



# Existence and Stability of Localized Structures in Hexagonal and Honeycomb Lattices

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In collaboration with: P.G.Kevrekidis, K.J.H.Law, I.Kourakis, D.J.Frantzeskakis,  
A.R.Bishop, R.S.MacKay

# Overview

- Definition of the Hexagonal and Honeycomb lattices

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  - Analytical results
  - Numerical results
  - Comparison of analytics with numerics

# Description of an oscillator-Terminology

An oscillator is described by a one degree of freedom Hamiltonian, with  $V'(0) = 0$  and  $V''(0) = \omega_p^2$ :

$$H = \frac{p^2}{2} + V(x)$$



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The action-angle variables are defined:

$$\begin{aligned} \dot{w} &= \omega \\ \dot{J} &= 0 \end{aligned} \rightarrow \begin{cases} w = \omega t + \vartheta \\ J = \text{const.} \end{cases}$$

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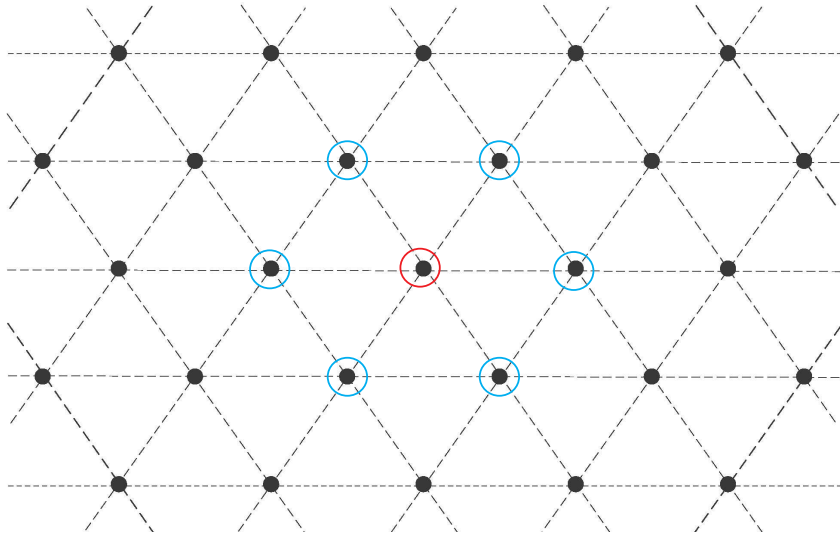
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Due to the symmetry:

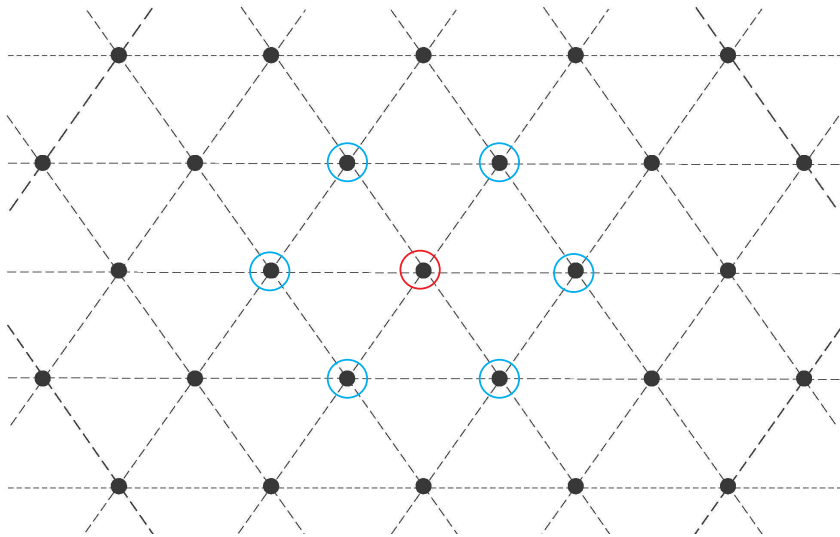
$$\begin{aligned} x(-t) &= x(t) \\ p(-t) &= -p(t) \end{aligned} \rightarrow x(t) = \sum_{n=0}^{\infty} A_n(J) \cos(nw)$$

# The Hexagonal Lattice



Each site has 6 neighbors

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Each site has **6** neighbors

The sites are coupled through  $\varepsilon$

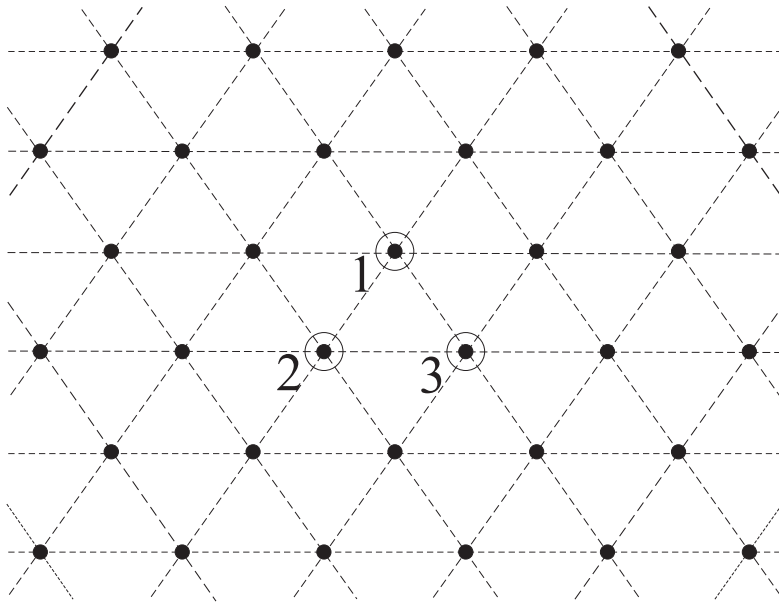
$\mathbb{S}$  is the set of sites

$\mathbb{G}_i$  is the set of neighbors of site  $i$

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

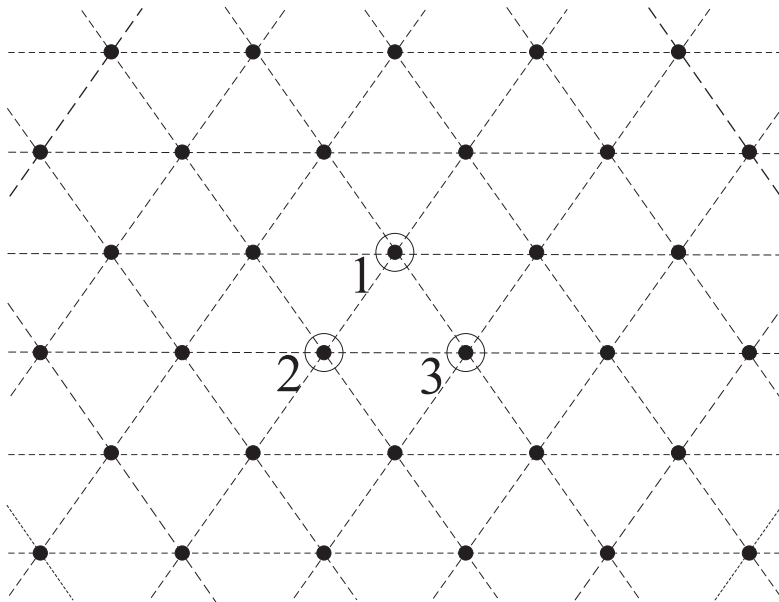
$$\ddot{x}_i = -V'(x_i) - \varepsilon \left( \sum_{j \in \mathbb{G}_i} x_j - \mathbf{6}x_i \right)$$

# Hexagonal Lattice-Anticontinuous Limit



In the anticontinuous limit  $\varepsilon = 0$  we consider 3 oscillators moving in periodic orbits with frequency  $\omega$ .

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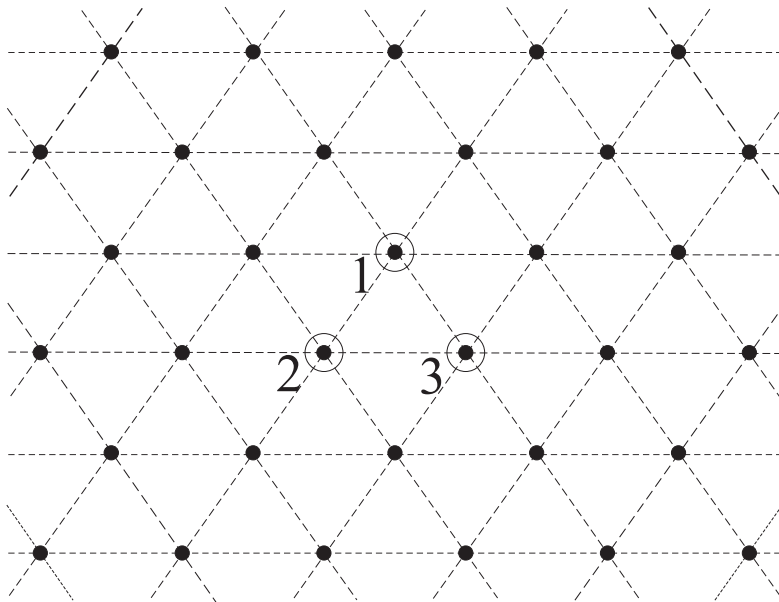
This motion is continued for  $\varepsilon \neq 0$  to a **3-site breather** if:

*VK and R.S.MacKay(2005)*

$$\frac{\partial \langle H_1 \rangle}{\partial \phi_i} = 0, \quad \frac{\partial^2 \langle H_1 \rangle}{\partial \phi_i \partial \phi_j} \neq 0, \quad \omega_p \neq m\omega, \quad \frac{d\omega}{dJ} \neq 0$$

where  $\langle H_1 \rangle = \oint H_1 dt$  and  $\phi_i = w_{i+1} - w_i$

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**Only 2 independent  $\phi_i$ :**  $\phi_1 = w_2 - w_1, \phi_2 = w_3 - w_2$



# Persistence condition for 3-site breathers

Using the previous terminology, the persistence condition becomes

$$\sin(n\phi_i) + \sin[n(\phi_1 + \phi_2)] = 0, \quad i = 1, 2 \quad n \in \mathbb{N}$$

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$\phi_{1,2} = 0 \quad \rightarrow \quad \text{in-phase tree-site breather}$

$\phi_{1,2} = \pi \quad \rightarrow \quad \text{out of phase tree-site breather}$

$\phi_{1,2} = \frac{2\pi}{3} \quad \rightarrow \quad \text{vortex breather}$

# Linear stability of a breather

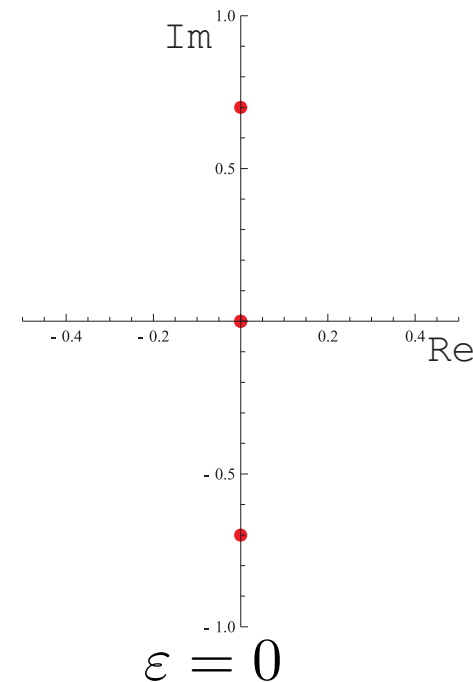
The **characteristic exponents**  $\sigma_i$  of the breather, which are related to the **Floquet multipliers**  $\lambda_i$  of the corresponding periodic orbit as  $\lambda_i = e^{\sigma_i T}$ . For linear stability **all**  $\sigma_i$  must lie in the imaginary axis.

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for  $\varepsilon = 0$  the exponents are concentrated in 3 bulks

- 3 pairs at unity
- all the rest in 2 bulks at  $\pm e^{\omega_p T}$

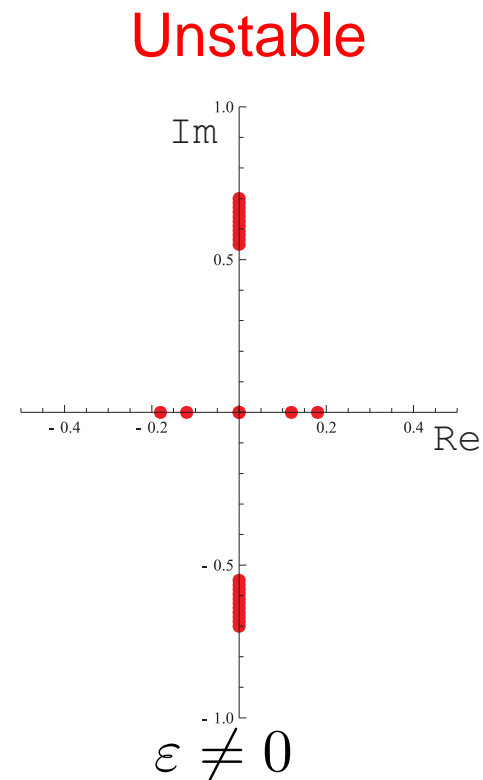


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for  $\varepsilon \neq 0$

- the **phonon band** is generated
- **two** pairs of exponents leave along the real axis

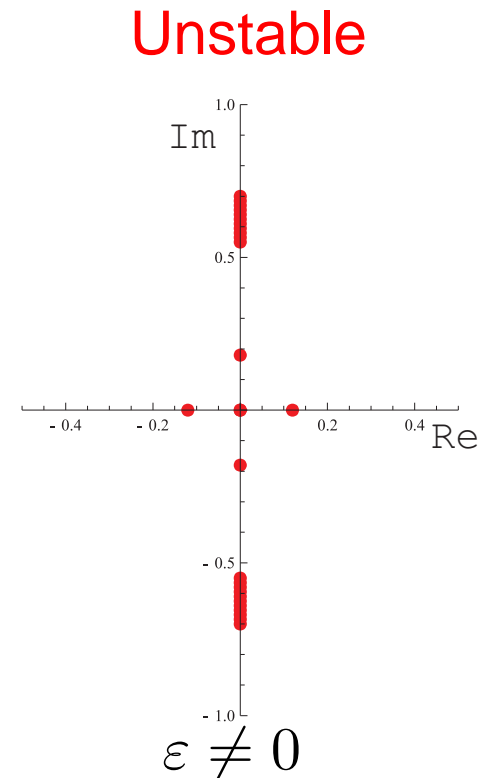


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for  $\varepsilon \neq 0$

- the **phonon band** is generated
- **one** pair of exponents leave along the real axis



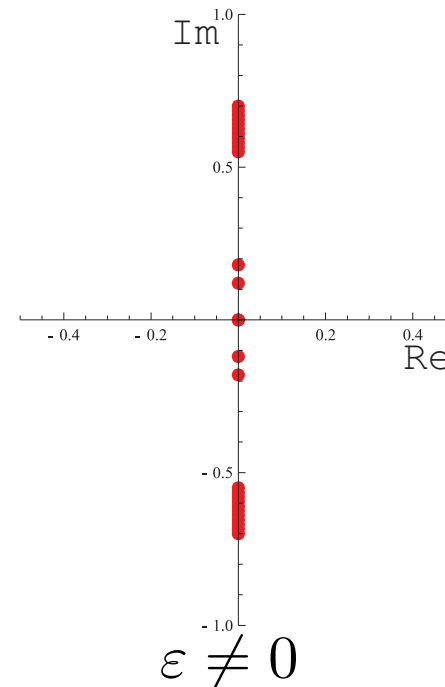
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Stable

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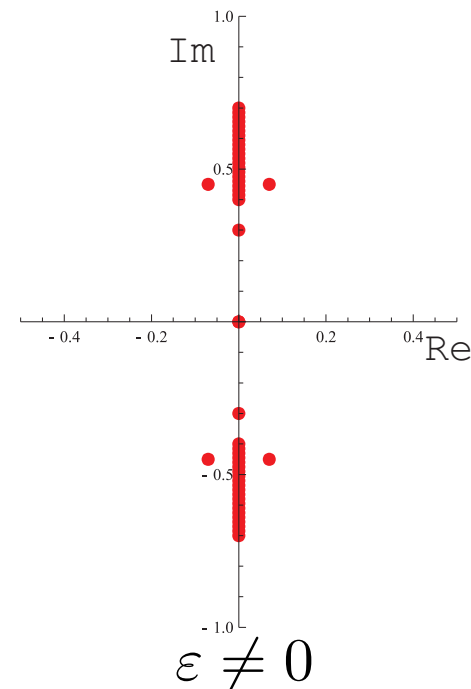
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The configuration remains stable until they collide with the phonon band for

$$\varepsilon = \varepsilon_{cr}$$

Unstable





# Stability in the hexagonal lattice

The  $\sigma_i$  are given up to leading order of approximation as eigenvalues of  $E = D^2 J H^{\text{eff}}$ , with  $H^{\text{eff}} = H_0 + \varepsilon \langle H_1 \rangle$  and

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$$\phi_i = 0 \quad \rightarrow \quad \sigma_i = \pm \sqrt{-3\varepsilon \frac{d\omega}{dJ} f(0)}$$

$$\phi_i = \pi \quad \rightarrow \quad \sigma_i = \begin{cases} \pm \sqrt{-\varepsilon \frac{d\omega}{dJ} (2f(0) + f(\pi))} \\ \pm \sqrt{-\varepsilon \frac{d\omega}{dJ} f(\pi)} \end{cases}$$

$$\phi_i = 2\pi/3 \quad \rightarrow \quad \sigma_i = \pm \sqrt{-3\varepsilon \frac{d\omega}{dJ} f(2\pi/3)}$$

# Stability for a specific example

For:  $\varepsilon > 0$  and  $V(x) = \frac{x^2}{2} - 0.27\frac{x^3}{3} - 0.03\frac{x^4}{4} \rightarrow \frac{d\omega}{dJ} < 0$

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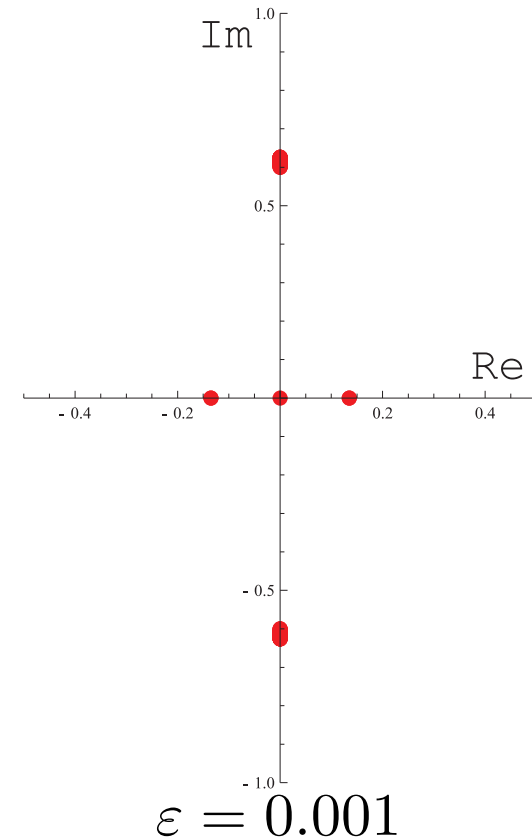
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In phase :  $\phi_i = 0$

$$f(0) = \sum_{n=1}^{\infty} n^2 A_n^2 > 0$$

$$\sigma_i = \sqrt{-3\varepsilon \frac{d\omega}{dJ} f(0)} \in \mathbb{R}$$

Unstable



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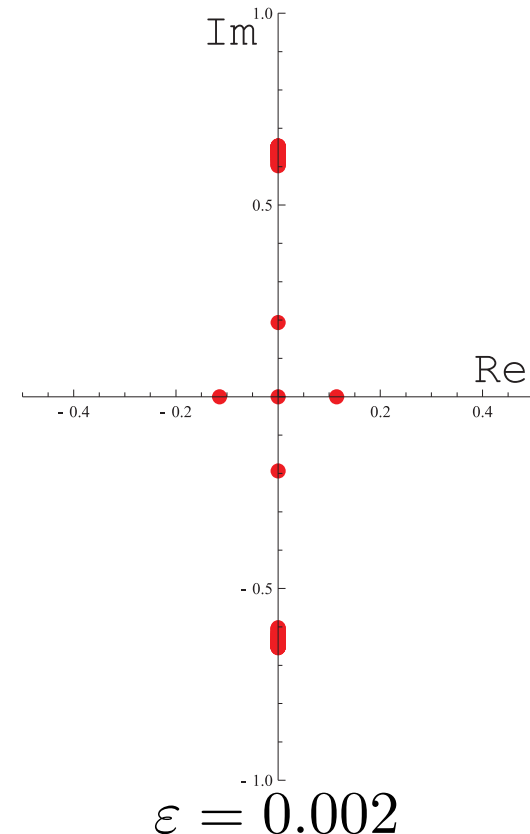
$$f(\pi) = \sum_{n=1}^{\infty} (-1)^n n^2 A_n^2 < 0$$

$$2f(0) + f(\pi) > 0$$

$$\sigma_{1,2} = \sqrt{-\varepsilon \frac{d\omega}{dJ} f(\pi)} \in \mathbb{I}$$

$$\sigma_{3,4} = \sqrt{-\varepsilon \frac{d\omega}{dJ} (2f(0) + f(\pi))} \in \mathbb{R}$$

Unstable



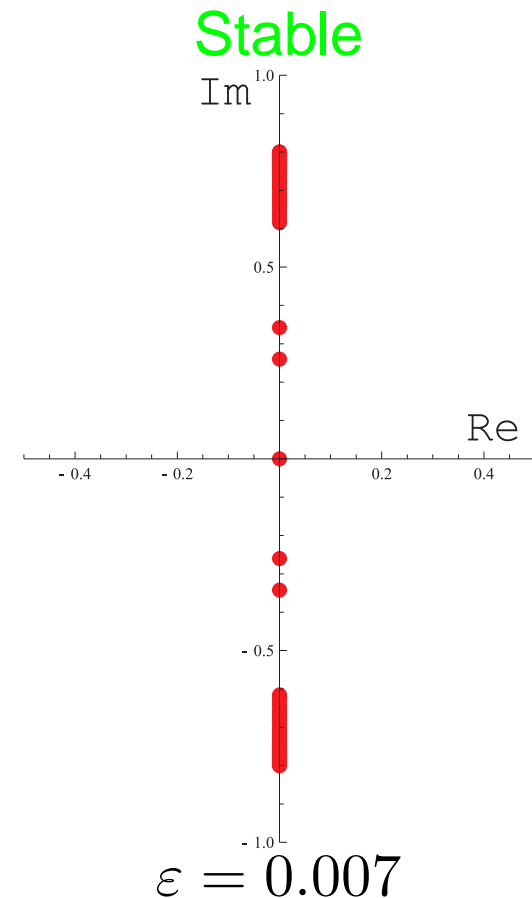
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**Vortex** :  $\phi_i = 2\pi/3$

$$f(2\pi/3) = \sum_{n=1}^{\infty} (-1)^n n^2 A_n^2 \cos(\pi/3) < 0$$

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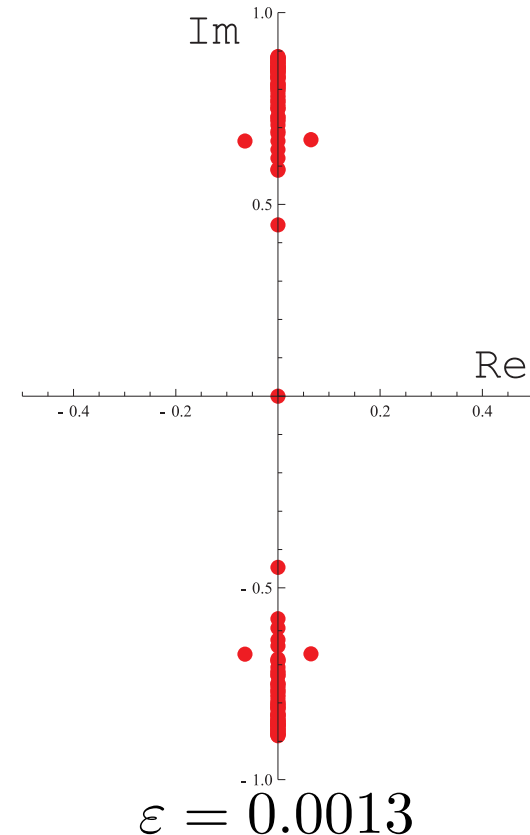
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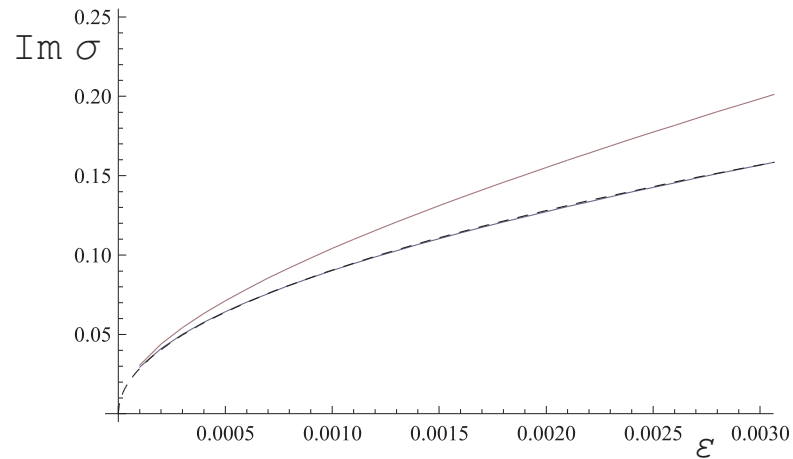
**Unstable**





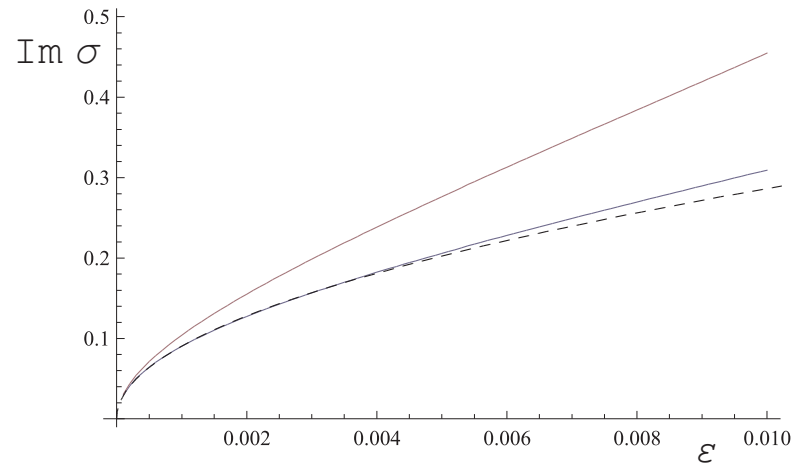
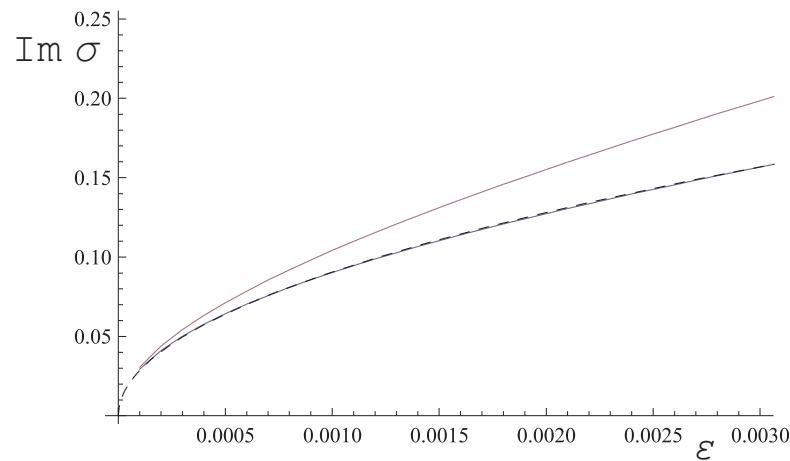
# Prediction vs Numerics

We draw our  $O(\sqrt{\varepsilon})$  prediction together with the numerical results



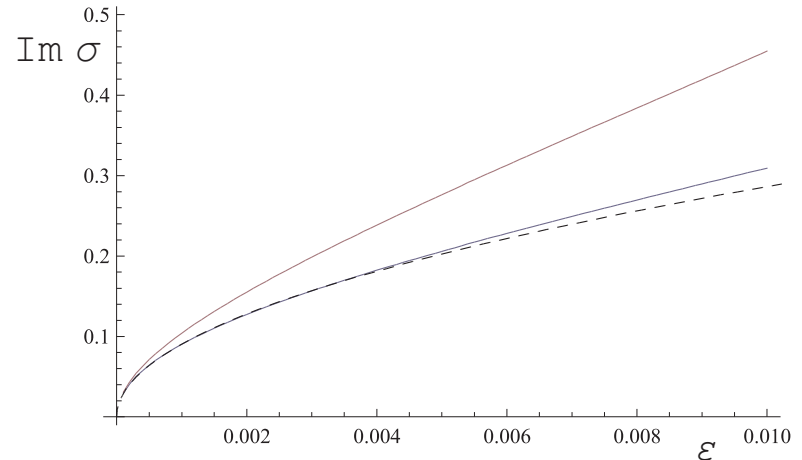
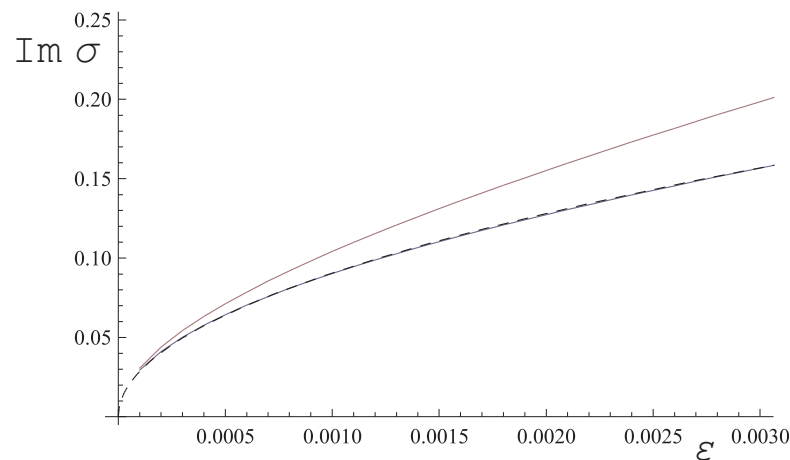
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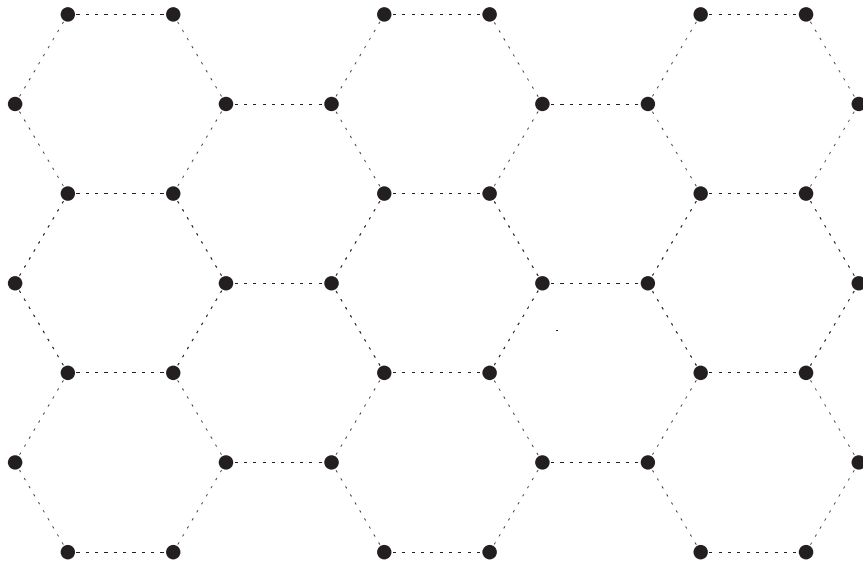
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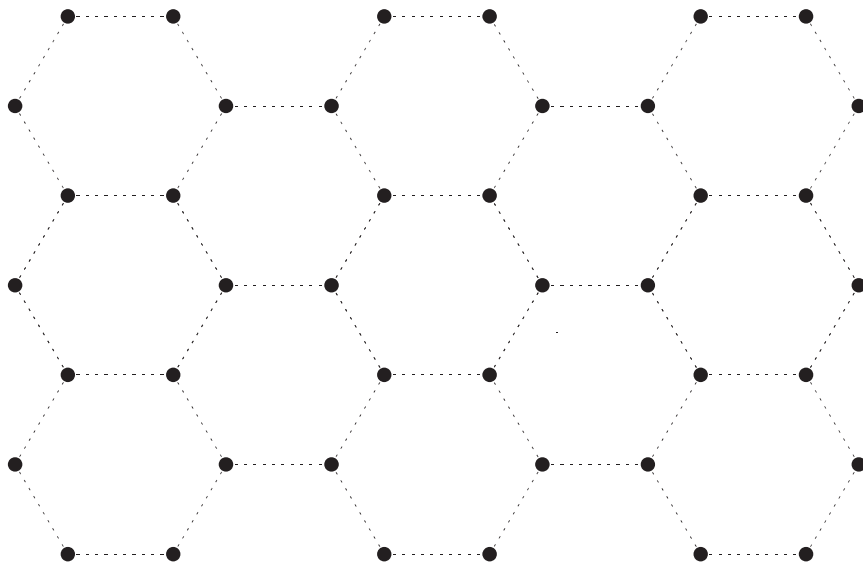
$O(\varepsilon)$  result would be useful! (Upcoming work with E.Meletlidou)

# The Honeycomb lattice



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The sites are coupled through  $\varepsilon$

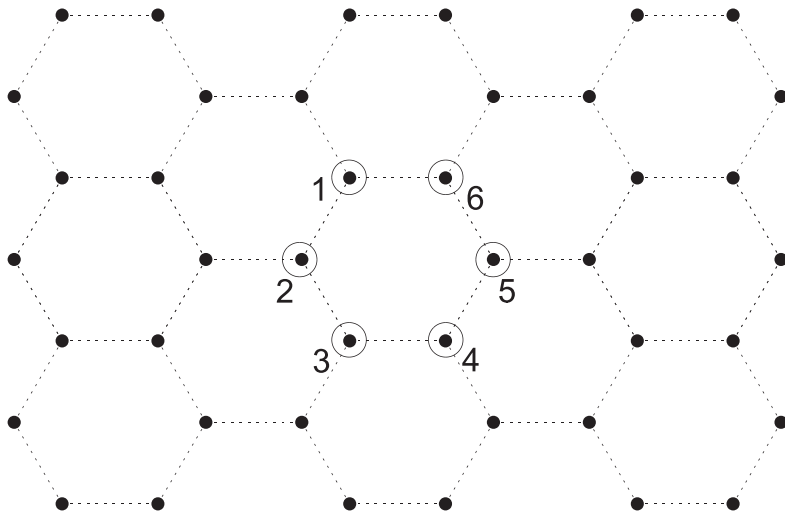
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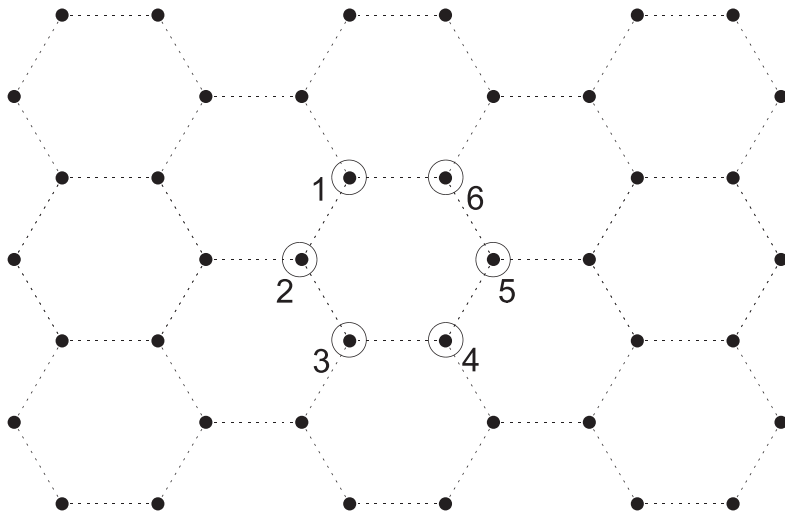
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In the anticontinuous limit  $\varepsilon = 0$  we consider 6 oscillators moving in periodic orbits with frequency  $\omega$ .

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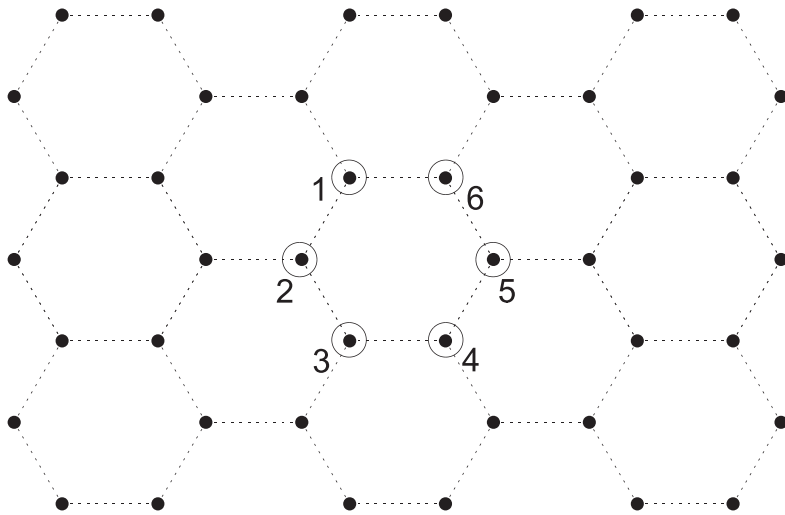
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This motion is continued for  $\varepsilon \neq 0$  to a **6-site breather** if:

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where  $\langle H_1 \rangle = \oint H_1 dt$  and  $\phi_i = w_{i+1} - w_i$

**5 independent  $\phi_i$ :**  $\phi_1 = w_2 - w_1$ ,  $\phi_2 = w_3 - w_2$ ,  $\phi_3 = w_4 - w_3$   
 $\phi_4 = w_5 - w_4$ ,  $\phi_5 = w_6 - w_5$



# Persistence conditions for 6-site breathers

The persistence conditions in this case become

VK, P.G.Kevrekidis, K.J.H.Law, I.Kourakis, D.J.Frantzeskakis, A.R.Bishop (In preparation)

$$\sin(n\phi_i) + \sin[n(\phi_1 + \phi_2 + \phi_3 + \phi_4 + \phi_5)] = 0, i \in 1..5, n \in \mathbb{N}$$

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Two groups of solutions:

The **6-site breathers**

$$\phi_i = 0, \pi \quad i = 1..5$$

The **vortex** breathers

$$\phi_i = s \frac{\pi}{3} \quad i = 1..5 \quad s \in \mathbb{N}$$

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$$\phi_i = 0 \quad \rightarrow \quad \text{in phase 6-breather}$$

$$\phi_i = \pi \quad \rightarrow \quad \text{out of phase 6-breather}$$

$$\phi_i = \frac{\pi}{3} \quad \rightarrow \quad \text{charge 1 vortex breather}$$

$$\phi_i = \frac{2\pi}{3} \quad \rightarrow \quad \text{charge 2 vortex breather}$$

# Stability in the Honeycomb lattice

Using again:

$$f(\phi) = \frac{1}{2} \sum_{n=1}^{\infty} n^2 A_n^2 \cos(n\phi)$$

$$\sigma_i = \begin{cases} \pm \sqrt{-\varepsilon \frac{d\omega}{dJ} f(\phi)} & i \in 1..4 \\ \pm \sqrt{3} \sqrt{-\varepsilon \frac{d\omega}{dJ} f(\phi)} & i \in 5..8 \\ \pm 2 \sqrt{-\varepsilon \frac{d\omega}{dJ} f(\phi)} & i \in 9, 10 \end{cases}$$

# Stability for a specific example

For:  $\varepsilon > 0$  and  $V(x) = \frac{x^2}{2} - 0.27\frac{x^3}{3} - 0.03\frac{x^4}{4} \rightarrow \frac{d\omega}{dJ} < 0$

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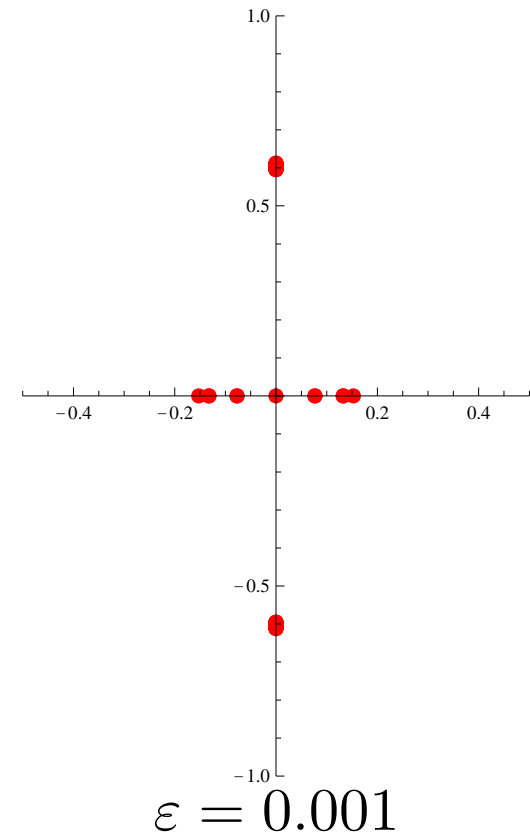
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In phase :  $\phi_i = 0$

$$f(0) = \sum_{n=1}^{\infty} n^2 A_n^2 > 0$$

$$\sqrt{-\varepsilon \frac{d\omega}{dJ} f(0)} \in \mathbb{R}$$

Unstable



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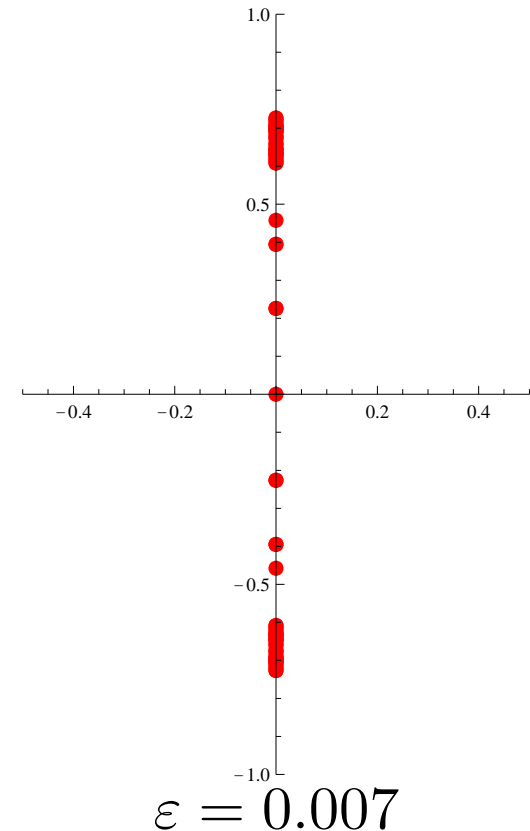
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Out of phase :  $\phi_i = \pi$

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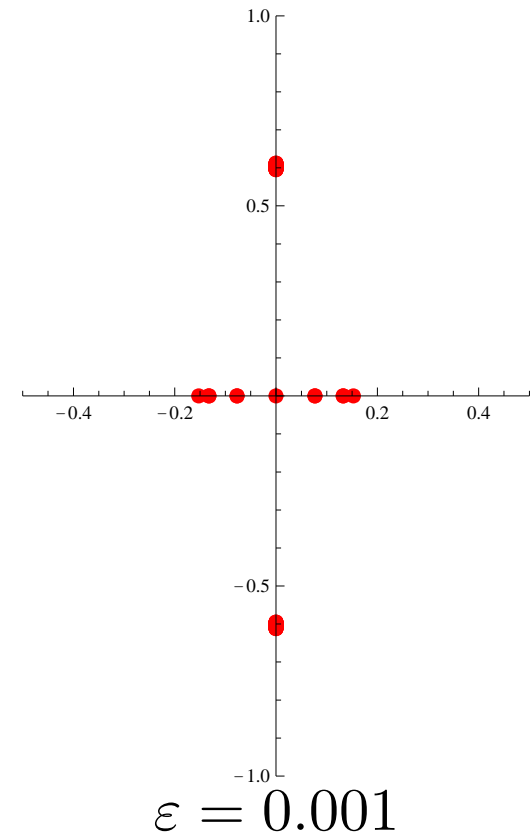
For:  $\varepsilon > 0$  and  $V(x) = \frac{x^2}{2} - 0.27\frac{x^3}{3} - 0.03\frac{x^4}{4} \rightarrow \frac{d\omega}{dJ} < 0$

Charge 1 Vortex :  $\phi_i = \pi/3$

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

$$\sqrt{-\varepsilon \frac{d\omega}{dJ} f\left(\frac{\pi}{3}\right)} \in \mathbb{R}$$

Unstable





# Stability for a specific example

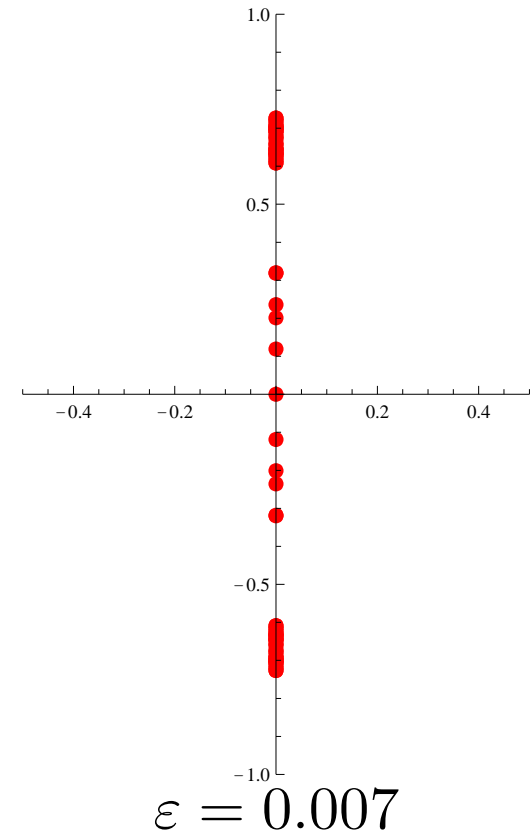
For:  $\varepsilon > 0$  and  $V(x) = \frac{x^2}{2} - 0.27\frac{x^3}{3} - 0.03\frac{x^4}{4} \rightarrow \frac{d\omega}{dJ} < 0$

**Charge 2 Vortex** :  $\phi_i = 2\pi/3$

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

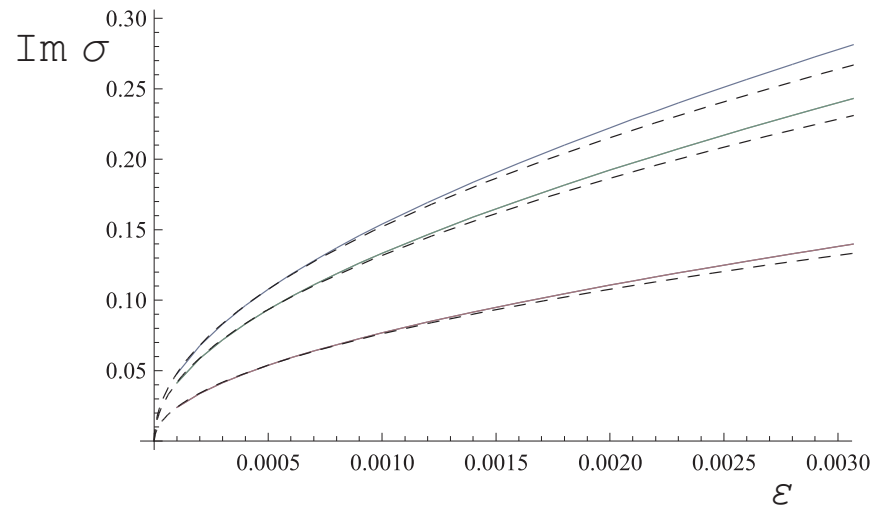
$$\sqrt{-\varepsilon \frac{d\omega}{dJ} f\left(\frac{2\pi}{3}\right)} \in \mathbb{I}$$

Stable



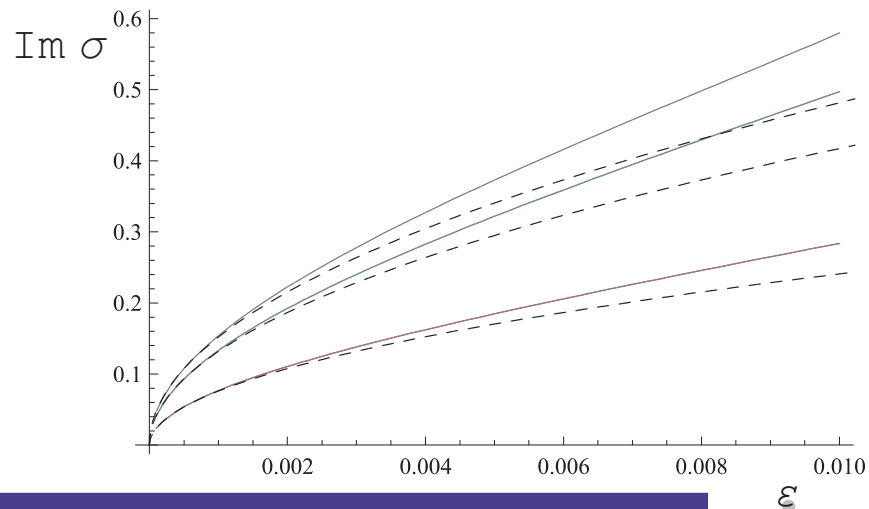
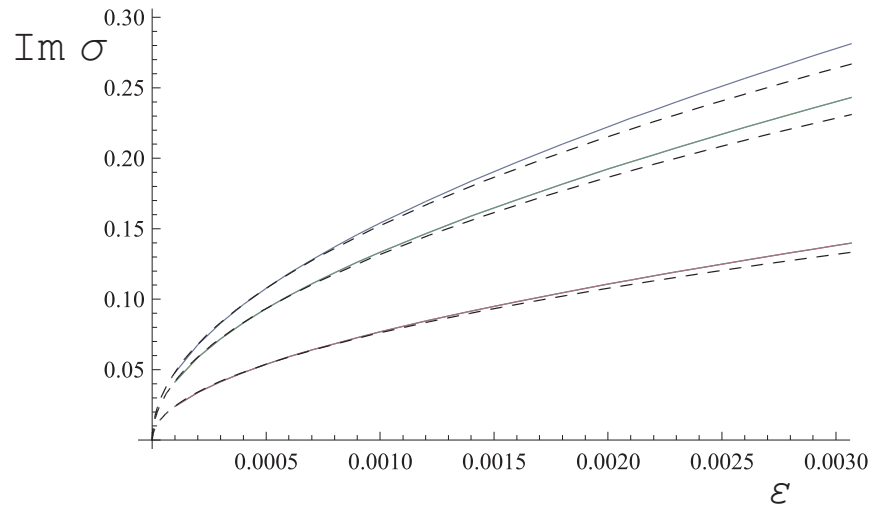
# Prediction vs Numerics

Out of phase



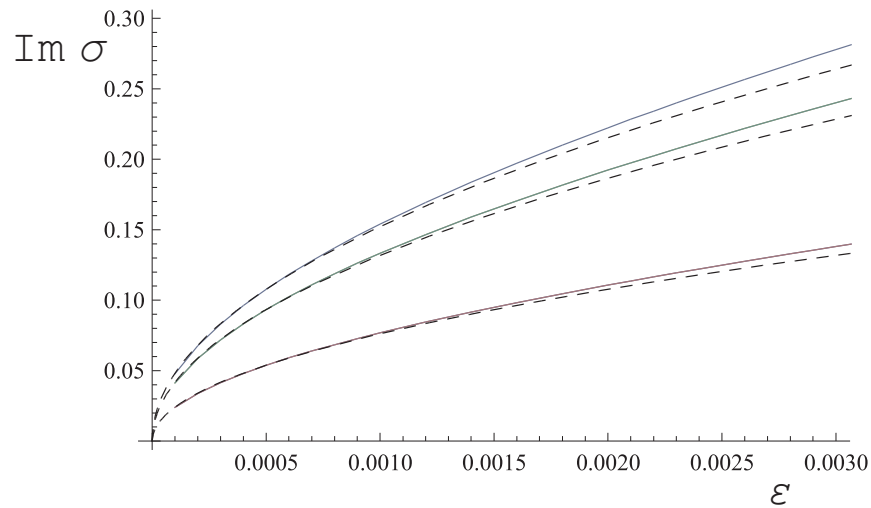
# Prediction vs Numerics

Out of phase

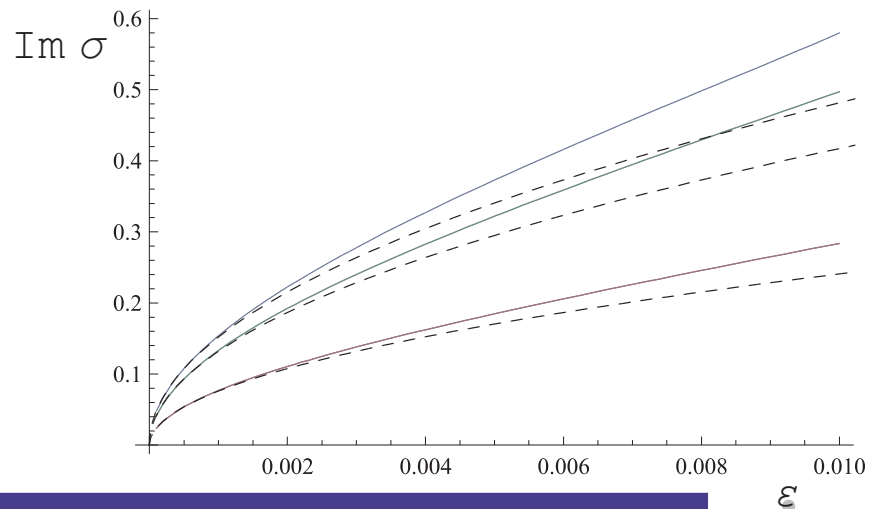
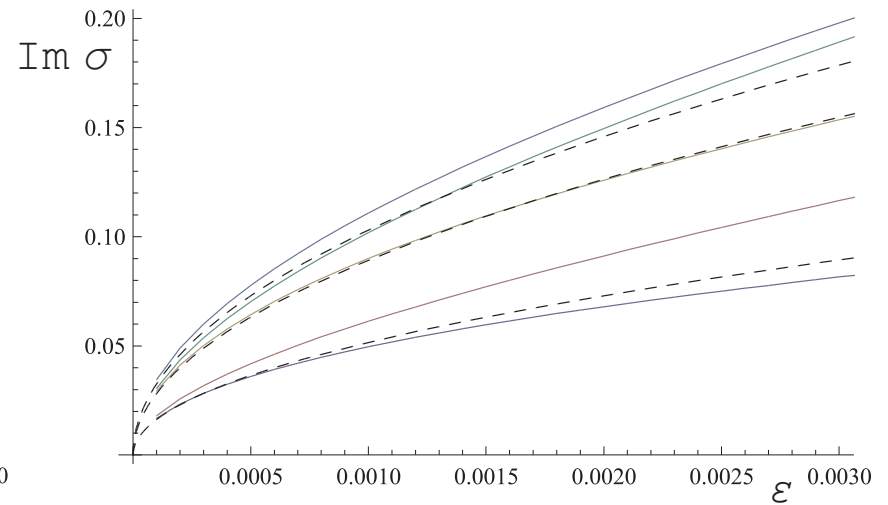


# Prediction vs Numerics

Out of phase

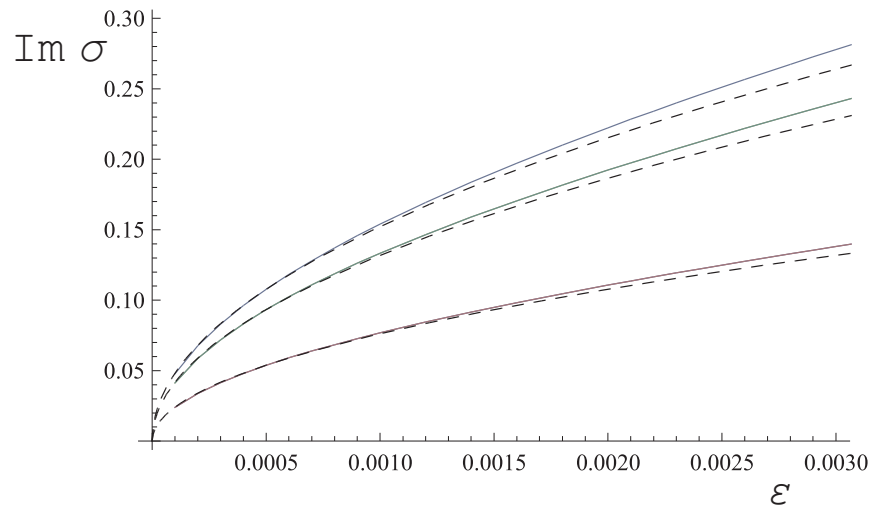


Vortex  $s = 2$

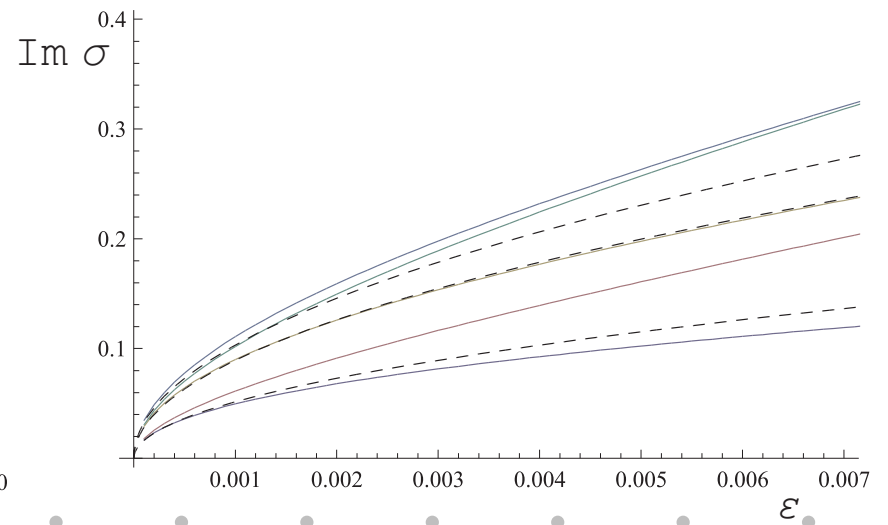
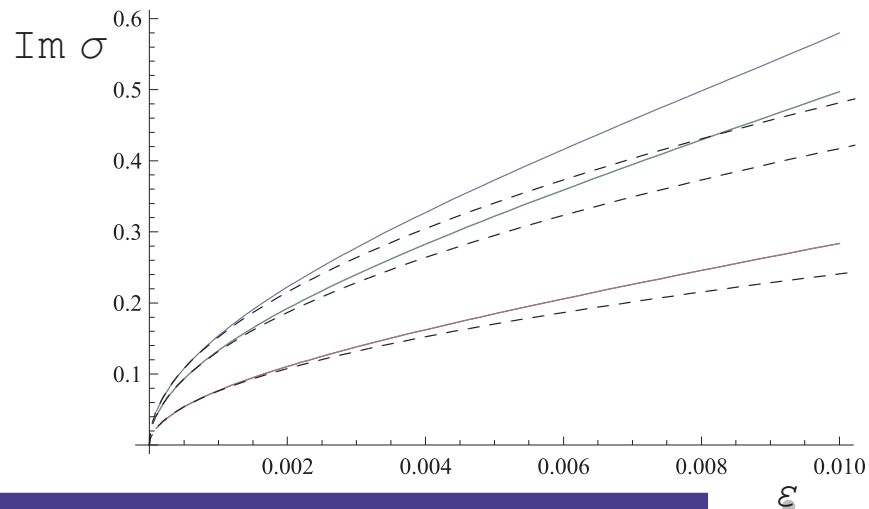
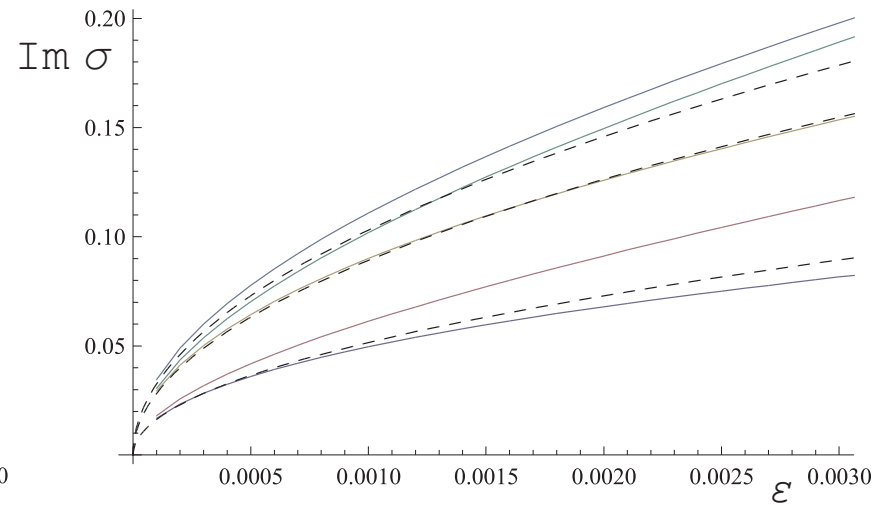


# Prediction vs Numerics

Out of phase



Vortex  $s = 2$



# Summary

- We prove existence of various localized structures in a Hexagonal and a Honeycomb lattice
- We predict their stability and ...
- ... provide  $O(\sqrt{\varepsilon})$  estimates of the corresponding characteristic exponents
- Comparison with the numerical results, satisfactory in most cases
- Using a DNLS description of the systems, we get similar results, K.J.H.Law, P.G.Kevrekidis, VK, I.Kourakis, D.J.Frantzeskakis, A.R.Bishop (submitted in PRE)