Wavelet Analysis of Breather Mode Behavior

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Abstract

Because of its potential to uncover shifting frequencies and phase information, a wavelet transformation may be the ideal tool with which to examine the frequency behavior of various kinds of nonlinear phenomena. We show here some preliminary examples of wavelet analysis of several previously examined discrete breather modes in two different models and various situations.

1. Introduction.

The behaviour of intrinsic localized modes (refered to in many papers as discrete breathers) is now well established (see [1] and references therein for a recent review of the current status of discrete breathers). In the following discussion the frequency content of discrete breathers existing on single and double mass chains of various lengths with different coupling were analyzed. The simulations were performed using a fifth order Runga-Kutta method with an energy conservation of better than 0.001% . Wavelet transforms were performed on the amplitude oscillations of the maximum energy site(s) on the chain as these oscillations evolved in time, using the continuous wavelet transform of Grossman and Morlet. For a function f on the line, this is defined by

$$Wf(t,\xi) = \int_{-\infty}^{\infty} f(x) w(\xi(x-t))\xi \, dx, \tag{1.1}$$

where $w(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{i2\pi x}\, e^{-x^2/2\sigma^2}$. The transform $Wf(t,\xi)$ gives information about the energy content of the signal f at time t and frequency ξ. In this paper we give spectrograms which are plottings of $|Wf(t,\xi)|$ for (typically) $0 \leq t \leq 72$ sec and $1 \leq \xi \leq 3$ Hz; the wavelet variance σ is typically chosen to be aproximately 8 sec. The spectrograms are rendered as density plottings; the density is always arbitrarily scaled to fit the available range of intensity values. Also the vertical scale is logarithmic, to show equal octaves of frequency equally spaced.

The underlying idea of the wavelet transform is similar to that of the "windowed" Fourier transform defined by

$$T_g(t,\xi) = \int_{-\infty}^{\infty} f(x) g(x-t) e^{i2\pi\xi x} \, dx;$$

this is the Fourier transform with a window function g inserted, which limits the calculation of frequency to an interval of time around time t. (The window function g can be chosen to be a Gaussian, which results in a Gabor transform.) The wavelet transform differs from this transform in that the "window" changes width as the frequency ξ is changed: for high frequencies, the window is narrow (which will catch rapid changes in frequency better); for low frequencies, the window is wider (which localizes frequency better, since more cycles of the complex exponential are visible in the integral). Thus the continuous wavelet transform is well-suited for localizing frequency and for localizing time; the windowed Fourier transform can often localize one well but not the other.

There is a limitation to how well time and frequency can both be localized with this method; in fact, this is the uncertainty principle, the mathematical form of which states that a function and its Fourier transform cannot both have small support. This limitation manifests itself in our renderings as a trade-off between how "blurry" the image is vertically (i.e., localization of frequency), and how blurry the image is horizontally (i.e., localization of time).

It should be noted that there are many variations in wavelet construction and application; often discrete wavelet transforms are used instead of continuous transforms. This amounts to computing $W(t,\xi)$ for a discrete set of (t,ξ) (often only ξ equal to powers of two are considered). The advantages of discrete wavelet transforms often include fast algorithms; here we use the continuous transform because we desire complete information about frequency as well as time. A good mathematical reference is Holschneider [2]. There is a large literature on wavelet analysis; see the Wavelet Digest [3] for bibliographies and other current information about this field.

In order to give an indication of the sensitivity of this method we show in Fig. 1, a wavelet analysis of an artificial test signal consisting of a superposition of two cosine terms about 1 Hz apart, one of which is slowing changing. The upper line shows a frequency shift of approximately 1% as can be seen from the white reference line.

2. Examples with single chains.

In a previous work [4] the behavior of a breather mode on a single chain of 100 atoms with a 2-3 on-site potential has been discussed with a Hamiltonian given by

$$H = \sum_n \left[\frac{1}{2}\dot{u}_n^2 + \frac{1}{2}k(u_n - u_{n-1})^2 + V(u_n) \right] , \tag{2.1}$$

where the potential is

$$V(u_n) = \omega_0^2 \left(\frac{u_n^2}{2} - \frac{u_n^3}{3} \right) . \tag{2.2}$$

In these expressions, the position of particle n is written as a dimensionless variable u_n; time and space have been scaled to have a unit mass for the particles. The parameter ω_0 measures the relative scale of the on-site potential and of the coupling energy. The simulations shown here have been performed with $\omega_0 = 2.2$ which is a moderately discrete case so that the breathers investigated here are localized on a few lattice sites, but are not completely trapped by the pinning potential due to the lattice.

The linear dispersion relation for this Hamiltonian is given by

$$\omega^2 = \omega_0^2 + 4k\sin^2(q/2) \tag{2.3}$$

where q is the linear wave vector and the lattice spacing is taken to be unity. As can be seen from the dispersion relation there is a gap below ω_0 in which there is the potential for stable discrete breathers to exist, providing they don't have a multiple of their frequency lying in the linear phonon band.

Approximate breather solutions can be found using a semi-discrete method and were used in the following as initial conditions . Input parameters for these solutions are the envelope velocity u_e and the amplitude A' (see [4] for details).

In [4] the results of the interaction of these moving breather with an excited mass impurity mode were examined. Breathers may reflect, pass through or be trapped by an excited impurity. It was suggested in that paper that both the frequencies of the breather and impurity mode and the relative phase have an effect on whether the breather is trapped, reflected or passes through. Here we examine the frequency shifts of the breather and a defect in the case of three identical breathers colliding with three identical excited impurity modes but starting the breathers at different distances. Parameter choices were initial breather amplitude of $A' = 0.28$ with speed $u_e = 0.2$ and an impurity mode amplitude of 0.1 and impurity mass of 1.05 times the non-defect mass. These parameters result in a frequency difference of about 0.03 Hz between the impurity mode and the breather in all three cases, initially. Starting the breather at different distances has the effect of changing the relative phase between the breather and impurity oscillations at the time of collision which changes drastically the outcome of the event.

In Fig. 2 we show the outcome of a collision where the breather starts at a distance of 20 sites away from the defect. Fig. 2a shows an energy contour plot of the collision as a function of time. In this case the breather (starting at location 70) collides with the impurity mode (at site 50) and is trapped (a longer simulation shows this trapped state to be quite stable). A wavelet analysis was preformed on the breather location as it moved towards the impurity and is shown in Fig. 2b. The bottom of the phonon band is shown in these figures by a line at at $\omega = 2.2$. Fig. 2c shows a wavelet analysis on the defect location. After the trapping the final state of breather plus impurity mode has shifted frequency to a lower frequency indicating a larger amplitude. The periodic spots on the spectrogram occuring after trapping indicate the presence of a second frequency of low amplitude very close to the new trapped breather frequency. These oscillations indicate that the trapped breather has new internal frequencies and so is not as stable as the breather before trapping.

In Fig. 3 we show the outcome of a collision where the breather starts at a distance of 21 sites away from the defect. As can be seen from the energy contour plot (Fig. 3a), this collision results in the breather passing through the impurity mode (longer simulations show the breather gradually leaving the defect site). The wavelet frequency analysis of the breather (Fig. 3b) shows that the frequency of the breather has shifted downward slightly, again indicating a gain of amplitude. A wavelet analysis starting at the defect and following the maximum energy site (Fig. 3c) shows that dring the collision a large number of freqencies are present, some of which are in the phonon band. The defect energy is no longer large enough to appear on the energy countour picture and the wavelet analysis in Fig. 3c follows the breather at times after the collision.

In Fig. 4 we show the outcome of a collision where the breather starts at a distance of 23 sites away from the defect. As can be seen, this collision results in the breather bouncing off of the impurity mode (Fig. 4a). The wavelet frequency analysis of the breather (Fig. 4b) shows that the effect of the collision raises the breather frequency slightly indicating a *loss* of energy. As can be seen from the energy contour, the breather has pushed the energy of the impurity mode off the impurity creating a second, smaller breather (this was not noted in [4]). A wavelet analysis was also preformed starting on the impurity site (Fig. 4c) and following the new breather as it leaves the impurity site. This figure shows this new breather has a slightly higher frequency than the original impurity mode.

Because the trapping/passing/reflection behaviour was seen in [4] for even further distances (for example launching at a distance of 24 sites away resulted in trapping again) it was postulated that the outcome (trapping, reflection, or passing) was primarily the result of the relative phase of the breather and impurity mode (assuming the frequenices were relatively close). It should be noted, however, that during the collision process the wavelent analysis shows different frequency behavior in the three cases. All three cases show frequencies in the phonon band during collision but in the trapping and passing cases there is a wide range of additional frequencies present during and after the collisions. In these two cases the defect site shows many new frequencies below (and above) the breather frequency and the breather after the collision shows new internal frequencies. In the case where the breather bounces off the impurity, however, relatively few additional frequencies appear during collision and there are no new internal frequencies after collision indicating a more stable outcome. The existence of these additional frequencies in some collisions may provide additional channels of interaction and indicate a rich phenomenology of the internal motions of the breather and impurity mode in these cases. This complicated frequency behavior is currently under investigation.

The collision of two breathers in this and similar models has been examined in a number of works (see [6] and [7] for example). It is known to be the case that a larger amplitude breather will take energy from a smaller breather on average during a collision. We show a wavelet analysis of the collision of two breathers with the same parameters as above but instead of an impurity mode, a second breather of amplitude $A' = 0.26$ is launched at the center of the chain with $u_e = 0.0$. As can be seen from the spectrograms, the frequency of the larger breather (Fig. 5b) shows a smaller range of frequencies during the collision than the smaller breather (Fig. 5c). The larger breather's frequency does not change much as a result of this interaction but the smaller breather's frequency shifts upward slightly, indicating a loss of energy. The significance of the larger frequency spread for the smaller breather during collision is not understood at present but it can be speculated that the result of such a frequency spread is a greater likelihood of energy sharing (via resonance interaction) with other oscillating objects (i.e. the larger breather).

The time evolution of modulational instability in this system has been investigated in [8]. We show here an example of the frequency shifts occuring during amplitude modulation. Fig. 6 shows a wavelet analysis of the evolution of a site on a chain with an initial (slightly perturbed) sine wave. A maximum energy site was chosen on the chain and a wavelet analysis of the evolution of the oscillations performed. After an interim state containing many frequencies this site became a localized breather mode. A second shift in frequency is seen later indicating further trapping of energy. These effects are further investigated in [9]. Figures from [9] and a quicktime movie of the spacial frequency shifts for a chaing with 600 points occurring during energy localization due to modulational instability can be found at

`Http://Physics.ius.indiana.edu/TalksPapers/Wavelet2/WaveletPics2.html`

3. Examples with double chains.

In a previous work [10] the behavior of a breather mode on a double chain of atoms linearly connected along their length with an inter-chain Morse potential has been discussed. The Hamiltonian for that model is given by given by

$$H = \sum_n \frac{1}{2}\left[\left(\frac{du_n}{dt'}\right)^2 + \left(\frac{dv_n}{dt'}\right)^2\right] + \frac{1}{2}k(u_{n+1} - u_n)^2 + \frac{1}{2}k'(v_{n+1} - v_n)^2 + D\left[\exp[-(u_n - v_n)] - 1\right]^2 \quad (3.1)$$

with k and k' the (scaled) upper and lower linear coupling (respectively) and u_n and v_n the upper and lower displacements from equilibrium (respectively). The dispersion relations of the small amplitude waves of frequency ω and wavevector q are given by

$$\omega^2 = 2(1 + 2K_+ \sin^2 \frac{q}{2}) \pm 2\sqrt{1 + 4K_-^2 \sin^4 \frac{q}{2}} \quad (3.2)$$

where the + sign corresponds to the optical branch and the − sign corresponds to the acoustic branch.

Exact stationary numerical solutions (using the the anti-continuum limit) and approximate analytical solutions (using the semi-discrete method) can be found for this model after a substitution of variables (see [10] for details). The existence of solutions does not, however, guarantee their stability. If harmonics of the breather freqency lie in or close to the linear phonon band the solutions will not be stable. Fig. 7a shows a wavelet analysis of the exact numerical solutions derived by the anti-continuum limit in a region of parameter space where the breather is expected to be stable ($k = 0.7$, $k' = 0.5$ and breather frequency $\omega_b = 1.95$). The bottom of the optical band at 2 Hz and top of the accoustic band at 1.54 are show by lines in the figure. Fig. 7b shows a wavelet frequency analysis of the central molecule in an approximate analytic solution given by the semi-descrete method in a region of stable parameter space ($k = 0.7$, $k' = 0.5$ and breather amplitude $A' = 0.5$). Clearly the approximate solution is less stable and has additional internal frequencies. Frequencies of an exact solution with parameters $k = 0.7$, $k' = 0.5$ and frequency $\omega_b = 1.5$ which is unstable because of harmonics lying in the phonon band is shown in Fig. 7c. An energy profile of this case gives no indication of the lack of stability of the solution whereas the wavelet transform clearly shows a frequency shift and extra internal frequencies, indicating an unstable solution.

The model shown in equation 3.1 was constructed to investigate the behavior of energy localization in a double chain model of DNA. It is thought that bending plays a role in local opening of DNA during the transcription process. Bending can be simulated in this model by changing the linear coupling parameters

k and k' relative to each other. It was found previously that local bending (where $k \neq k'$ in a region of the chain) could reflect, trap or pass a breather. In Fig. 8a we show the energy contour plot of an breather temporarily trapped in a region of bending. Here $k = k' = 0.6$ except between sites 100 and 120 where k gradually changes to 0.1 and k' gradually changes to 1.1 and back. As can be seen from the wavelet spectrogram (Fig. 8b) the frequency shifts upward while in the bent region. It can also be seen that the final state is quite stable but during entry into the bent region frequenies show up in the phonon band, indicating a slight loss in energy during the transition into the bent region. The significance of these kinds of frequency shifts for trapping of breathers in regions where the chain has a bend is under investigation.

4. Conclusions.

We have given here some preliminary results which show the utility of applying a wavelet transform to analyze the frequency of discrete breather modes in various mass chain models. Clearly new information about stability and the frequency content of breather modes interacting with impurities, other breathers and site dependent changes in the lattice structure is available using this technique. While the current work is still at a preliminary stage, we feel the examples given in this paper demonstrate the potential of the wavelet method for revealing the dynamics of nonlinear behaviour in discrete systems.

References

[1] S. Flach and C.R. Willis, "Discrete Breathers," to be published in Physics Reports (1997).

[2] M. Holschneider, Wavelets, An Analysis Tool (Clarendon Press, Oxford, 1995).

[3] The URL of the Wavelet Digest is `http://www.wavelet.org/wavelet/index.html`.

[4] K. Forinash, M. Peyrard and B. Malomed, Phys. Rev. B 49 (1994) 3400.

[6] T. Dauxois, M. Peyrard and C.R. Willis, Physica D 57 (1992) 267.

[6]2 T. Dauxois, M. Peyrard, and C. R. Willis; Phys. Rev. E 48 (1993) 4768 .

[7] O. Bang and M. Peyrard; Phys. Rev. E 53 (1996) 4143.

[8] Y.S. Kivshar, M. Peyrard, Phys. Rev. A 46 (1992) 3198.

[9] K. Forinash, C. Lang ; Frequency Analysis of Discrete Breather Modes Using a Continuous Wavelet Transform', submitted to Physica D.

[10] K. Forinash, T. Cretegny and M. Peyrard; Phys. Rev. E 55 (1997) 4740.

Figure Captions

Fig. 1: Wavelet analysis of a test signal with a superposition of two cosine terms about 1 Hz apart, the higher of which shifts by about 1% during the time shown.

Fig. 2: Contour energy plot (a) and wavelet analysis (b, c) of a breather trapped on an excited mass defect in a single chain. Spectrogram (b) shows the frequency of the larger breather, picture (c) shows the defect frequency.

Fig. 3: Contour energy plot (a) and wavelet analysis (b, c) of a breather passing through an excited mass defect (located at site 50) in a single chain. Wavelet picture (b) is of the larger breather, picture (c) is

the defect mode but follows the breather after collision.

Fig. 4: Contour energy plot (a) and wavelet analysis (b, c) of a breather reflecting from an excited mass defect in a single chain. Spectrogram (b) is of the larger breather, picture (c) is the defect before the collsion and follows the new breather after collision.

Fig. 5: Contour energy plot (a) and wavelet analysis (b, c) of a two breather collision in a single chain. Wavelet picture (b) is of the larger breather, picture (c) is the smaller breather.

Fig. 6: Wavelet analysis of a region undergoing modulational instability on a single chain. Intial conditions were a perturbed sine wave and the analysis was performed on a location of largest energy as it evolved.

Fig. 7: Wavelet analysis of the stability of (a) exact numerical solutions in stable parameter space, (b) approximate breather solutions in stable parameter space and (c) exact numerical breather in unstable parameter space on a two chain model.

Fig. 8: Contour energy plot (a) and wavelet analysis (b) of a breather reflecting from a bend (differing k and k') in a two chain model. The bend is located between sites 100 and 120.