Existence and stability of multisite breathers in honeycomb and hexagonal lattices

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Abstract

We study the existence and stability of multisite discrete breathers in two prototypical non-square Klein–Gordon lattices, namely a honeycomb and a hexagonal one. In the honeycomb case we consider six-site configurations and find that for soft potential and positive coupling the out-of-phase breather configuration and the charge-two vortex breather are linearly stable, while the in-phase and charge-one vortex states are unstable. In the hexagonal lattice, we first consider three-site configurations. In the case of soft potential and positive coupling, the in-phase configuration is unstable and the charge-one vortex is linearly stable. The out-of-phase configuration here is found to always be linearly unstable. We then turn to six-site configurations in the hexagonal lattice. The stability results in this case are the same as in the six-site configurations in the honeycomb lattice. For all configurations in both lattices, the stability results are reversed in the setting of either hard potential or negative coupling. The study is complemented by numerical simulations which are in very good agreement with the theoretical predictions. Since neither the form of the on-site potential nor the sign of the coupling parameter involved have been prescribed, this description can accommodate inverse-dispersive systems (e.g. supporting backward waves) such as transverse dust-lattice oscillations in dusty plasma (Debye) crystals or analogous modes in molecular chains.

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(Some figures in this article are in colour only in the electronic version)
1. Introduction

Over the past decade, there has been a considerable increase of interest in the study of discrete or quasi-discrete systems in a wide range of areas in physics. Among the numerous themes of intense theoretical and experimental interest, one can refer to the DNA double-strand dynamics in biophysics [1], coupled waveguide arrays and photorefractive crystals in nonlinear optics [2–4], breathing oscillations in micromechanical cantilever arrays [5], Bose–Einstein condensates in optical lattices in atomic physics [6], granular crystals [7], and so on.

These studies have been conducted predominantly in one-dimensional (1D) systems or in higher dimensions, but chiefly in the context of square lattices. In the latter, a wide variety of novel and interesting phenomena have been revealed, both theoretically and experimentally. Pertinent examples include, among others, the prediction and observation of dipole [8], and necklace [9] solitons, discrete vortices [10, 11], rotary solitons [12, 13], higher order Bloch modes [14] and gap vortices [15], as well as two-dimensional Bloch oscillations and Landau–Zener tunnelling [16].

More recently, the dynamics of non-square lattices have become a focal point of interest, both in the context of periodic photonic structures [17–20], and in that of quasi-crystalline [21] or completely disordered lattices [22]. While most of the above works had a view towards applications based on photorefractive crystals, there exist many other applications where such non-square lattices may be relevant. In particular, for the hexagonal and honeycomb lattices considered herein, we note that they have already been showcased in recent experiments in two-dimensional waveguide arrays (e.g. in glass) [23], in optical lattices acting on Bose–Einstein condensates [24], as well as in Debye crystals formed in dusty plasmas [25, 26]. Interestingly, in the latter case (dusty plasma crystals), the horizontal propagation of transverse (off-plane) vibrations gives rise to an inverse-optic dust-lattice mode (a backward wave) [27, 28] which is described by a Klein–Gordon-type equation like the one we shall focus on below, yet upon formally considering a negative coupling coefficient (‘spring constant’). In this case, nonlinearity is provided by the (anharmonic) plasma sheath potential, while discreteness is expressed by the (small value of the) ratio of a characteristic coupling frequency (related to electrostatic Debye interactions). Remarkably, both ab initio theoretical considerations and experimental findings suggest that the sheath on-site potential is intrinsically anharmonic and in fact strongly asymmetric, so that existing theories involving even (symmetric) polynomial functions for the on-site potential do not apply in this case. Further contribution to nonlinearity is furnished by Debye-type (screened Coulomb) electrostatic inter-dust-particle interactions, yet the associated anharmonicity is of lesser order of magnitude for the transverse mode and can be neglected. Details on dusty plasma modelling can be found, e.g. in [29, 30], while the experimental setting is described in [28, 31].

The above experimental developments have prompted further theoretical work towards the goal of understanding the structures that may emerge in such non-square lattices and their corresponding stability. An example of this type is the recent work of [32], where this analysis was performed in the framework of the discrete nonlinear Schrödinger (DNLS) equation, a prototypical model widely perceived as relevant to optical systems.

The aim of the present work, motivated by models of dusty plasma lattices [25, 26], is to extend the considerations in [32] to nonlinear Klein–Gordon lattices of the hexagonal and honeycomb type. We stress the fact that no assumption will be made on the (anharmonic) substrate potential or the sign of the coupling parameter involved in the description. In particular, inverse-dispersive systems (supporting backward propagating waves in the linear limit) such as transverse oscillations in dusty plasma crystals are straightforward to accommodate in this description (by reverting, say, the sign of the ‘spring’ coupling coefficient
to negative). Within this framework, we offer a systematic analysis of the type of solutions that arise in six-site contours in honeycomb lattices and three-site as well as six-site contours in hexagonal lattices (for the latter lattice, see also earlier work in [26, 33]). In the six-site contours, we illustrate that solutions with higher topological charge \( S \) (namely \( S = 2 \)) are more dynamically robust than lower topological charge ones (namely \( S = 1 \)). This is true for soft nonlinearities and positive coupling (or hard nonlinearities and negative coupling), while the results are reversed if either the nature of the nonlinearity or the sign of the coupling is changed. It is interesting to note that similar findings have been reported not only in DNLS-type chains [32] but also in continuum photorefractive crystals [34] (where they have recently been confirmed experimentally [35]). Furthermore, in-phase and out-of-phase structures are also examined. The former are found to be unstable, while the latter are potentially linearly stable. In the three-site, hexagonal configuration, both in- and out-of-phase structures are unstable, while the vortex one may be stable. Again, this is true for soft nonlinearities and positive coupling (or hard nonlinearities and negative coupling), while all the results, besides the out-of-phase case, are reversed if either the nature of the nonlinearity or the sign of the coupling are changed. Finally, in the six-site configurations in the hexagonal lattice, the stability results are the same as in the case of six-site configurations in the honeycomb lattice.

Our paper is structured as follows. In section 2, we analyse the six-site honeycomb contour, while in section 3, we briefly review the findings for the three-site hexagonal contour. Section 4 contains the comparison with numerical results. Finally, section 5 contains a summary of our findings and a brief discussion of future directions.

2. Existence of multisite breathers in a honeycomb Klein–Gordon lattice

We consider a honeycomb lattice (see the prototypical example of figure 1) with on-site potential and linear nearest neighbour interaction. This system is described by a Klein–Gordon Hamiltonian of the form

\[
H = H_0 + \varepsilon H_1 = \sum_{i \in \mathcal{S}} \frac{p_i^2}{2} + V(x_i) + \frac{\varepsilon}{2} \sum_{i,j \in \mathcal{G}} (x_j - x_i)^2,
\]

where \( \mathcal{S} \) is the set of all the oscillators and \( \mathcal{G} \) is the set of neighbouring pairs of oscillators.

In the anti-continuum (AC) limit \( \varepsilon = 0 \) we consider the six encircled oscillators of figure 1 as moving in periodic orbits with the same period \( \omega_i = \omega \), while the rest of the oscillators lie at equilibrium \((x_i, p_i) = (0, 0)\). This periodic and trivially localized motion is continued, for \( \varepsilon \neq 0 \) small enough, to provide multisite breathers, if the phase differences between successive oscillators \( \phi_i \) are such that they correspond to critical points of the effective Hamiltonian \( H_{\text{eff}} \) [37]. To leading order of approximation, the effective Hamiltonian becomes

\[
H_{\text{eff}}^{\text{ac}}(I, \phi, A) = H_0(I, A) + \varepsilon \langle H_1 \rangle(I, A, \phi_i),
\]

where \( I, A, \phi_i \) are canonical variables which are defined by the transformation

\[
\begin{align*}
\vartheta &= w_1, \\
A &= \sum_{j=1}^{6} J_j \\
\phi_i &= w_{i+1} - w_i, \\
I_i &= \sum_{j=i+1}^{6} J_j, \quad i = 1, \ldots, 5
\end{align*}
\]

with \( J_j, w_i \) being the action-angle variables. The average value of \( H_1 \), namely \( \langle H_1 \rangle = \frac{1}{\tau} \int H_1 \, dt \), is calculated along the unperturbed orbit. Note that since the motion of a single oscillator for \( \varepsilon = 0 \) can be described by \( J_i = \text{const} \) and \( w_i = \omega t + w_{0i} \), the variables \( \phi_i \) can
be considered as the phase differences between two successive oscillators. Since we consider six oscillators in the AC limit and \( \phi_6 = -\sum_{i=1}^5 \phi_i \), we get only five independent \( \phi_i \). Then, the configurations of the AC limit that will be continued to provide the multisite breathers correspond to simple roots of the system of equations

\[
\frac{\partial \langle H_1 \rangle}{\partial \phi_i} = 0, \quad i = 1, \ldots, 5
\]

provided, of course, the non-resonance of the frequency of the breather \( \omega_b \) with the frequency \( \omega_p \) of the system’s linear spectrum, namely \( k \omega_b \neq \omega_p \), and the anharmonicity of the single uncoupled oscillator, i.e. \( \partial \omega / \partial J \neq 0 \). This result is in accordance with the findings of [38] (see also [33]).

In order to calculate \( \langle H_1 \rangle \) we use the fact that the motion of each oscillator in the AC limit can be described by a cosine Fourier series due to the time-reversibility (viz. \( x(-t) = x(t) \), \( p(-t) = -p(t) \)),

\[
x_i(t) = \sum_{n=0}^{\infty} A_{nJ} \cos(n\omega_i t),
\]

where \((J, \omega)\) are the action-angle variables for the specific oscillator. Using this fact, and the canonical transformation (2), \( \langle H_1 \rangle \) becomes

\[
\langle H_1 \rangle = -\frac{1}{2} \sum_{n=1}^{\infty} A_n^2 [\cos(n\phi_1) + \cos(n\phi_2) + \cos(n\phi_3) + \cos(n\phi_4) + \cos(n\phi_5) + \cos[n(\phi_1 + \phi_2 + \phi_3 + \phi_4 + \phi_5)]].
\]

So, condition (3) becomes

\[
\sum_{n=1}^{\infty} n A_n^2 [\sin(n\phi_i) + \sin[n(\phi_1 + \phi_2 + \phi_3 + \phi_4 + \phi_5)]] = 0, \quad i = 1, \ldots, 5,
\]

which leads to two groups of solutions. The first one is

\[
\phi_i = 0 \quad \text{or} \quad \pi, \quad i = 1, \ldots, 5,
\]

which determines the time-reversible solutions according to the terminology of [36], while the second kind of solutions

\[
\phi_i = S \frac{\pi}{3}, \quad i = 1, \ldots, 5 \quad \text{and} \quad S \in \{1, 2\}
\]
determines the non-time-reversible solutions, i.e. vortex breather solutions of topological charge $S$. This kind of solutions can be distinguished from the previous one because it possesses a nonzero energy flux [39]. The form and the time evolution over a period of the above-mentioned motions can be found in [40].

The stability of the above-mentioned solutions is determined through the corresponding Floquet multipliers $\lambda_i$ (see e.g. [41]). The characteristic exponents of the breather are defined as $\lambda_i = e^{\sigma_i T}$. The nonzero characteristic exponents of the central oscillators are given as eigenvalues of the stability matrix $E = \Omega D^2 H^{\text{eff}}$, where $\Omega = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}$ is the symplectic structure matrix and $O, I$ are the $5 \times 5$ zero and identity matrices, respectively. The leading-order approximation of $E$ is given by

$$E_1 = \begin{pmatrix} -\varepsilon \frac{\partial^2 \langle H_1 \rangle}{\partial \phi_i \partial I_j} & -\varepsilon \frac{\partial^2 \langle H_1 \rangle}{\partial \phi_i \partial \phi_j} \\ \frac{\partial^2 H_0}{\partial I_i \partial I_j} + \varepsilon \frac{\partial^2 \langle H_1 \rangle}{\partial I_i \partial I_j} & \frac{\partial^2 \langle H_1 \rangle}{\partial \phi_i \partial \phi_j} \end{pmatrix} .$$ (5)

If all the eigenvalues of matrix $E$ lie on the imaginary axis, then the corresponding breather is linearly stable. If the eigenvalues of $E_1$ are simple to leading order in $\varepsilon$ and lie on the imaginary axis, then the eigenvalues of $E$ will also lie in the imaginary axis, due to continuity reasons. If the eigenvalues of $E_1$ are not simple in the leading order, then the higher order terms of the approximation could push the eigenvalues of $E$ outside the imaginary axis and, thus, lead to complex instability. However, this cannot happen if the symplectic signature of $E_1$ is definite [42] and the breather remains stable for $\varepsilon$ small enough. This signature is definite if the quadratic form $x^T E_1 x$ has the same sign for every vector $x \in \mathbb{R}^{10}$.

Note that, although the above conditions certify linear stability for small values of $\varepsilon$, for higher values of $\varepsilon$ a characteristic exponent of the central oscillators can collide with the linear spectrum causing instability through a Hamiltonian–Hopf bifurcation, as it can be seen in some of our numerical results below (see also [41]).

2.1. The four configurations under consideration

We consider four representative configurations of the AC limit which lead to the corresponding multisite breathers. For all of the ones we consider, it is true that $\omega_i = \omega \Leftrightarrow J_i = J$ and $\phi_i = \phi, i = 1, \ldots, 5$. More precisely, we consider the in-phase configuration, $\phi = 0$, the out-of-phase one, $\phi = \pi$, the charge-one vortex breather $\phi = \pi/3$ and the charge-two vortex breather $\phi = 2\pi/3$. Using (2), we obtain for the various elements of matrix $E_1$

$$\begin{align*}
\frac{\partial^2 H_0}{\partial I_i \partial I_j} &= \begin{cases} 2 \frac{\partial^2 H_0}{\partial J^2} = 2 \frac{\partial \omega}{\partial J}, & j = i \\
-\frac{\partial^2 H_0}{\partial J^2} = -\frac{\partial \omega}{\partial J}, & j = i + 1 \\
0 & \text{otherwise}
\end{cases} \\
\frac{\partial^2 \langle H_1 \rangle}{\partial \phi_i \partial \phi_j} &= \begin{cases} 2 f(\phi), & j = i \\
 f(\phi), & j \neq i, \quad \text{with} \quad f(\phi) = \frac{1}{2} \sum_{n=1}^{\infty} n^2 A_n^2 \cos(n\phi)
\end{cases}
\end{align*}$$
\[ \frac{\partial^2 \langle H_1 \rangle}{\partial I_i \partial I_j} = \begin{cases} 2g_1 - 3g_2, & j = i \\ -2g_1 - 2g_2, & j = i + 1 \\ g_1, & j = i + 2 \end{cases} \]

with

\[ g_1 = \frac{1}{2} \sum_{n=1}^{\infty} \left( \frac{\partial A_n}{\partial J} \right)^2 \cos(n\phi) \]

\[ g_2 = \frac{1}{2} \sum_{n=1}^{\infty} \frac{\partial^2 A_n}{\partial J^2} \cos(n\phi) \]

\[ \frac{\partial^2 \langle H_1 \rangle}{\partial I_i \partial \phi_j} = \begin{cases} k, & j = i + 1 \\ 0, & j \neq i + 1 \end{cases} \]

with \( k = \frac{1}{2} \sum_{n=1}^{\infty} n A_n A_n \sin(n\phi) \).

Below, we examine separately each of the four principal configurations under investigation.

Up to leading order of approximation, the eigenvalues of the stability matrix \( E_1 \) correspond to the \( O(\sqrt{\epsilon}) \) approximation of the characteristic exponents, and they are given, for all the configurations under consideration, by the expressions

\[ \sigma_{\pm 1, \pm 2} = \pm \sqrt{-\epsilon} \frac{\partial \omega}{\partial J} f, \quad \sigma_{\pm 3, \pm 4} = \pm 3 \sqrt{-\epsilon} \frac{\partial \omega}{\partial J} f, \quad \sigma_{\pm 5} = \pm 2 \sqrt{-\epsilon} \frac{\partial \omega}{\partial J} f. \]  

(6)

It may be added for rigor that we have chosen to keep the sign of the coupling strength \( \epsilon \) arbitrary, bearing in mind that inverse dispersive systems, such as transverse dust-lattice vibrations (briefly discussed above), require negative values of \( \epsilon \) to be considered (in contrast with the ordinary Klein–Gordon formulation). Thus, \( \epsilon \) may be either negative or positive throughout this text, unless otherwise stated.

2.1.1. The in-phase multibreather \( \phi = 0 \). We first examine the in-phase (\( \phi = 0 \)) configuration. In this case we obtain \( \frac{\partial^2 \langle H_1 \rangle}{\partial I_i \partial \phi_j} = 0 \), which simplifies the calculations of the characteristic exponents \( \sigma_i \) in equation (6). Since for continuous periodic functions the size of Fourier coefficients \( A_n \) is exponentially decreasing as a function of \( n \), \( f \) converges—in this case—to a positive number:

\[ f = f(0) = \frac{1}{2} \sum_{n=1}^{\infty} n^2 A_n^2 > 0. \]

Hence, the nature of the exponents (and the linear stability) hinges on the product \( \epsilon \frac{\partial \omega}{\partial J} \). If it is negative (as is the case for soft nonlinearities and positive couplings, or for hard nonlinearities and negative couplings), the exponents are real and the corresponding breather is unstable. If \( \epsilon \frac{\partial \omega}{\partial J} > 0 \) we also have to check the corresponding symplectic signature to ensure that the exponents will remain on the imaginary axis. It can be proved (but the calculations are rather lengthy) that this signature is definite if \( \epsilon \frac{\partial \omega}{\partial J} > 0 \). So, in this case the resulting breather is linearly stable for \( \epsilon \) small enough in order to avoid collisions with the linear spectrum.

2.1.2. The out-of-phase multibreather, \( \phi = \pi \). For \( \phi = \pi \), the stability matrix \( E_1 \) and its eigenvalues \( \sigma_i \) are the same as before, but in this case it is

\[ f = f(\pi) = \frac{1}{2} \sum_{n=1}^{\infty} n^2 A_n^2 (-1)^n < 0. \]

Due to the Hamiltonian nature of the single oscillator it is \( A_1 > 4A_2 \) and since the absolute value of the terms is exponentially decreasing, \( f \) converges to a negative number. Following similar arguments as in the previous section we conclude that for \( \epsilon \frac{\partial \omega}{\partial J} < 0 \) (under the physical conditions discussed in the previous subsection), the breather is linearly stable, while it is unstable otherwise.
2.1.3. The vortex breather of charge $S = 1$, $\phi = \pi/3$. In the case of the vortex with charge $S = 1$ ($\phi = \pi/3$), the terms $\frac{\partial^2}{\partial I_i \partial \phi_j}$ are not identically zero, but the corresponding characteristic exponents are still, to leading order of approximation, given by equation (6). For the polynomial potentials typically used, $f$ converges to a positive number:

$$f = f\left(\frac{\pi}{3}\right) = 12 \sum_{n=1}^{\infty} n^2 A_n^2 \cos\left(\frac{n\pi}{3}\right) > 0.$$  

Thus, following the arguments of the previous sections for $\varepsilon \frac{\partial \omega}{\partial J} < 0$ it turns out that the vortex breather is linearly unstable, while for $\varepsilon \frac{\partial \omega}{\partial J} > 0$ the breather is linearly stable.

2.1.4. The vortex breather of charge $S = 2$. The stability matrix $E_1$ and its eigenvalues ($\sigma_i$) are the same as before, but since for $\phi = 2\pi/3$, it is found that

$$f = f\left(\frac{2\pi}{3}\right) = 12 \sum_{n=1}^{\infty} n^2 A_n^2 (-1)^n \cos\left(\frac{n\pi}{3}\right) < 0.$$  

Thus, we conclude that the corresponding breather is linearly stable if $\varepsilon \frac{\partial \omega}{\partial J} < 0$, while otherwise it is unstable. Note that the symplectic signature arguments mentioned in subsection 2.1.1 are still valid.

3. Existence and stability of three-site and six-site breathers in a hexagonal Klein–Gordon lattice

Let us start by briefly reviewing the theory of [26, 33], as a preamble to the systematic comparison with numerical results in the following section. The Klein–Gordon Hamiltonian is of the form of equation (1), but now each site has six neighbours instead of three as before.

We consider an AC limit of three oscillators, as per the contour shown in figure 2. In this case, there exist only two independent $\phi$’s since $\phi_3 = w_1 - w_2 = -\phi_1 - \phi_2$. The persistence conditions for three-site breathers in these lattices are

$$\sum_{n=1}^{\infty} n A_n^2 [\sin(n\phi_i) + \sin(n(\phi_1 + \phi_2))] = 0, \quad i = 1, 2.$$
Seeking zeros of the curly bracket in the above expression, we will consider the in-phase configuration with \( \phi_i = 0 \), the out-of-phase one with \( \phi_i = \pi \), and the vortex breather with \( \phi_i = \frac{2\pi}{3} \). The form and time evolution over a period of these motions can also be found in [40]. To leading order of approximation, the corresponding characteristic exponents are given by the following expressions—for the in-phase configuration:

\[
\sigma_{\pm 1, \pm 2} = \pm \sqrt{-3\varepsilon \frac{\partial \omega}{\partial J} f(0)},
\]

for the out-of-phase configuration:

\[
\sigma_{\pm 1} = \pm \sqrt{-\varepsilon \frac{\partial \omega}{\partial J} [2f(0) + f(\pi)]}, \quad \sigma_{\pm 2} = \pm \sqrt{-3\varepsilon \frac{\partial \omega}{\partial J} f(\pi)},
\]

and, finally, for the vortex configuration:

\[
\sigma_{\pm 1, \pm 2} = \pm \sqrt{-3\varepsilon \frac{d\omega}{dJ} f(2\pi/3)},
\]

where the function \( f(\phi) \) is defined as in the previous section.

In the case of the six-site configurations, the characteristic exponents results are the same as in the honeycomb lattice and are given by equations (6). This is because our theory is a first order one, while the influence of the extra sites in this case would be visible in the higher order of the expansion of the exponents.

4. Numerical results

We perform a set of numerical computations in order to demonstrate the validity of our results. Although the theoretical analysis above is completely general, in what follows, we consider a particular choice of an on-site potential and breather frequency. More specifically, the potential under consideration is a quartic one of the form

\[
V(x) = \frac{a}{2}x^2 + \frac{b}{3}x^3 + \frac{c}{4}x^4
\]

with \( a = 1, b = -0.27, c = -0.03 \). For this set of parameters \( \frac{\omega}{J} < 0 \). We will consider the orbit with the frequency \( \omega = 7.43409 \) which corresponds to the amplitude of oscillation \( x_{\text{max}} = 1.949275 \); thus, \( J = 1.20306 \) and \( \frac{\omega}{J} = -0.224556 \). For the same orbit we obtain \( f(0) = 1.423404, f(\pi) = -1.279544, f(\frac{\pi}{3}) = 0.638983 \) and \( f(\frac{2\pi}{3}) = -0.710913 \).

We point out that a positive value was considered in our numerical investigation below. Recalling that the value of \( \varepsilon \) may be either positive or negative (see discussion above), one should therefore keep in mind that the qualitative predictions (on breather stability) to follow are directly reversed if either the sign of \( \varepsilon \) or the sign of \( \frac{\omega}{J} \) are reversed (to negative/positive, respectively). They obviously remain unchanged if both quantities change sign.

4.1. Honeycomb lattice

4.1.1. In-phase, six-site breather. First we consider the in-phase configuration \( (\phi_i = \phi = 0) \). As mentioned in section 2.1.1, all the characteristic exponents \( \sigma_i \) of the central oscillators are real to leading order of approximation. We calculate the breather for increasing values of \( \varepsilon \) and numerically compute the corresponding characteristic exponents. In figure 3 we show the theoretically predicted values (cf equation (6)), depicted by dashed lines, together with the ones calculated by the numerical simulation, depicted by solid lines. In this figure, as well as in the following ones, only the positive \( \sigma_i \) is shown. It is observed that the theoretical and
Figure 3. The real part of the characteristic exponents $\sigma_i$ for the in-phase honeycomb configuration for increasing values of $\epsilon$. The solid lines represent the values obtained numerically, while the dashed ones represent the $O(\sqrt{\epsilon})$ theoretical prediction.

Figure 4. The imaginary part of the characteristic exponents $\sigma_i$ for the out-of-phase honeycomb configuration for increasing values of $\epsilon$. The solid lines represent the values obtained numerically, while the dashed ones represent the $O(\sqrt{\epsilon})$ theoretical prediction.

numerical branches almost coincide for small values of $\epsilon$, while for larger values of $\epsilon$, where the higher order terms of $\sigma_i$ become significant, the lines start to deviate from each other. We also note that instead of having five branches of numerical $\sigma_i$, we have only three. This happens because the branches of the $\sigma_{1,2}$ pair, as well as the $\sigma_{3,4}$ pair coincide (these double pairs will be hereafter denoted by thicker lines), which means that the higher order terms of the approximation also coincide.

4.1.2. Out-of-phase, six-site breather. The next configuration is the out-of-phase one, i.e. $\phi_i = \phi = \pi$. As it has already been discussed in section 2.1.2, this is a linearly stable configuration. Indeed, we have numerically calculated the corresponding characteristic exponents for increasing values of the coupling constant $\epsilon$ and accordingly confirmed that all of them lie on the imaginary axis, as it was expected. The calculated value of the exponents, as well as the theoretical $O(\sqrt{\epsilon})$ prediction, are shown in figure 4. We note again that, for small values of $\epsilon$, the theoretical (dashed) and the numerical (solid) curves coincide, and for larger values of $\epsilon$, where the higher order terms become significant, they start to diverge.
4.1.3. Charge \( S = 1 \), six-site vortex breather. We now consider the six-site vortex configuration with \( \phi_i = \phi = \pi/3 \), i.e. with \( S = 1 \). As discussed in section 2.1.3, this configuration is unstable. Indeed, the numerical simulation shows that all the characteristic exponents of the central oscillators have nonzero real part, as predicted by the \( \mathcal{O}(\sqrt{\epsilon}) \) estimation of equation (6) (cf also with the DNLS case of [32]). Those among the exponents of equation (6) which are double, also possess a nonzero imaginary part which is due to higher order contributions of the approximation of \( \sigma_i \). The calculated value of their real part with respect to \( \epsilon \) is shown in the left frame of figure 5, together with the theoretical estimate. Note that the numerical (solid) line and the theoretical (dashed) line diverge less than in the previous two cases. In addition, in the right frame of figure 5 the positive imaginary part of the exponents with the double real part is shown. Interestingly, many of these findings (presence of imaginary parts in the next order and higher quality of agreement of the real part of the first-order predictions) are also present in the DNLS equation for these solutions [32] (cf also the square-lattice case in [43]).

4.1.4. Charge \( S = 2 \), six-site vortex breather. The configuration with \( \phi_i = \phi = 2\pi/3 \), i.e. the \( S = 2 \) vortex breather is linearly stable, as it has already been discussed in section 2.1.4. Indeed, the numerical simulation confirmed that the characteristic exponents of the central oscillators are all imaginary and their value with respect to the value of \( \epsilon \) is shown in figure 6, together with the theoretical prediction. Note that in this case the higher order splits the double eigenvalue pairs, similarly to the case of the DNLS setting [32].

4.2. Hexagonal lattice

4.2.1. In-phase, three-site breather. First, we consider the in-phase configuration (\( \phi_i = \phi = 0 \)). The corresponding characteristic exponents are shown in figure 7. The solid line represents the value of the exponent which is acquired from the numerical simulation, while the dashed one represents the theoretical prediction acquired from equation (7). Note once again in this case the coincidence (also to higher orders) of the double pair of exponents.

4.2.2. Out-of-phase, three-site breather. The next configuration under consideration is the out-of-phase one (\( \phi_i = \phi = \pi \)). This is a linearly unstable configuration, since, as seen from equation (8), one of the characteristic exponents will be real while the other will be imaginary. This is also shown in panels (a) and (b) of figure 8, where the imaginary and real parts of
Figure 6. The imaginary part of the characteristic exponents $\sigma_i$ for the charge $S = 2$ vortex breather honeycomb configuration for increasing values of $\varepsilon$. The solid line represents the values obtained numerically, while the dashed ones represent the $O(\sqrt{\varepsilon})$ theoretical prediction.

Figure 7. The real part of the characteristic exponents $\sigma_i$ for the in-phase three-site hexagonal configuration is shown for increasing values of $\varepsilon$. The solid line represents the values obtained numerically, while the dashed ones represent the $O(\sqrt{\varepsilon})$ theoretical prediction. Note that the double pair does not appear to split for the couplings considered.

the exponents are respectively shown. It is observed that, for small values of $\varepsilon$, one of the exponents is purely imaginary while the other is real. When $\varepsilon$ acquires the value $\varepsilon \simeq 0.014$, a Hamiltonian–Hopf bifurcation occurs, which forms a complex quadruplet of exponents and the corresponding exponent acquires a nonzero real part (this collision with a mode of the continuous spectrum also leads to the apparent non-smoothness of the line in panel (a)).

4.2.3. Vortex three-site breather. The last three-site configuration under consideration is the vortex of topological charge $S = 1$ ($\phi_i = \phi = 2\pi/3$). This configuration is a stable one as can be seen from equation (9). In figure 9 the values of the characteristic exponents, which are both imaginary, are shown. We see in this case that the two branches corresponding to the numerical acquired values of the exponents are distinct, although we have only one theoretical prediction (i.e. the double pair splits). This fact implies that the higher order terms contributing to these exponents are different. Note also that for $\varepsilon \simeq 0.019$, a collision of one of the pairs with the linear spectrum, leading to the emergence of an eigenvalue quartet through a Hamiltonian–Hopf bifurcation. Note that we do not consider the topological charge.
Figure 8. The imaginary (a) and the real part (b) of the characteristic exponents $\sigma_i$ for the out-of-phase three-site hexagonal configuration for increasing values of $\varepsilon$. The solid lines represent the values obtained numerically, while the dashed ones represent the $O(\sqrt{\varepsilon})$ theoretical prediction. Note the Hamiltonian–Hopf bifurcation at $\varepsilon \simeq 0.014$, leading to the formation of a quartet.

Figure 9. The imaginary part of the characteristic exponents $\sigma_i$ for the vortex three-site hexagonal configuration for increasing values of $\varepsilon$. The solid lines represent the values obtained numerically, while the dashed ones represent the $O(\sqrt{\varepsilon})$ theoretical prediction. Note the numerical splitting of the double pair and the Hamiltonian–Hopf bifurcation inducing collision for $\varepsilon \simeq 0.019$.

$S = 2 (\phi_i = \phi = 4\pi/3)$ configuration in our study. This happens because the $S = 2$ case does not produce any physically distinct motion, instead it provides the same motion as the $S = 1$ case with the reverse rotation direction.

4.2.4. In-phase six-site breather. We now consider six-site breathers. The first configuration we study is the in-phase one ($\phi_i = \phi = 0$). As is already predicted, this configuration is unstable. The corresponding characteristic exponents are shown in figure 10. The solid line represents the value of the exponent which is acquired from the numerical simulation, while the dashed one represents the theoretical prediction acquired from equation (6). Note once again in this case the coincidence (also to higher orders) of the exponents which have been predicted to be double in the leading order of approximation. Although the theoretical estimation of the exponents is the same as in the in-phase honeycomb configuration, their actual value is different because of the different behaviour of the higher order terms.

4.2.5. Out-of-phase six-site breather. The next configuration under consideration is the out-of-phase one ($\phi_i = \phi = \pi$), which is linearly stable for small values of $\varepsilon$. Indeed as shown in
Figure 10. The real part of the characteristic exponents $\sigma_i$ for the in-phase six-site hexagonal configuration for increasing values of $\varepsilon$. The solid lines represent the values obtained numerically, while the dashed ones represent the $O(\sqrt{\varepsilon})$ theoretical prediction.

Figure 11. The imaginary part of the characteristic exponents $\sigma_i$ for the out-of-phase six-site hexagonal configuration for increasing values of $\varepsilon$. The solid lines represent the values obtained numerically, while the dashed ones represent the $O(\sqrt{\varepsilon})$ theoretical prediction. Note the numerical splitting of the double pair and the Hamiltonian–Hopf bifurcation inducing collision for $\varepsilon \approx 0.011$.

4.2.6. $S = 1$, six-site vortex breather. We now consider the charge $S = 1$ vortex configuration ($\phi_i = \phi = \pi/3$), which is anticipated to be linearly unstable, since the theoretical prediction (6) implies that all the exponents will be real in $O(\sqrt{\varepsilon})$. As in the corresponding case in the honeycomb lattice, the symplectic signature arguments do not hold and the exponents, which are predicted to have double real part in leading order of approximation, also have a nonzero imaginary part and split, forming two complex quartets, for $\varepsilon$ arbitrarily small. This behaviour is shown in figure 12. In the left frame the real part of the exponents $\sigma_i$ is shown together with $O(\sqrt{\varepsilon})$. In the right frame the imaginary part of the exponents is shown. Note that there is no theoretical prediction for the imaginary part of the exponents, since this is a higher order effect.

4.2.7. $S = 2$, six-site vortex breather. The last configuration under consideration is the $S = 2$ vortex breather ($\phi_i = \phi = 2\pi/3$) which is linearly stable. Indeed, as shown in figure 13, the
numerical simulation confirmed that the characteristic exponents of the central oscillators are all imaginary; their dependence on $\varepsilon$ is depicted in the figure, together with the corresponding theoretical prediction. Note that, in this case, the higher orders of the characteristic exponents development causes the splitting of those which have double imaginary part up to leading order of approximation.

5. Conclusions

We have studied the existence and stability of multisite discrete breathers in two prototypical examples of non-square two-dimensional lattices. The lattice types under consideration were a honeycomb and a hexagonal one. We have considered six-site contours in the honeycomb lattice and three-site as well as six-site ones in the hexagonal case. We have categorized these solutions in terms of those having zero or nonzero energy flux between their bonds, obtaining, respectively, regular discrete breather as well as vortex breather structures.

Our analysis has offered a systematic analysis of the linear stability of the discrete excitations supported in the prototypical lattices studied. In the honeycomb lattice case we have considered six-site configurations and have shown that, for soft potential and positive coupling,
the out-of-phase breather configuration and the charge-two vortex breather are linearly stable, while the in-phase and charge-one vortex states are unstable. In a hexagonal lattice, and in the case of soft potential and positive coupling, the in-phase three-site configuration is unstable and the charge-one vortex is linearly stable. The out-of-phase three-site configuration here is always unstable, while the stability results for all other configurations in both lattice cases are reversed in the setting of either hard potential or negative coupling (but not both). The stability results in the six-site hexagonal case coincide with the ones acquired in the honeycomb lattice configuration.

Our study was complemented by numerical computations which have been shown to be in very good agreement with theoretical predictions. In order to consider larger amplitude multibreather configurations, we would need a higher order theory which is a natural subject for future investigation. This higher order treatment could also lead us to an improved approximation in the calculation of the characteristic exponents considered herein.

Our results are of relevance in 2D discrete systems characterized by a nonlinear substrate potential, namely including molecular chains as well as dusty plasma (Debye) lattices. Any particular form/type of on-site potential can fit in our description. Finally, we stress that the scope of our formulation includes inverse-dispersive (backward wave supporting) systems, such as transverse oscillations in dusty plasma crystals.

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