Static and moving breathers in a DNA model with competing short–range and long–range dispersive interactions

J Cuevas, F Palmero, B Sánchez–Rey and JFR Archilla

Group of Nonlinear Physics (GFNL), University de Sevilla, Spain

http://www.us.es/gfnl

Work done in collaboration with Yu B Gaididei

Bogolyubov Institute for Theoretical Physics, Kiev, Ukraine

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Abstract

So far, all the studies on breathers on DNA have considered models with either short–range or long-range interaction. However, none of them have considered both kinds of interactions.

When both interactions are taken into account, there appear a great number of phenomena, and some of them are considered here.

One of these phenomena consists in that short–range interaction provide the existence of moving breathers, a fact that does not occur when only long–range interactions are taken into account.

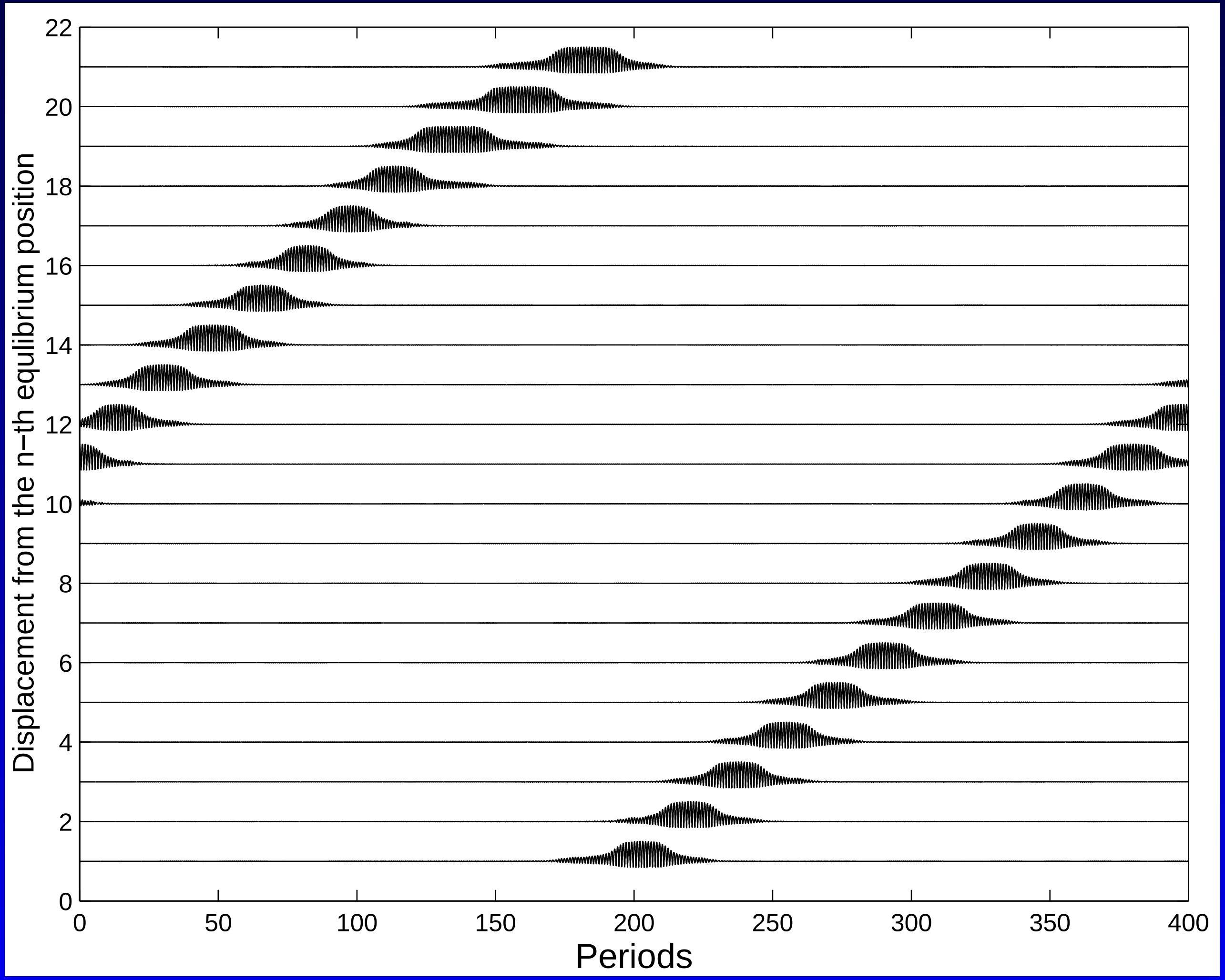
Other phenomena studied here are the existence, stability and shape of static breathers and the properties of moving breathers.

Introduction

- There exist in DNA two important sources of interaction:
  1. Stacking forces $\longrightarrow$ Nearest–neighbour interaction (NNI)
  2. Dipole–dipole forces $\longrightarrow$ Long–range interaction (LRI)
- The introduction of NNI is necessary to make a breather movable.
- The LRI reduces the range of existence of static and moving breathers
- The LRI hinders the mobility of breathers

Moving breather

This is a moving breather in a system with both NNI and LRI:



Description of the model

- Modification of the Peyrard–Bishop model with long-range interaction
- Hamiltonian: $H = T + U_{BP} + U_{NN} + U_{LR}$
- Terms in the Hamiltonian:
  - Kinetic Energy: T
  - Energy due to the openings of base pairs (on–site potential): $U_{BP} = \sum_n V(u_n)$. $V(u_n)$ is the Morse potential:

$$V(u) = \frac{1}{2}(e^{-u} - 1)^2$$

  - Coupling terms $U_{NN} + U_{LR}$

Coupling terms

- Nearest–neighbour interaction (NNI):

$$U_{NN} = \frac{1}{2} C \sum_n (u_{n+1} - u_n)^2$$

- Long–range interaction (LRI):

$$U_{LR} = \frac{1}{2} \sum_{m,n} J_m u_{n+m} u_n$$

$$J_m = \begin{cases} \dfrac{J}{|m|^3} & \text{for } 1 \leq |m| \leq (N-1)/2 \\ 0 & \text{otherwise} \end{cases}$$

Parameters

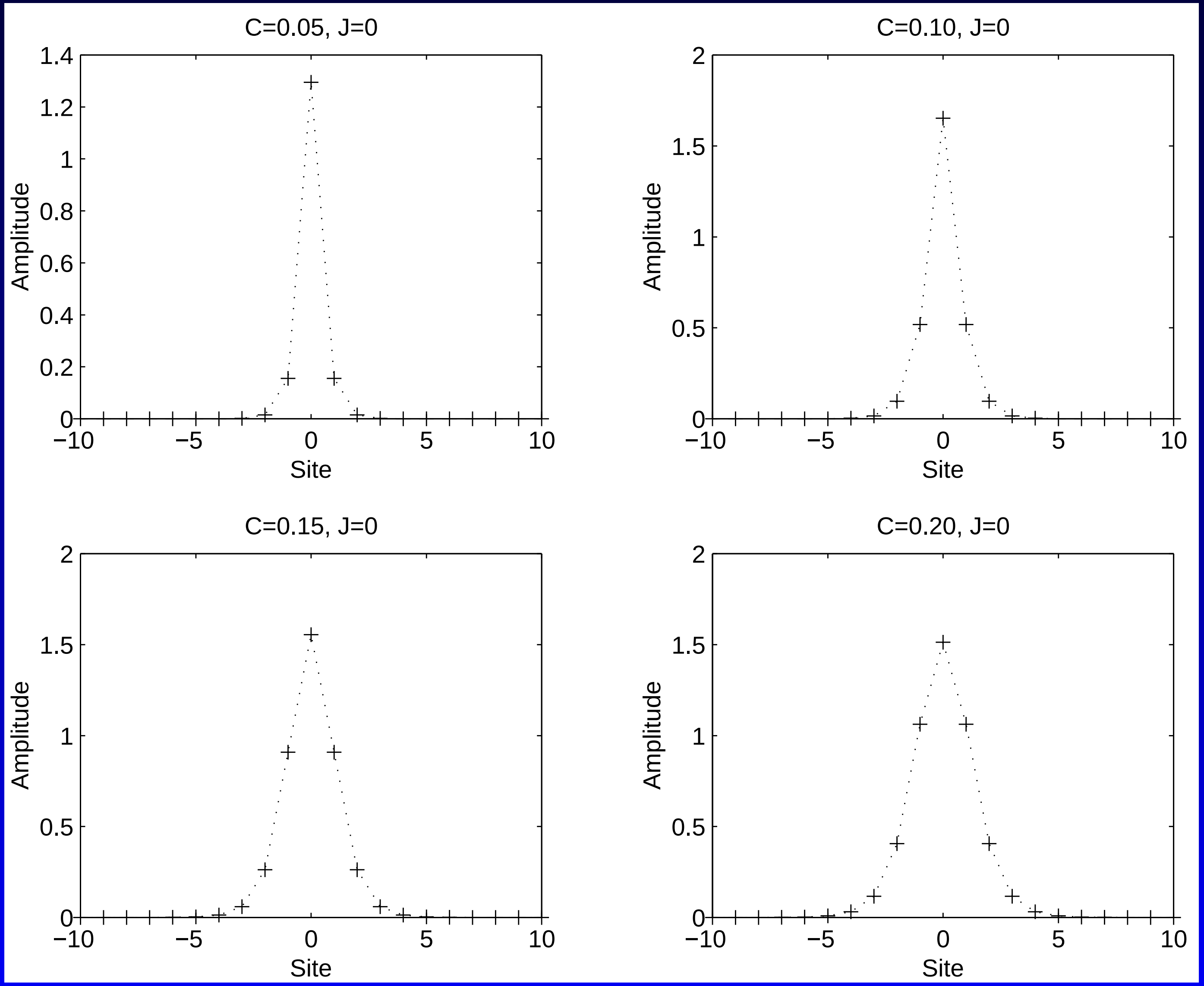
- C is the NNI coupling parameter
- J is the LRI coupling parameter

Origin of the terms:

- Nearest-neighbour term: stacking forces
- Long-range term: dipole–dipole forces

Vibration pattern I

Breather with only NNI: Bell pattern

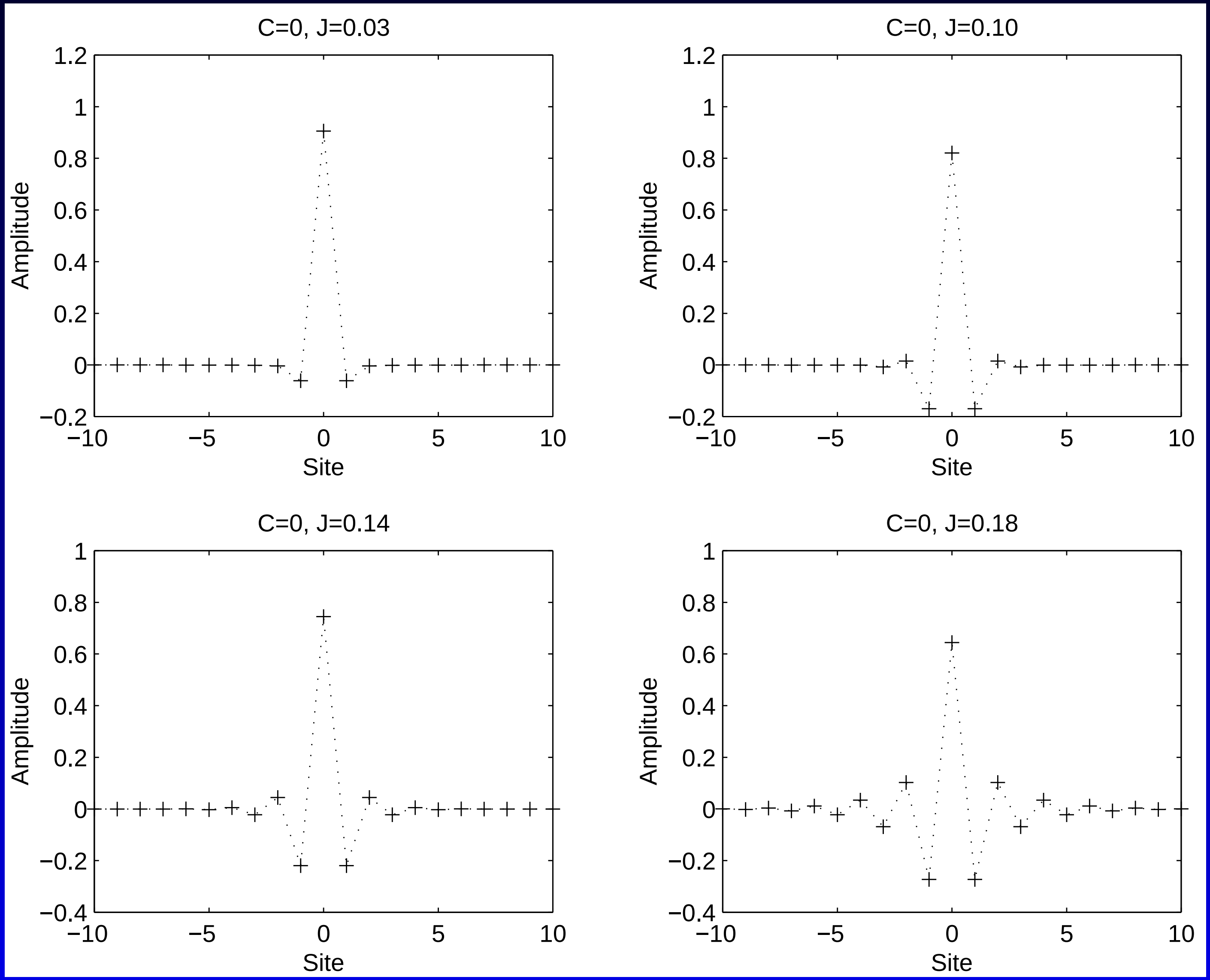


Vibration pattern II

Breather with only LRI

- Low LRI: All particles vibrate in anti-phase with respect to the central one
- Medium LRI: The particles in even sites start to vibrate in phase
- High LRI: Zigzag pattern of vibration

Different patterns with LRI



Main bifurcations I

General description when C and J are varied

- Stability bifurcations:
  There is a change of stability of the breather. A Floquet exponent corresponding to a localized mode abandons (or returns to) the unit circle. Necessary for the existence of moving breathers
- Breather extinctions:
  The breather is not continuable any longer when a Jacobian eigenvalue becomes zero.

Main bifurcations II

The NNI and LRI parameters, C and J, are varied

Different cases:

- Only NNI: Breathers are movable: there exist only stability bifurcations.
- Only LRI: Breathers are not movable: there exist only breather extinctions. NNI must be included in order to obtain moving breathers in a system with LRI.
- General case: There exists a critical value of J above which no stability bifurcation occurs.

Obtaining moving breathers

A static breather is moved by perturbing its velocity components. However, the static breather and the perturbation must fulfill several conditions [2,3]

1. Existence of two complementary stability bifurcations for the 1–site and 2–site breathers with bifurcation loci fairly close together. The static–breather parameters must be in a region near these bifurcation loci.
2. The static breather has to be perturbed with the velocity components of the localized mode that abandons the Floquet circle at the stability bifurcation.

Concept of effective mass

- The breather effective mass (m^*) is a quantitative measure of the mobility.
- It is found [2]that the translational velocity of a moving breather (v) is proportional to the modulus of the initial perturbation (v_I).
- The effective mass is defined by the equation:

$$\frac{1}{2}\, m^* v^2 = \frac{1}{2}\, v_I^2$$

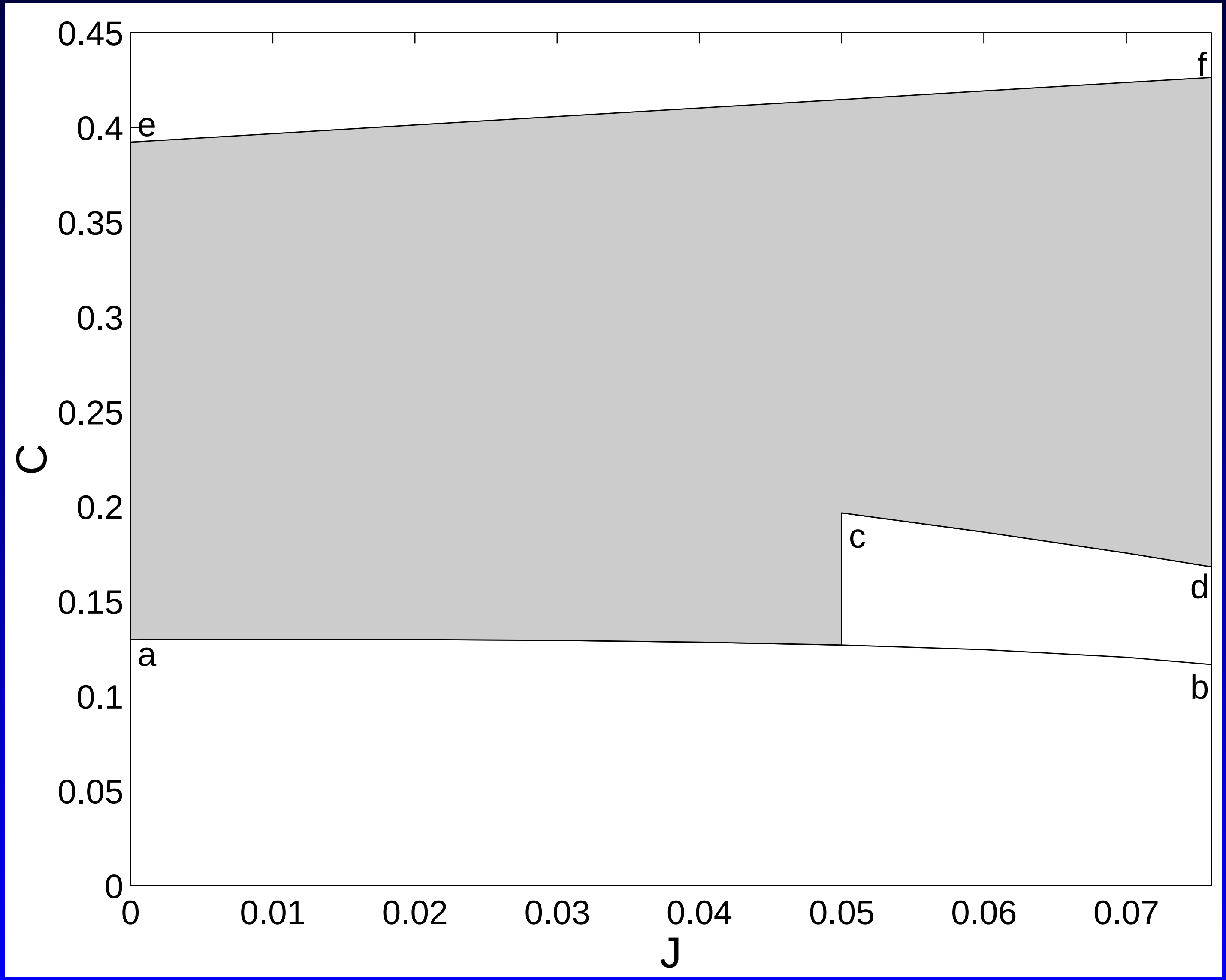
Moving breathers

Range of existence

- There is a maximum value of the LRI parameter J above which there are no mobile breathers. This value is higher for 2–site breathers than for 1–site breathers and is independent of the size of the system.
- For low J, breathers can be made movable for values of C above the first stability bifurcation
- For high J, the 1–site breathers can only be moved in the proximity of the first stability bifurcation curve and above the second one; the 2–site breathers can only be moved above the second stability bifurcation curve.

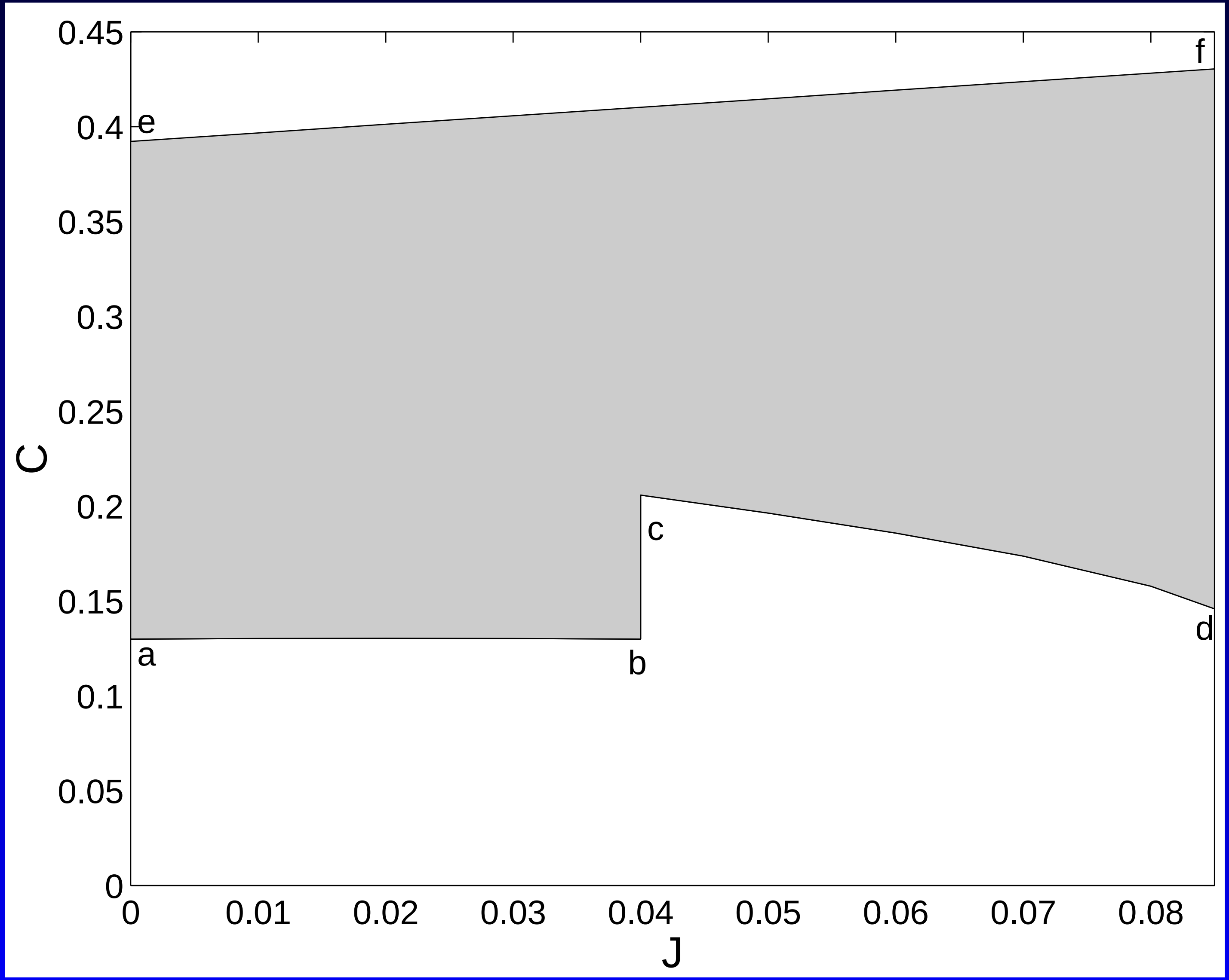
Range of existence I

Moving breathers obtained from a 1–site breather



Range of existence II

Moving breathers obtained from a 2–site breather

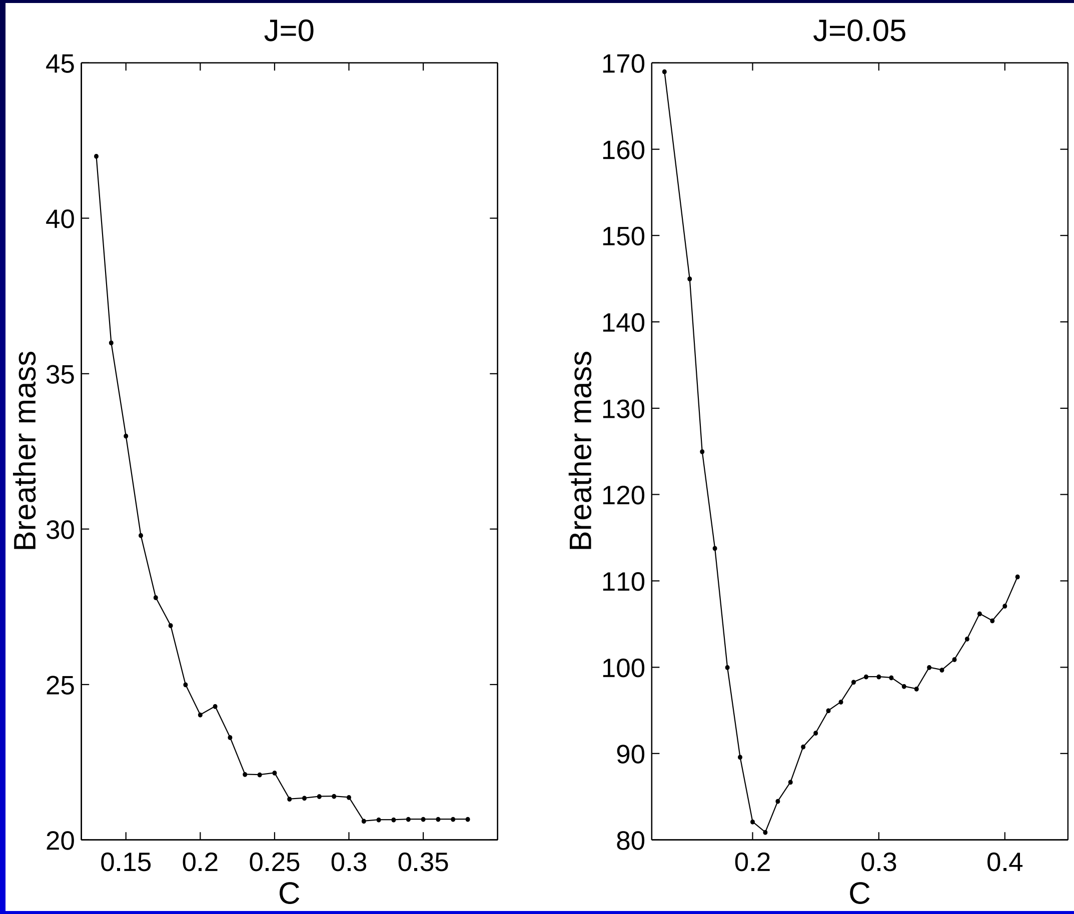


Mobility

- The breather effective mass has its maximum value in the vicinity of the first stability bifurcation curve
- This maximum value increases with the LRI parameter J
- The long–range interaction emphasizes the discreteness of the system. In other words, the smoothness of the movement decreases when J increases.

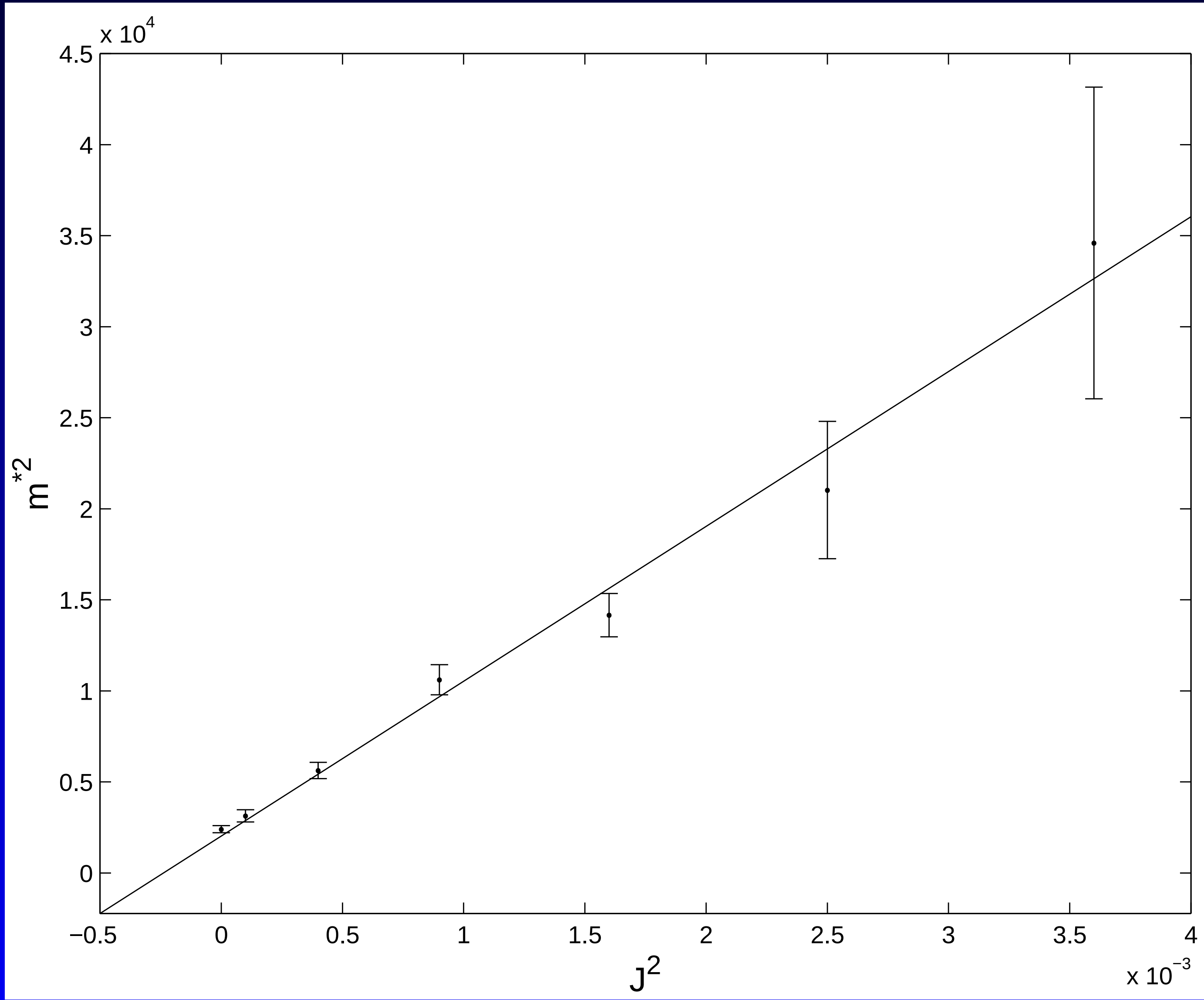
Breather effective mass

Variation of with the NNI parameter C at constant LRI parameter J



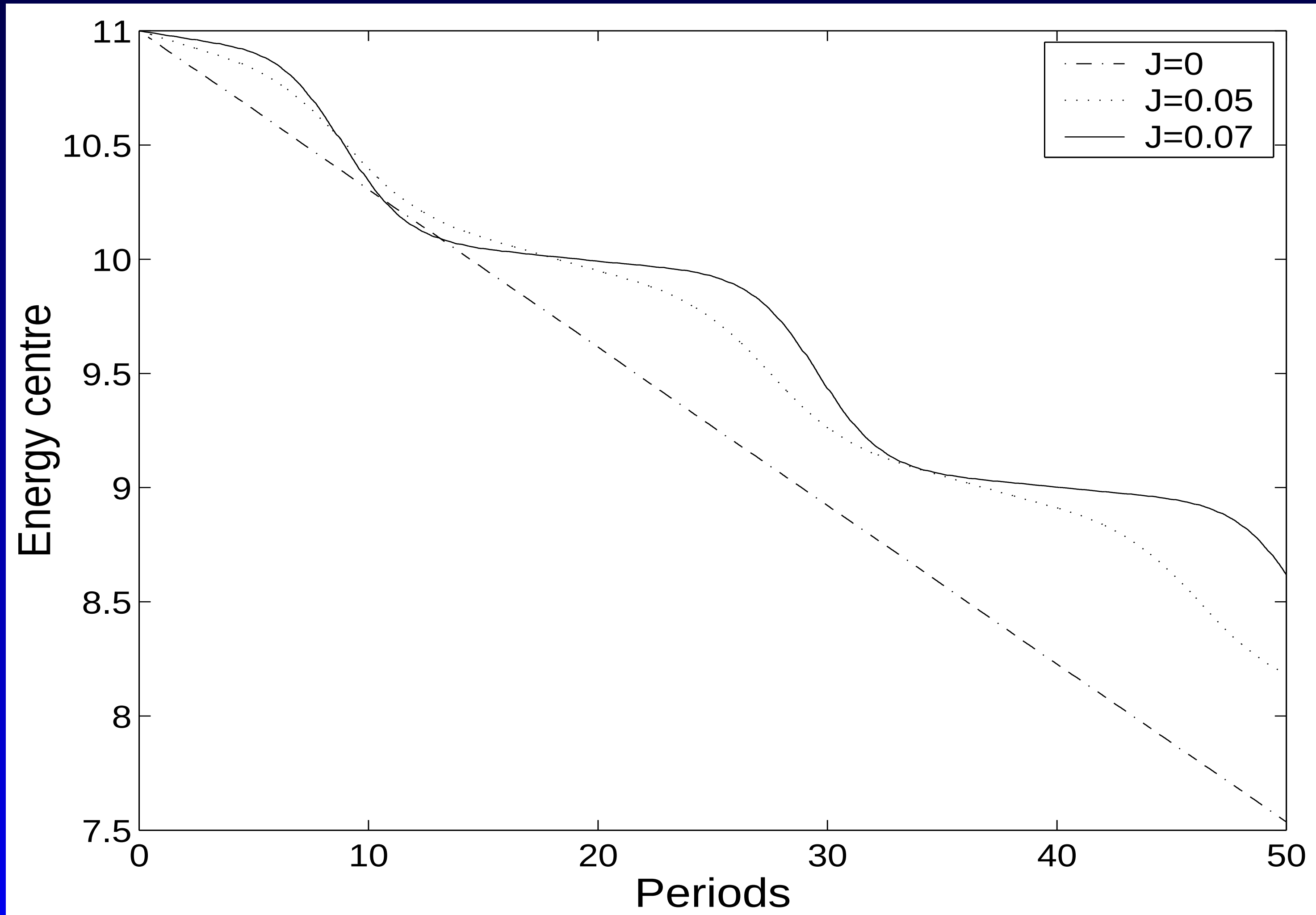
Maximum breather mass

For different values of J



Energy centre

For different values of J being the value of C the corresponding to the maximum breather mass

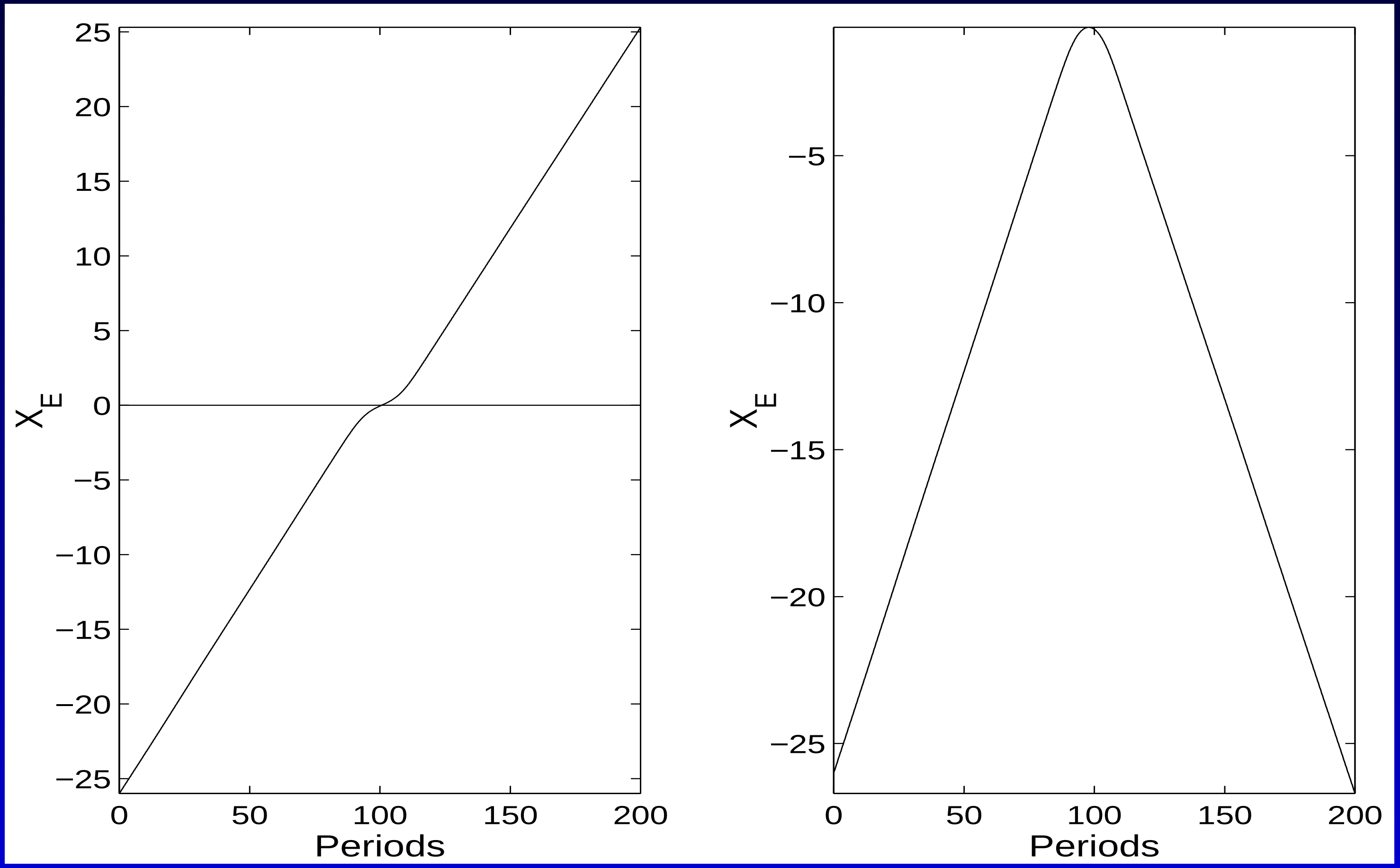


Further developments

- Moving breathers are studied in a bent chain [4]
- At constant velocity, there exists a critical value of the curvature below which the breather cross the bending point.
- Above this curvature the breather is reflected.

Motion of the energy centre

For low and high curvature



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