

Twisted localized modes

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In a number of recent papers the so-called twisted localized mode of the discrete nonlinear Schrödinger equation has been proposed. Herein, we study the existence and stability properties of such modes. We analyze the persistence of quasiperiodic modes and study the domains of existence and numerical stability of the exact form of such solutions. We identify the bifurcations through which they lose their stability and follow the behavior of the intrinsic localized modes and their eigenmodes even in the unstable regime.

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I. INTRODUCTION

In the past two decades a significant amount of research has been dedicated to the study of energy localization in nonlinear lattices [1]. In particular the subject of *intrinsic localized modes* (ILM's) has drawn considerable attention as it offers appealing insight into a variety of problems ranging from the nonexponential energy relaxation in solids [2] to the local denaturation of the DNA double strand [3]. Also, within materials science [4] and nonlinear optics applications [5] the subject has drawn a new focus.

Recently, a lot of theoretical work [6–8] has been devoted to the study and understanding of the dynamic and thermodynamic properties of the nonlinear modes that arise in these discrete systems. One of the most interesting results of this intense study is the striking difference between the discrete solitary-wave modes and their continuum counterparts. In particular, many of the characteristic phenomena related to these waves, such as the modulational instability of plane waves [6] or the formation and stability of solitons [9], occur in discrete systems very differently from their continuum counterparts. Furthermore, discreteness provides abundant possibilities for more complex modes than expected in the continuum limit.

Keeping in mind that in the discrete problem there is a multitude of additional modes that most likely serve as asymptotic states for the system dynamics [10], we will analyze the existence, dynamics, and stability of a mode recently proposed by a number of researchers. This odd, symmetric mode was first studied for small systems in [11,12]. For infinite-dimensional systems, it was first mentioned as a sub-case of the ILM's studied in [13] and briefly also in [14]. The first focused attempt to study such ILM's was however, by Darmanyan, Kobayakov, and Lederer (DKL) [15]. Herein, we will expand on the results of DKL and attempt to display some of the very interesting features that these modes possess. As a simple benchmark system for this study, we will use the ubiquitous discrete nonlinear Schrödinger (DNLS) equation that has appeared in a variety of contexts in the study of discrete nonlinear lattices [3,5,7,11].

II. TWISTED MODE

The DNLS equation has the form

$$i\dot{u}_n = -C\Delta_2 u_n - |u_n|^2 u_n, \quad (1)$$

where $u_n(t)$ is the complex field under study, the subscript n indexes the lattice sites, the overdot denotes temporal partial derivative, C is the lattice coupling constant, and, finally, $\Delta_2 u_n = u_{n+1} + u_{n-1} - 2u_n$ is the discrete Laplacian [16]. We will be interested in ILM's of the form $u_n(t) = \exp(it)\psi_n$ [17] that reduce the dynamical problem to a static one due to the monochromatic gauge symmetry of the equation. The two most studied modes of the DNLS equation are (1) the stable Sievers-Takeno mode (ST) [18]—a site-centered mode, and (2) the unstable Page (P) [19] mode centered between sites.

However, recently DKL [15] proposed a different mode, which they called the *twisted unstaggered* mode of the form $u_n(t) = \exp(it)(\dots, \alpha, 1, -1, -\alpha, \dots)$ (as normalized by its maximum amplitude; $\alpha > 0$). The analysis of this mode and its staggered version $u_n(t) = \exp(it)(\dots, -\alpha, 1, 1, -\alpha, \dots)$ are exactly symmetrical, so we will consider only the former.

This mode arises naturally from the anticontinuum limit ($C=0$) [20]. Apart from the explicit construction of such twisted modes a main issue that will be of concern to this study will be their stability. Interestingly enough, earlier references on the subject left this question without a definitive answer. In particular, it was argued (but not proved) [13] that all twisted modes should be unstable. On the contrary, in [14] a perturbative result was used to argue the stability of such modes for small C and numerical verification was claimed but not demonstrated (Ref. [25] of [14]). We intend to resolve this issue in a decisive way demonstrating the regimes of stability and instability of these modes as well as indicating the mechanisms through which instability will arise. In order to perform linear stability analysis around it, we use the rotating wave frame (RWF)

$$u_n(t) = \exp(it)[\psi_n + v_n(t)] \quad (2)$$

along with the ansatz $v_n = a_n \exp(-i\omega t) + b_n \exp(i\omega t)$. This leads to the linear stability equations

$$\omega a_n = -C\Delta_2 a_n - 2|\psi_n|^2 a_n - a_n - \psi_n^2 b_n^*, \quad (3)$$

$$-\omega b_n = -C\Delta_2 b_n - 2|\psi_n|^2 b_n - b_n - \psi_n^2 a_n^*. \quad (4)$$

We first solve the static equation

$$-\psi_n = -C\Delta_2 \psi_n - |\psi_n|^2 \psi_n \quad (5)$$

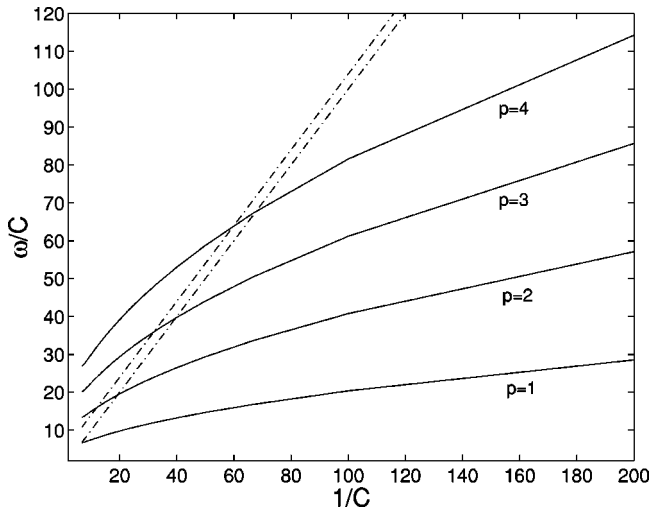


FIG. 1. The frequency of the S mode (scaled by C) eigenfrequency and its harmonics (second, third, and fourth) shown as solid lines as a function of the (scaled) fundamental frequency. The phonon band edge $1/C$ and $4+1/C$ are shown for comparison in dashed-dotted lines. In the intervals for which the harmonics are in the phonon band, the nonlinear resonances described in the text are present.

using Newton-Raphson iteration with an appropriate initial condition to obtain the exact twisted mode. We then use Eq. (3) and the complex conjugate of Eq. (4) to solve the ensuing matrix eigenvalue problem for $(\omega, \{a_n, b_n^*\})$.

We thus find that for $C \in [0, 0.146]$ the ILM's spectrum consists of two eigenmodes at $\omega = 0$. An additional even-parity shape eigenmode S of nonzero frequency exists in the gap between $\omega = 0$ and $\omega = 1$. The latter represents the lower edge of the phonon band since the spatially extended waves of this band obey the dispersion relation $\omega = \pm[1 + C(2 - 2 \cos k)]$. Following previous expositions on the subject [21], we scale the fundamental frequency, $\Lambda = 1$, and the eigenmode frequencies ω by the coupling constant C . In Fig. 1 we show the shape mode frequency variation with respect to the phonon band (indicated by dash-dot lines). We also show the variation of the S mode harmonics for the interval of stability of the exact twisted mode.

As was found for the DNLS equation in Ref. [21] and for the equivalent static problem of the discrete sine-Gordon (SG) and ϕ^4 equations in Ref. [22], the existence of a p th harmonic of a discrete eigenmode inside the phonon band leads to a $t^{-1/(2p-2)}$ rate of decay of the localized energy into extended wave ripples. For the twisted mode, the fourth harmonic of S is in the band for $C \in [0.0147, 0.0167]$ signaling a $t^{-1/6}$ decay. Similarly for $C \in [0.0252, 0.0313]$ the third harmonic generates a $t^{-1/4}$ decay and for $C \in [0.0518, 0.0834]$ the second harmonic induces a $t^{-1/2}$ decay. Perhaps more interestingly, for intervals between the mentioned ones, no harmonics are resonating with the extended modes. This signifies that an original perturbation of the exact ILM in the S eigendirection, rather than decaying, will sustain a persistent oscillation [named *breather on breather* (BOB) in Ref. [23]]. These modes are genuinely single-frequency time-periodic modes in the rotating wave

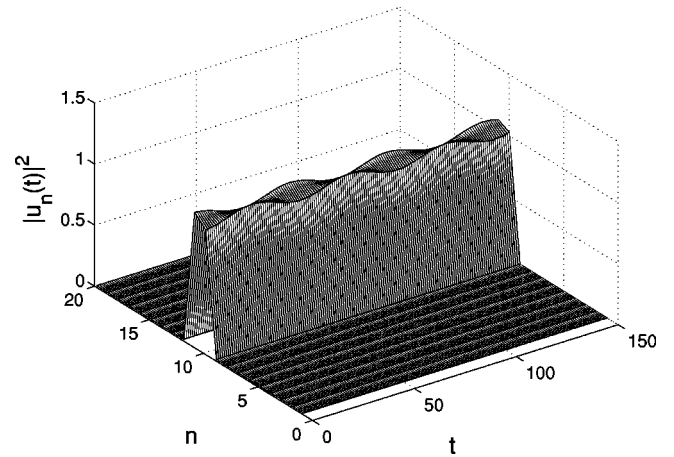


FIG. 2. An example of a BOB mode for $C = 0.02$. The modulus of a solution $\exp(it)\psi_n$ would obviously be static in time. However, the genuinely periodic nondecaying oscillation indicates the existence of a secondary S frequency. This frequency is associated with a spatial projection along the S eigenfunction that creates a spatially localized, time periodic structure (a breather) on the “background” of another such structure, hence a (nondecaying due to the absence of resonances) BOB.

frame, whereas they are quasiperiodic two-frequency modes for the original dynamical problem. In order to rigorously prove the existence of such modes, one can directly adjust (in the rotating wave frame where the problem is static) the arguments of Sec. 5.1 of [22]. This demonstrates that the only condition for the rigorous proof of existence of BOB's is the nonresonance condition for their internal mode frequencies in the RWF, which is satisfied between the above mentioned intervals. Such modes are seen to persist in the dynamics of numerical experiments as can be seen in Fig. 2 for $C = 0.02$. Our long-time simulations have indicated that BOB's generically persist [as is also suggested by Fig. 3(a) of [15]] in the long-time dynamics of the system. This conclusion is in full agreement with what one would expect from the findings of Sec. 6 of [22], where breathers on kinks (BOK's) were studied. These numerical results suggest that these coherent structures (BOK's and BOB's) are stable for, at least, intermediate time scales and in any event, certainly for time scales relevant for realistic experimental realizations of the systems under study. A rigorous proof of stability of such structures would involve the Floquet theory; that is a quite interesting but rather technical endeavor beyond the scope of the present work (one of which was) to rigorously prove the existence and numerically demonstrate the stability (at least for relevant time scales and for the appropriate values of the coupling constant, see Sec. III) of these ILM's. It is worth noting that these modes can be genuinely quasiperiodic, persisting in the long-time asymptotics of the system while the regular DNLS modes (such as ST) can sustain only metastable BOB's as explained in [23]. It is therefore likely that the twisted modes and their persistent internal oscillations often appear spontaneously in dynamical simulations [10] and experiments.

Useful insight into the nature of the twisted mode can be obtained by considering the two (out of phase) components

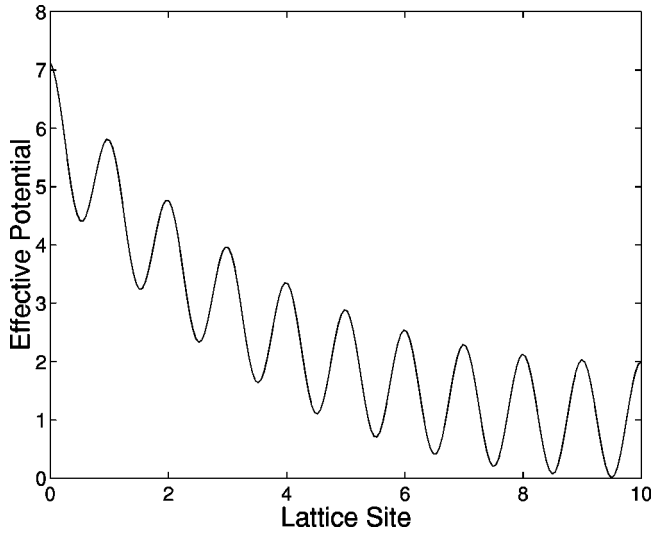


FIG. 3. Sketch of effective potential between two oppositely phased components of the twisted mode.

separately. In this case, analogously to what was discussed in [24], it is, in principle, possible to construct a potential determining the center of mass motion of a single component. Generally, there will be two separate contributions to this potential arising from (1) the (repulsive) interaction of the two components and (2) from the translational barrier created by the discreteness [often referred to as the Peierls-Nabarro periodic potential (PNP)]. A sketch of the overall potential is given in Fig. 3 (compare with Fig. 2 of Ref. [24]). It is evident that the twisted mode exists due to the PNP as this is the source of the local minima observed in Fig. 3. Approaching the continuum limit, the PNP will vanish while the repulsive interaction persists and therefore the twisted mode will not survive in the continuum limit as the two components will be free to separate. The oscillation of the internal mode of the twisted ILM can be viewed as a small amplitude oscillation of a point particle in one of the local minima of the potential in Fig. 3. Therefore the frequency of the internal mode, as shown in Fig. 1, is a measure of the curvature of the potential at this local minimum. It is important to note that although this ‘‘center of mass’’ picture offers insight into the existence properties of the twisted ILM and its internal mode, it cannot fully account for the quantitative details of the stability properties of the infinite-dimensional dynamical system. Hence, we use numerical linear stability analysis to probe such details more carefully.

III. BIFURCATION SCENARIO

As the first harmonic ($p=1$) of the S mode approaches the band and eventually hits it at $C \approx 0.14604$, an instability emerges from a bifurcation of a quartet of modes that now have a nonzero imaginary frequency component ω_i . The positions of the eigenvalues in the spectral plane very close to the onset of this instability are shown in Fig. 4. This behavior is rather unusual for the regular ST and P modes whose bifurcations to instability occur primarily through the origin onto the imaginary axis of the spectral plane. Herein, the

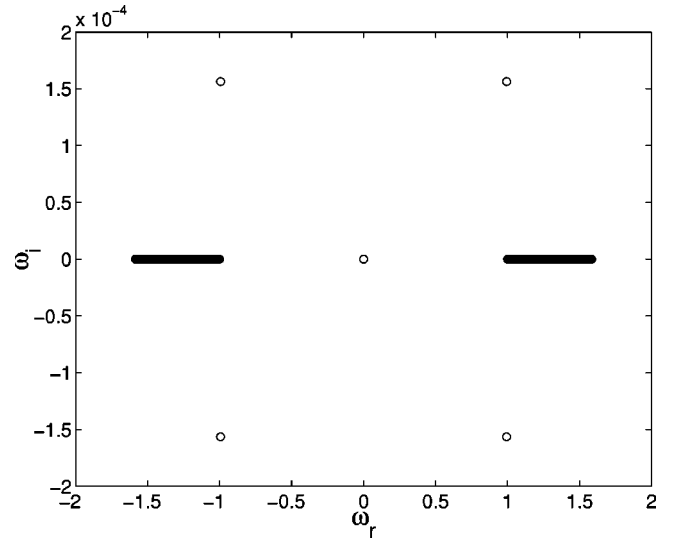


FIG. 4. The spectrum around the exact twisted mode at the onset of the first instability $C=0.14604$. Shown is the spectral plane (ω_r, ω_i) . The quartet bifurcation is clearly visible. There are two more modes at $\omega=0$ and a phonon band with $\omega \in \pm[1, 1+4C]$

complexity of a noncontinuum mode gives rise to the much more complex behavior of quartet generation in order to produce the instability. Furthermore, as was pointed out in Ref. [21], the regular modes when approaching the phonon band eventually merge with it without causing an instability, whereas clearly this is not the case here. It is also interesting to note that, given the structure of the discrete eigenvalue problem $\omega^2 v_i = [H]v_i$ (where $[H]$ is a Hermitian matrix), when linearizing around static nonuniform steady states in the discrete SG and ϕ^4 models, a quartet bifurcation is impossible due to discreteness. Hence, this is a phenomenon particular to the DNLS equation. This is a feature observed for *bright* modes of the DNLS equation. Prior to this work, such an oscillatory instability, reminiscent of a Hopf bifurcation (common to parabolic dissipative systems) had been observed for bright modes in the Bragg-gap solitons of the generalized Thirring model [25]. In the DNLS equation, it was very recently observed [26] that dark staggered modes of the discrete problem become unstable via such an instability with increase of the coupling strength.

After splitting, the quartet of modes moves symmetrically in the complex plane up to a maximum bifurcation and thereafter moves towards the real axis. This scenario is very similar to the one described in Ref. [26].

Due to the sparse population of the phonon band for any finite system (the trajectory of the imaginary part of which is shown in Fig. 5 for a system with $N=100$ sites), the eigenvalue may return to a gap in the spectrum. In that case, it reenters the axis (in the case of $N=100$ this happens for $C=0.769$); however, as C is increased, it encounters the closest eigenvalue of the band and collides with it. The collision results in the reexiting of the eigenvalue from the real axis (the ‘‘reentrant instabilities’’ of Ref. [26]) and a cascade of such phenomena results (in analogy to Fig. 2 of Ref. [26]). Calculations with larger lattices have verified a picture similar to Fig. 2 of [26] for the twisted modes. In the case of the

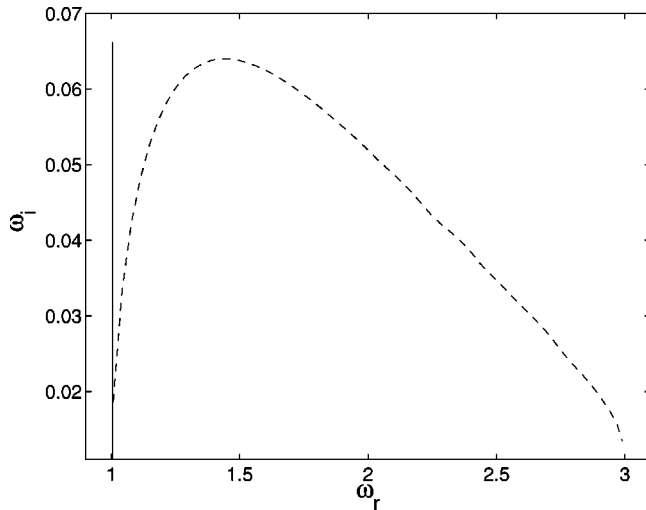


FIG. 5. The dashed line shows the behavior of the (absolute value of the) imaginary part of the quartet eigenvalue as a function of (the absolute value of) its real part (i.e., showing its trajectory in the spectral plane). The excursion along the spectral plane entails a maximum bifurcation and an eventual return to the real axis for $C \approx 0.769$. The solid line indicates the (invariant) position $\omega_r = 1$ of the edge of the phonon band. Note that the solid line is meant only as a guide to the eye as to where the phonon band edge lies (i.e., the phonon band edge mode always has $\omega_i = 0$).

infinite system (for which the phonon band contains no gaps), the approach of the quartet eigenfrequency to the real axis is only asymptotic.

However, in the interval between the bifurcation from and the return to the real axis of the quartet modes, there are further interesting phenomena. In particular, for $C > 0.41$, a mode that was sitting at the edge of the phonon band now bifurcates along the real axis to become a localized eigenmode. This mode moves all the way to the origin of the spectral plane to bifurcate along the imaginary axis of the plane giving rise to an additional unstable eigenmode. The bifurcation occurs at $C \approx 0.714$. Moreover, another eigenmode emerges from the phonon band, for $C > 0.6$ and moves towards the origin reaching it for $C \approx 0.77$. (The behavior of these two modes that are bifurcating from the band edge is shown in Fig. 6.) For higher values of the coupling constant, the twisted modes are highly unstable and hence of no particular interest.

IV. DISCRETE INTEGRABLE LIMIT

In the previous section we saw how the approach to the continuum limit of this discrete ILM occurs. Another interesting aspect worth exploring is the approach to the *discrete integrable limit*, as represented by the Ablowitz-Ladik (AL)NLS equation [27]

$$i\dot{u}_n = -C\Delta_2 u_n - |u_n|^2(u_{n+1} + u_{n-1}). \quad (6)$$

In order to study how the twisted mode and its stability change on approaching the discrete integrable limit, we used homotopic continuation, studying an interpolant between the

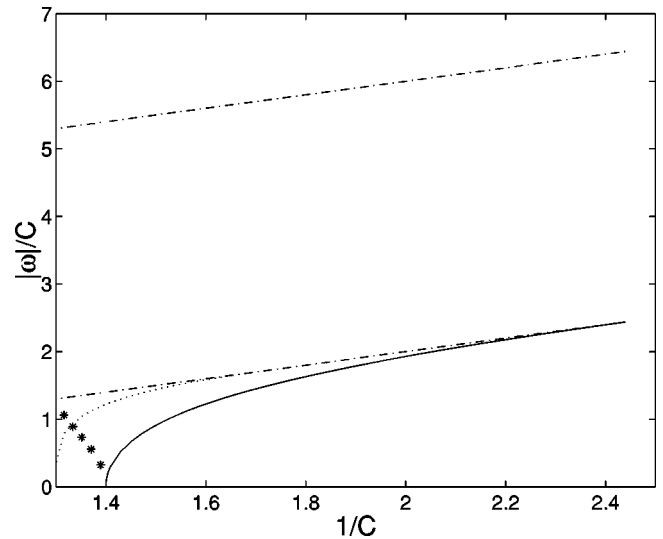


FIG. 6. The additional two eigenmodes that are bifurcating from the phonon band (shown by dash-dot lines) along the real line are shown. The first eigenmode (solid line) bifurcates along the real line for $C \approx 0.410$ and hits the origin to enter along the imaginary axis (the stars indicate the magnitude of this, now imaginary, eigenvalue) for $C > 0.714$. The second eigenmode (dotted line) bifurcates for $C > 0.6$ and arrives at the origin for $C \approx 0.77$.

two limits as the homotopic parameter ϵ is varied; a convex combination of the DNLS and AL-NLS nonlinearities is as follows:

$$i\dot{u}_n = -C\Delta_2 u_n - |u_n|^2[2(1 - \epsilon)u_n + \epsilon(u_{n+1} + u_{n-1})]. \quad (7)$$

Clearly, the $\epsilon = 0$ limit (from which we start the continuation) coincides with the DNLS equation, while the $\epsilon = 1$ limit coincides with AL-NLS equation. In addition to studying the twisted mode standing waves, we set up the analogs of Eqs. (3) and (4) to study stability.

The homotopic continuation was performed for a typical value of the coupling constant ($C = 0.1$) for which the mode is stable in the DNLS equation (by using different values of C , the generic nature of the scenario presented below was verified). It is observed that the mode continues to be stable until $\epsilon \approx 0.085$. The scenario up to this point is strongly reminiscent of the one encountered approaching the continuum limit. In particular the internal-mode frequency approaches the edge of the phonon band and eventually collides with it, generating a quartet of eigenvalues. The quartet of modes then moves symmetrically in the complex plane until $\epsilon \approx 0.235$ where it eventually returns to the real line *beyond* the phonon band. Note that this is the most important difference between the continuum limit and the integrable limit approach. For the case of the continuum, as the value of the lattice spacing is decreased, the width of the phonon band gradually increases and eventually becomes semi-infinite extending from a minimum frequency ($\omega = \Lambda \equiv 1$) to $\omega = \infty$. On the contrary, this is not true for the discrete integrable

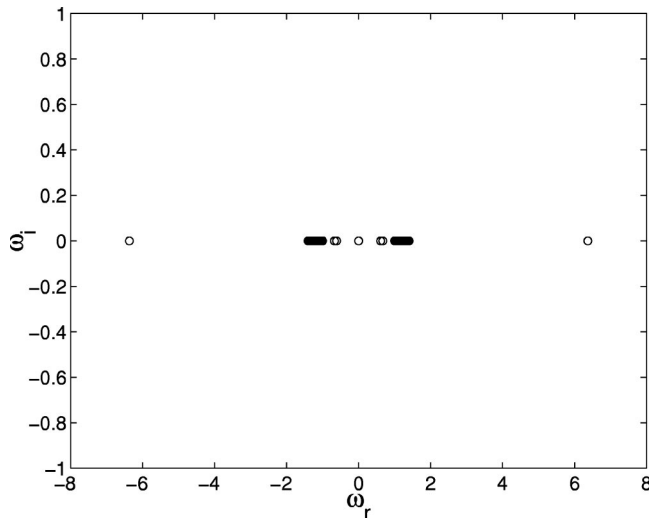


FIG. 7. The eigenvalues at the spectral plane (ω_r, ω_i) are shown for the case approaching the integrable limit for $\epsilon=0.6$, just prior to the termination of the branch. One can clearly discern the modes at 0 (of multiplicity 2), the phonon band (dense group of circles), the two pairs of modes that have bifurcated off the lower edge of the band, as well as the mode with $\omega=6.367$, which is the mode that has returned to the real line beyond the upper edge of the phonon band.

limit where the width of the phonon band remains constant, allowing the stability of the twisted mode to be reestablished. This was also verified numerically by full-scale integration of the ILM initial condition for $\epsilon > 0.235$. As ϵ is further increased, at $\epsilon \approx 0.395$ a pair of modes bifurcates off of the lower edge of the phonon band, followed at $\epsilon \approx 0.465$ by a second pair. The eventual collision of one of these with the origin of the spectral plane results in the saddle-node bifurcation terminating this branch of twisted mode solutions at $\epsilon_{cr} \approx 0.61$. The spectral plane of the stability analysis around the (still stable) mode at $\epsilon=0.6$ is given in Fig. 7.

From the above, we conclude that the approach to the discrete integrable limit is in certain ways reminiscent of the approach to the continuum limit; however, the specifics of the lattice system account for a (significant) difference that permits the mode to exist and be stable even at relatively high values of the relevant homotopic parameter.

V. SUMMARY

Summarizing, we have seen that the twisted modes proposed in [15] in media with cubic nonlinearity have very interesting properties.

(i) Contrary to the regular (ST and P) modes of the DNLS equation, they can sustain exact breather on breather solutions, which are genuinely quasiperiodic solutions of Eq. (1). These modes are naturally conforming to the symmetries of the problem and, as suggested by Fig. 3(a) of [15] as well as by our numerical results, are natural candidates for the long-time asymptotic states of the system. They are also rather different from the single-humped, integrability-related (constructed via the Hirota method) and rather unstable (to phase perturbations) quasiperiodic modes of the ALNLS equation constructed in [28].

(ii) Contrary to the regular modes of the DNLS equation and the discrete SG and ϕ^4 kinks [22,29,30], the “collision” of discrete eigenmodes with the phonon band does not occur in a smooth way, but rather entails a quartet bifurcation for a finite value of the coupling constant.

(iii) Additional modes leave the phonon band to give rise to localized eigenmodes and to eventually produce instabilities through the origin, the last of which will eventually destroy the mode for large values of the coupling constant.

(iv) The approach of the modes to the discrete integrable limit is in many respects reminiscent of that to the continuum limit. However, the differences between the bandwidths of the phonon band in the two cases account for some different phenomena and the stability of the mode even relatively close to the integrable limit.

The fact that these twisted modes have a number of interesting and significantly different properties than regular DNLS modes warrants further efforts to better understand their significance and influence in relevant experimental situations.

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