oscillations, the lower one – to the inphase motion. Now let us study the spectrum of linear oscillations above the inhomogeneous static solution of Eq. 3 (analogue of a kink). First we have to find the static distribution for small values of \( \lambda \). We suppose that this distribution has a form: \( u_1 = u^0_1, u_2 = 2\pi - u^0_1, u^0 = \alpha \lambda + \beta \lambda^2 + O(\lambda^3) \), and we should determine the corresponding constants, \( \alpha \) and \( \beta \), in the dependence \( u^0(\lambda) \). Expanding the sine in Taylor series and equalizing coefficients at the same powers of \( \lambda \) we find:

\[
u^0 = 2\pi \lambda - 4\pi \lambda^2 + \ldots. \tag{4}
\]

Then we linearize the initial set of dynamical equations around small quantities \( v_1 = u_1^0 + v_1 e^{i\omega t}, v_2 = 2\pi - u_1^0 + v_2 e^{i\omega t} \). The consistency condition gives the spectral dependencies: for the lower inphase mode \( \omega_0^2 = \cos u^0 \), that is the analogue of PN mode in a large system, and for the antiphase mode \( \omega_1^2 = \cos u^0 + 2\lambda \) – the analogue of the second antisymmetric internal mode. The analytical form for the frequencies, which is valid for the small \( \lambda \) values, is as follows:

\[
\omega_0^2 = 1 - 2\pi^2 \lambda^2 + \ldots, \quad \omega_1^2 = \omega_0^2 + 2\lambda. \tag{5}
\]

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

The frequency dependence \( \omega_1(\lambda) \) grows linearly with \( \lambda \), but then, as \( \lambda \) becomes larger, this growth slows down showing an ultimate tendency of this mode to get inside the gap below. The value of \( \lambda \) for which this dependence crosses the band threshold can be roughly estimated as \( \lambda_d \approx 1/\pi^2 \). One also notes that the frequency of PN-mode, \( \omega_0 \), drops to zero for \( u^0 = \pi/2 \). This manifests the well known fact that for the finite size chain there occurs an instability when the characteristic spatial scale of a kink overgrows the size of a system (see e.g. Ref. 7, 8). For a large system the PN-mode softens at some critical value \( \lambda_c \sim L^2 \), where \( L \gg 1 \) is the system size. For two pendulums, setting \( u_1^0 = \pi/2 - U, u_2^0 = 3\pi/2 + U \), \( U \ll 1 \), one finds the frequency dependencies near the critical point: \( \omega_1^0 \approx (\lambda_c - \lambda)/2\lambda_c^2 \), with \( \lambda_c \approx 1/\pi \), and \( \omega_1^2 = \omega_0^2 + 2\lambda \). We see that at the critical point \( \omega_1^2(\lambda_c) = 2/\pi \ll 1 \), i.e. the frequency remains inside the gap. Thus we expect that this internal mode dependence for a big system does not return back to the
spectrum for large values of \( \lambda \) and continues to be the internal mode for the whole interval of kink stability except for the extremely weak coupling. The splitting of this mode dependence from the continuum spectrum is of the order of \( \lambda^{-1} \) for large values of coupling parameter \( \lambda \).

The systems containing more sites enable us to study the "degree of localization" since we now have the outer and inner (core) sites. Let us mark the sites in the kink core (the middle of a chain) by numbers "1" and "-1", their neighbor sites by "2" and "-2" etc. For the case of four pendulums the "kink" solution for small \( \lambda \) is given by:

\[
\begin{align*}
u_0^0 & \approx 2\pi \lambda^2 + \ldots, \\
u_1^0 & \approx 2\pi \lambda - 8\pi \lambda^2 + \ldots, \\
\end{align*}
\]  
(6)

and the obvious solution symmetry, \( u_{-i} = 2\pi - u_i \), gives the field distribution for the remaining sites. In this limit the spectral dependencies for two lowest modes are:

\[
\begin{align*}
\omega_0^2 & \approx 1 - \pi^2 \lambda^2, \\
\omega_1^2 & \approx 1 + (2 - \sqrt{2})\lambda - \frac{\pi^2}{2} (2 - \sqrt{2}) \lambda^2. \\
\end{align*}
\]  
(7a)

(7b)

Putting \( \omega_1(\lambda) = 1 \) in Eq. (7b) one gets the rough estimate for the point where this frequency dependence enters the "quasicontinuum" spectrum: \( \lambda_0 \approx 2/\pi^2 \). In the same way one could deal with the systems of bigger size (see below).

The spectra and amplitude ratio dependencies on \( \lambda \) for four and six pendulums are given in Fig. 2. As the number of sites grows, the spectrum peculiarities, seen in Fig. 1, become more and more pronounced. In the panels (b) and (d) of Fig. 2, we present the dependencies for the ratios of the oscillation amplitudes for different pairs of neighbor sites, \( v_{i+1}/v_i \), for PN (zeroth) mode and first antisymmetric mode. Both modes display the tendency for localization in the kink core with the growth of \( \lambda \), but coming closer to the critical point \( \lambda_c \) they become localized worse because of the large kink width. Compared with the first antisymmetric mode, the PN-mode appears to be localized better. These dependencies have a minima for some intermediate value of coupling, where the inhomogeneity brought by the kink is pronounced well enough to sustain the modes localization well and the outer side, the kink width is still not large.

Large systems. Now suppose that our system has \( 2N \) sites. The static distribution for the kink is again given by \( u_i^0 = 2\pi \lambda + O(\lambda^2), u_n^0 = O(\lambda^n) \). Then we substitute \( u_n(t) = u_n^0 + v_n e^{i\omega t} \), and linearize the system obtained with respect to \( v_n \), noting that for the antisymmetric modes the symmetry is \( v_n = -v_{-n} \). After that one gains the following linear system:

\[
\begin{align*}
(\omega^2 - 3\lambda - \cos u_0^0)v_1 + \lambda v_2 & = 0, \\
\vdots & \\
(\omega^2 - 2\lambda - \cos u_0^0)v_n + \lambda(v_{n-1} + v_{n+1}) & = 0, \\
\vdots & \\
(\omega^2 - \lambda - \cos u_N^0)v_N + \lambda v_{N-1} & = 0,
\end{align*}
\]  
(8)

For the symmetric modes \( (v_n = v_{-n}) \) the first equation of system (8) is to be replaced with

\[
(\omega^2 - \lambda - \cos u_0^0)v_1 + \lambda v_2 = 0.
\]  
(9)

For small \( \lambda \) we use the approximate expressions for \( u_0^0 \), and in the leading approximation substitute \( \cos u_0^0 \rightarrow 1 - 2\pi^2 \lambda^2 \), \( \cos u_n^0 \rightarrow 1 \) for \( n > 1 \). This means that we effectively replaced the kink with two isotopic impurities located at sites 1 and -1, the "strength" of which alters with the change of \( \lambda \). Seeking the solution in the form \( v_n = A e^{i\kappa n} + B e^{-i\kappa n} \), with constant \( A \) and \( B \), one obtains the spectral dependence for \( \omega(\kappa) \) in form (8), where \( \kappa = ik \). Then using the consistency condition after some straightforward algebra we arrive at the relation which defines the allowed values of \( \kappa \) for antisymmetric modes:

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

Expanding this relation in the vicinity of \( \kappa = 0 \) \( (\kappa N \ll 1) \) up to \( \kappa^5 \) we determine the allowed values of \( \kappa \) for the frequency of first antisymmetric mode, \( \omega_1 \), and for the next, third mode, \( \omega_3 \), from the biquadratic equation:

\[
a = 1(\lambda - \lambda_d) + 5(2N^2 + N^4)(\lambda - \lambda_d) - 5\lambda(2N^3 + N) + \frac{60}{}, \\
b = (\lambda - \lambda_d)/3 + N^2(\lambda - \lambda_d) - N\lambda, \\
c = 2(\lambda - \lambda_d),
\]
and the detachment point is $\lambda_d = 1/\pi^2$. The notable fact, which can be extracted from Eq. (10), is the following: if $\lambda$ is close to zero, $\lambda \ll N^{-1}$, we have $\kappa^2 = -k^2 \sim N^{-2}$, and for this values of coupling parameter one finds the expressions for frequency dependencies as:

$$\omega^2 \approx 1 + 2\lambda(3 - \sqrt{3})N^{-2}, \quad (11a)$$
$$\omega^2 \approx 1 + 2\lambda(3 + \sqrt{3})N^{-2}. \quad (11b)$$

So, initially, for small $\lambda$, the lowest antisymmetric mode, Eq. (11a), goes up being inside the spectrum. 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 $\lambda_d$. 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:

$$\omega^2 \approx 1 - 2(\lambda - \lambda_d)N^{-1}, \quad (12a)$$
$$\omega^2 \approx 1 - 4(\lambda - \lambda_d)N^{-1} + 6\lambda_dN^{-2}. \quad (12b)$$

The second derivative of $\omega_1$ at the point $\lambda = \lambda_d$ involves the term independent on $N$: $d^2\omega_1/d\lambda^2 = -\lambda_d^3$. 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 (11a,12a) it becomes evident what brings about the peculiarity as $\lambda$ approaches $\lambda_d$, i.e. as the first antisymmetric mode detaches from the spectrum. For $\lambda$ close to zero we have $d\omega_{1,3}/d\lambda \sim N^{-2}$, whereas in the vicinity of $\lambda_d$ 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 $\lambda$ changes to more rapid ($\sim N^{-1}$) decrease in the close vicinity of $\lambda_d$. The dependencies for the modulus of derivatives at $\lambda = \lambda_d$ on the number of sites shown in Fig. 3 For $N' = 2N \geq 30$ they are in a good agreement with analytical results (12a). With the increase of $N$ this agreement becomes better as much as we omitted the higher with respect to $N^{-1}$ terms in Eqs. (12). In the region $\lambda < \lambda_d$ there must be an extremum point $\lambda_{ext}$, $d\omega_{1,3}/d\lambda|_{\lambda_{ext}} = 0$, for both dependencies $\omega_{1,3}(\lambda)$, at which the monotonic growth changes to decreasing. These extremum points, $\lambda_{ext}$, tend to $\lambda_d$ 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. 3 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 $\kappa$ becomes as follows:

$$e^{-\kappa} + 2\pi^2\lambda - 3 - 4\lambda\sinh^2\frac{\kappa}{2} = 0. \quad (13)$$

Expanding this relation we arrive at the dependence:

$$\kappa_1 = 2\lambda_d^{-1}(\lambda - \lambda_d), \quad \text{and then one finds the expression for the frequency of the antisymmetric localized mode as:}$$

$$\begin{cases}
\omega_1^2 = 1, & \text{for } \lambda < \lambda_d, \\
\omega_1^2 \approx 1 - 4\lambda_d^{-1}(\lambda - \lambda_d)^2, & \text{for } \lambda > \lambda_d,
\end{cases} \quad (14)$$

in consistency with the result for 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, $l_1 \sim (\lambda - \lambda_d)^{-1}$.

Proceed to studying the symmetric modes. The relation which defines the allowed values of $\kappa$ for those reads:

$$(1 + 2\pi^2\lambda) \sinh[\kappa(N - 1)] - 2(1 + \pi^2\lambda) \sinh[\kappa N] + \sinh[\kappa(1 + N)] = 0. \quad (15)$$

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

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

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

$$g = -2\lambda.$$ 

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

$$\omega_0^2 \approx 1 - 2\lambda_d^{-1}\lambda N^{-1}, \quad \omega_1^2 \approx 1 + 6\lambda N^{-2}. \quad (16)$$

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

FIG. 3: The dependencies for the modulus of 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. (12). The inset shows the dependence of deviation $\lambda_d - \lambda_{ext}$ of the extremal point from the detachment point as a function of number of sites $N' = 2N$. 

\[ \text{FIG. 3:} \text{ The dependencies for the modulus of derivative at the point } \lambda = \lambda_d \text{ on the number of sites for the first (antisymmetric) mode and for the next, third mode. The digits correspond to the mode number. Dashed curves for each mode show the analytical prediction obtained by virtue of Eqs. (12). The inset shows the dependence of deviation } \lambda_d - \lambda_{ext} \text{ of the extremal point from the detachment point as a function of number of sites } N' = 2N. \]
For the infinite system the relation for $\kappa$ is written as follows:

$$e^{-\kappa} + 2\pi^2\lambda - 1 - 4\lambda \sinh^2 \frac{\kappa}{2} = 0. \quad (17)$$

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

$$\omega_0^2 \approx 1 - 4\lambda^{-2}\lambda^3, \quad (18)$$

which is in agreement with this dependence given in Ref.[4]. The localization distance now is: $l_0 = \kappa^{-1} \sim \lambda^{-3/2}$. Thus we can infer that the localization for PN-mode with the growth of coupling value $\lambda$ develops faster than for antisymmetric internal mode, as it was pointed above while considering small size systems (cf. Fig.4 right panels).

The results for the frequency dependencies could also be obtained with the use of Green function (Lifshitz) technique for a linear chain with impurities, (see the monograph [9]), which was employed in Refs.3 4. However, for the sake of getting simple analytical expressions one should replace the kink solution with the finite number of effective impurities. In the case of two impurities model, utilized in the current paper, one would obtain exactly the same results. In fact, the usage of the two impurities model means that we retain only leading terms in powers of parameter $\lambda$.

To sum up, we investigated the features of spectrum and kink internal modes of DSGE focusing on the effect of detachment of an internal mode from the quasicontinuous spectrum. We note that the two-impurities model, used for our analysis, gives a somewhat different value for the detachment point ($\lambda_d = \pi^{-2}$, while the numerically estimated value for DSGE is $\lambda_d \approx 0.26$). This is explained by the fact that the value of $\lambda_d$ is nonzero, whereas we had to use the asymptotical expansions valid for $\lambda \to 0$. This means the higher order terms with respect to $\lambda$ should always result in the corrections to the analytically obtained value of $\lambda_d$. However the two impurities model allowed us to obtain analytical results describing the spectrum peculiarities, which are in good agreement (qualitative and even quantitative for large $N$) with the numerical ones. 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 $\lambda$ the first mode belongs to the spectrum. The initial weak growth ($\sim N^{-2}$) of lowest antisymmetric modes frequencies with the value of $\lambda$ then changes to more rapid ($\sim N^{-1}$) decreasing. The extremum point $\lambda_{ext}$ approaches the detachment point $\lambda_d$ as the number of sites gets bigger. At $\lambda = \lambda_d$ the first antisymmetric mode drops into the spectrum gap. The higher antisymmetric mode come closer and closer to the preceding symmetric modes with the increase of coupling but this tendency weakens with the growth of mode number. The symmetric modes do not display any peculiarity at $\lambda_d$.

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