Breathers in curved chains with long–range interaction

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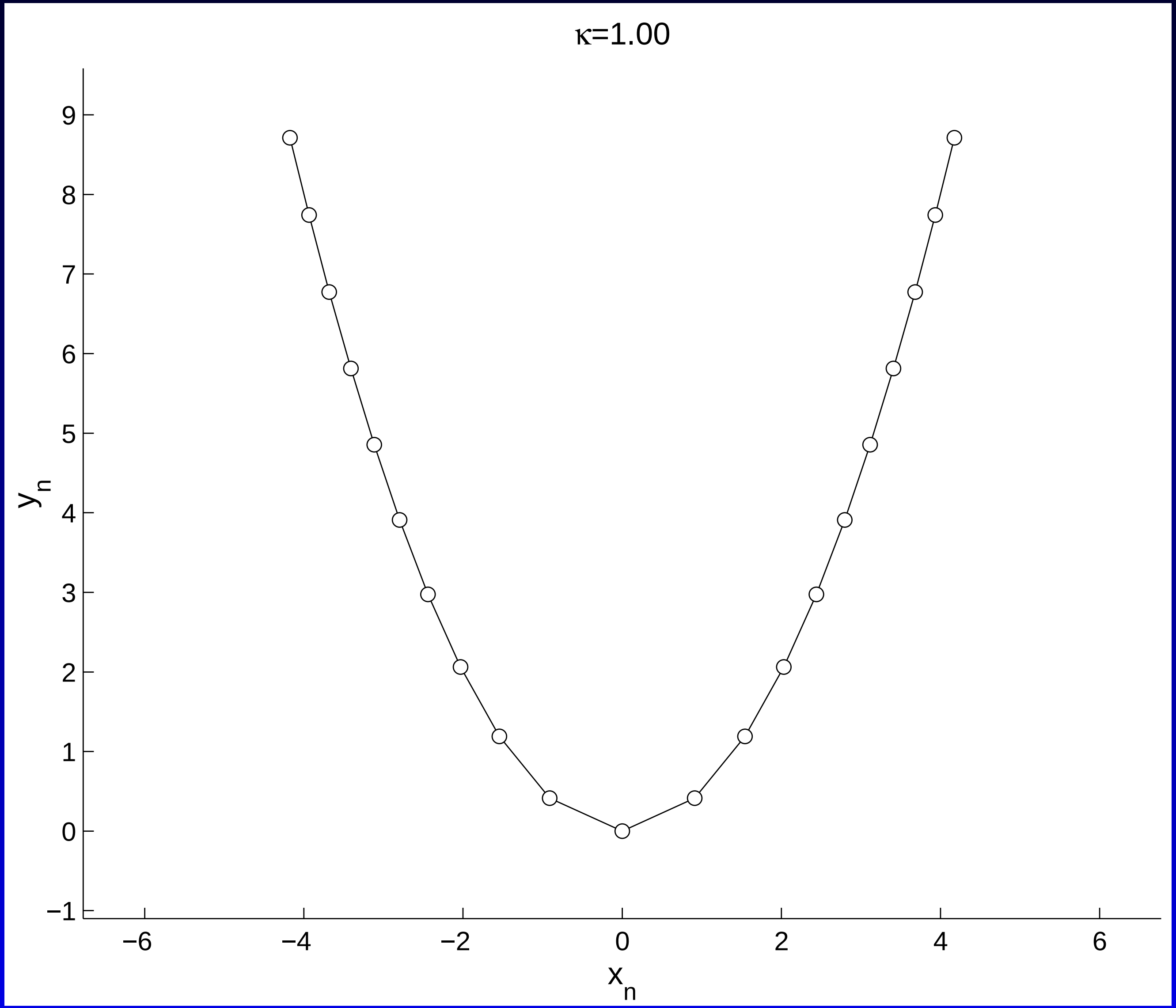
Work supported by the hospitality of IMM, DTU, and by the European Commission under the RTN project, HPRN-CT-1999-00163 (LOCNET) during 2000–2001

Sketch of the models



Klein–Gordon models

- Variants of the Peyrard–Bishop model for DNA
- Simplifying hypotheses:
  We neglect:
  - Stretching
  - Stacking interaction
  - helicity
  - inhomogeneity

  We suppose:
  - Curvature of the chain within a plane
  - Shape fixed in time and approximated to a parabola
  - Movement of the bases perpendicular to the plane

First model

- Soft on–site potential and attractive interaction
- Hamiltonian:

$$H = \sum_{n=1}^{N} \Big(\frac{1}{2}\, \dot{u}_n^2 \; + \frac{1}{2}\omega_0^2\, u_n^2 - \frac{1}{4}\, u_n^4$$

$$+ \frac{1}{4}\, \varepsilon \sum_{m=1}^{N} J_{nm} (u_n - u_m)^2 \Big)$$

- Coupling coefficients:

$$J_{n\,m} = \frac{1}{|\vec{r}_n - \vec{r}_m|^3} \quad n \neq m \quad ; \quad J_{n\,n} = 0$$

Breathers

- Dynamical equations:

$$\ddot{u}_n + \omega_0^2\, u_n - u_n^3 + \varepsilon \sum_{m=1}^{N} J_{n\,m}(u_n - u_m) = 0$$

$$n = 1, \ldots, N$$

- Breathers:

$$u_n = z_{0,n} + \sum_{k=1}^{k_m} 2\, z_{k,n}\, \cos(k\, \omega_{\mathrm{b}}\, t)$$

Stability

- Newton operator:

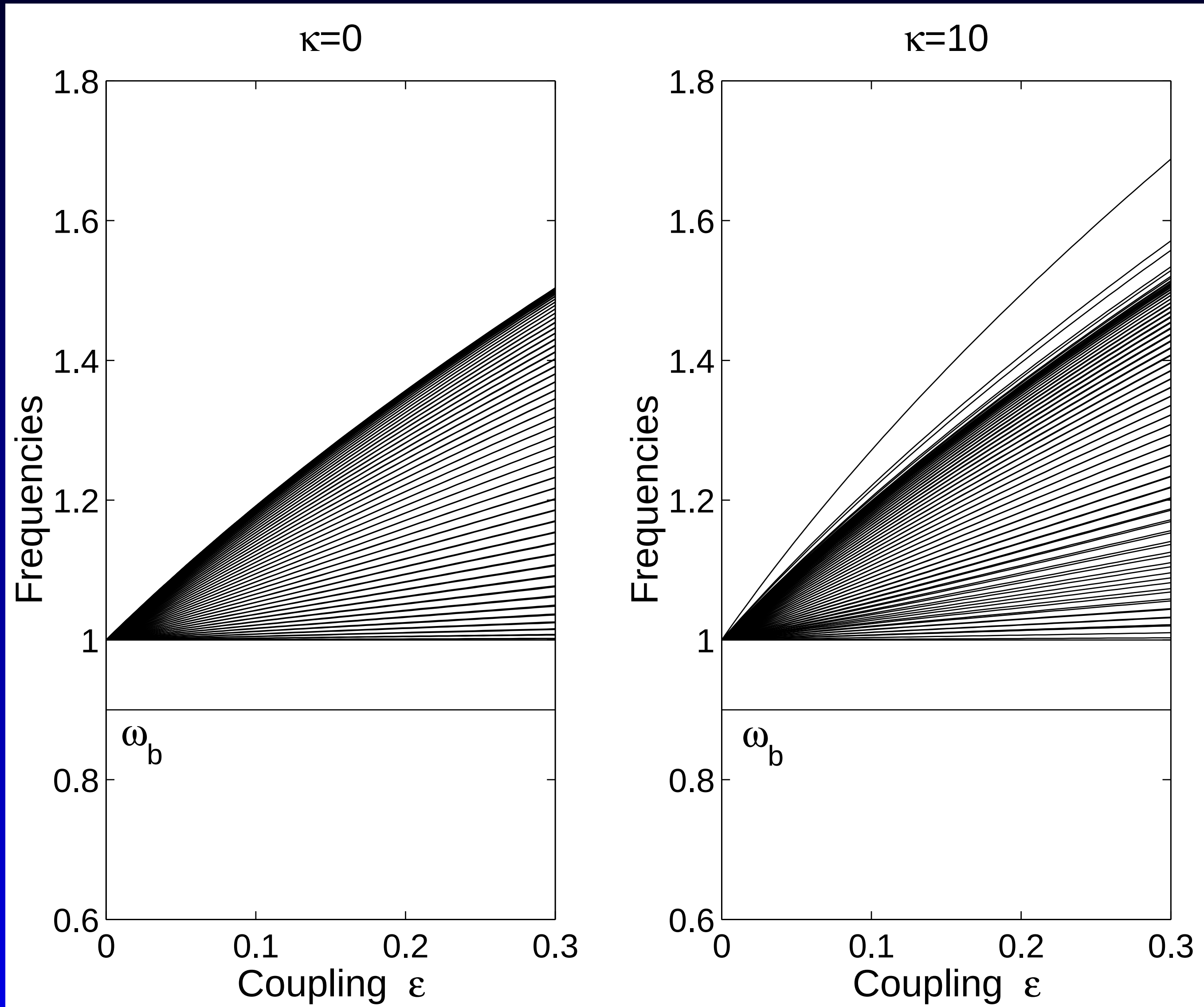
$$(\mathcal{N}(u(t),\varepsilon)\cdot\xi)_n \equiv \ddot{\xi}_n + \omega_0^2\,\xi_n - 3\,u_n^2\,\xi_n + \varepsilon\sum_{m=1}^{N} J_{nm}(\xi_n - \xi_m) = 0$$

- Floquet operator:

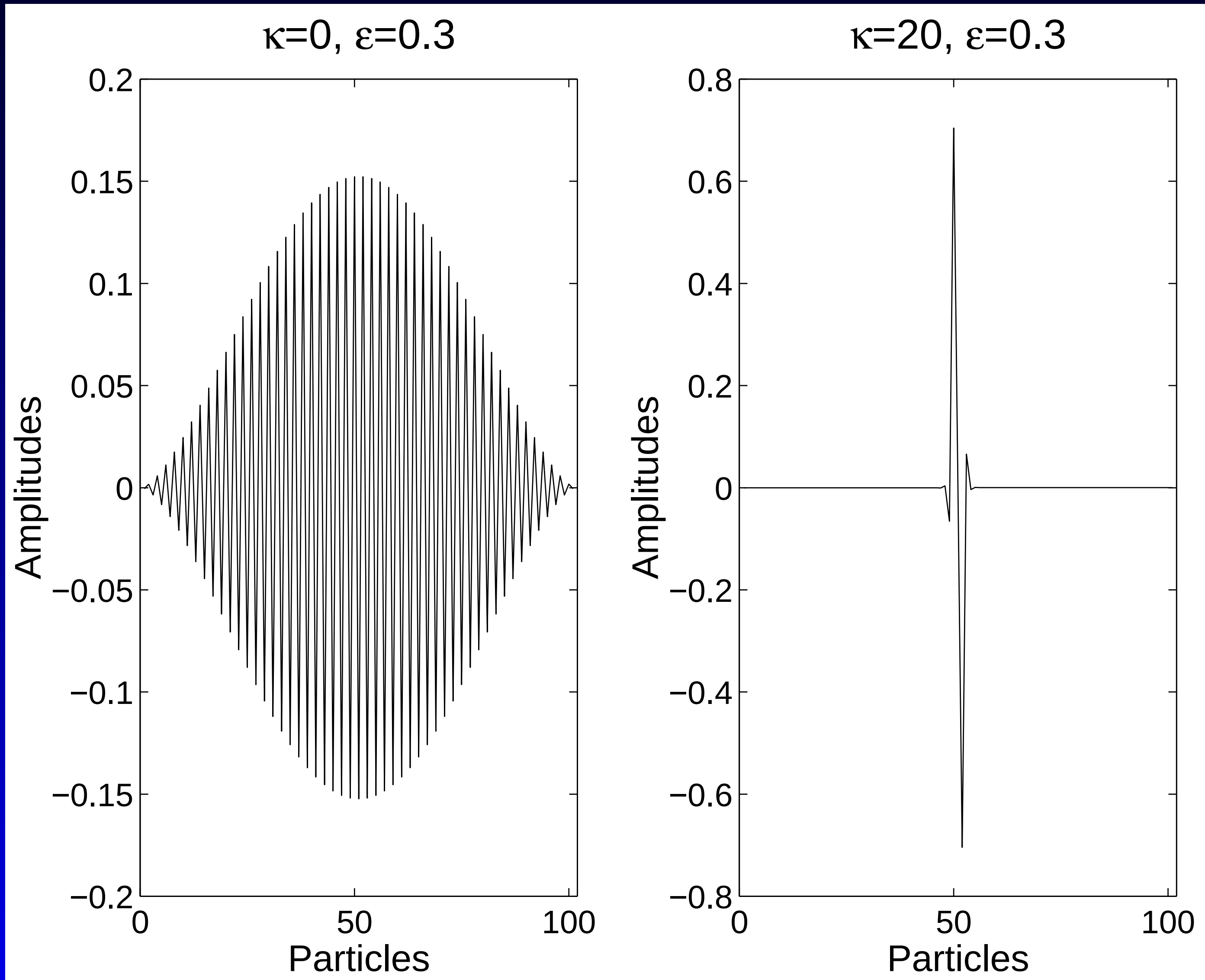
$$\begin{bmatrix} \{\xi_n(T)\} \\ \{\dot{\xi}_n(T)\} \end{bmatrix} = \mathcal{F}_0 \begin{bmatrix} \{\xi_n(0)\} \\ \{\dot{\xi}_n(0)\} \end{bmatrix}$$

- *Breathers are stable if every eigenvalue λ_j of $\mathcal{F}_0$ has $|\lambda_j| = 1$*

Linear Spectrum

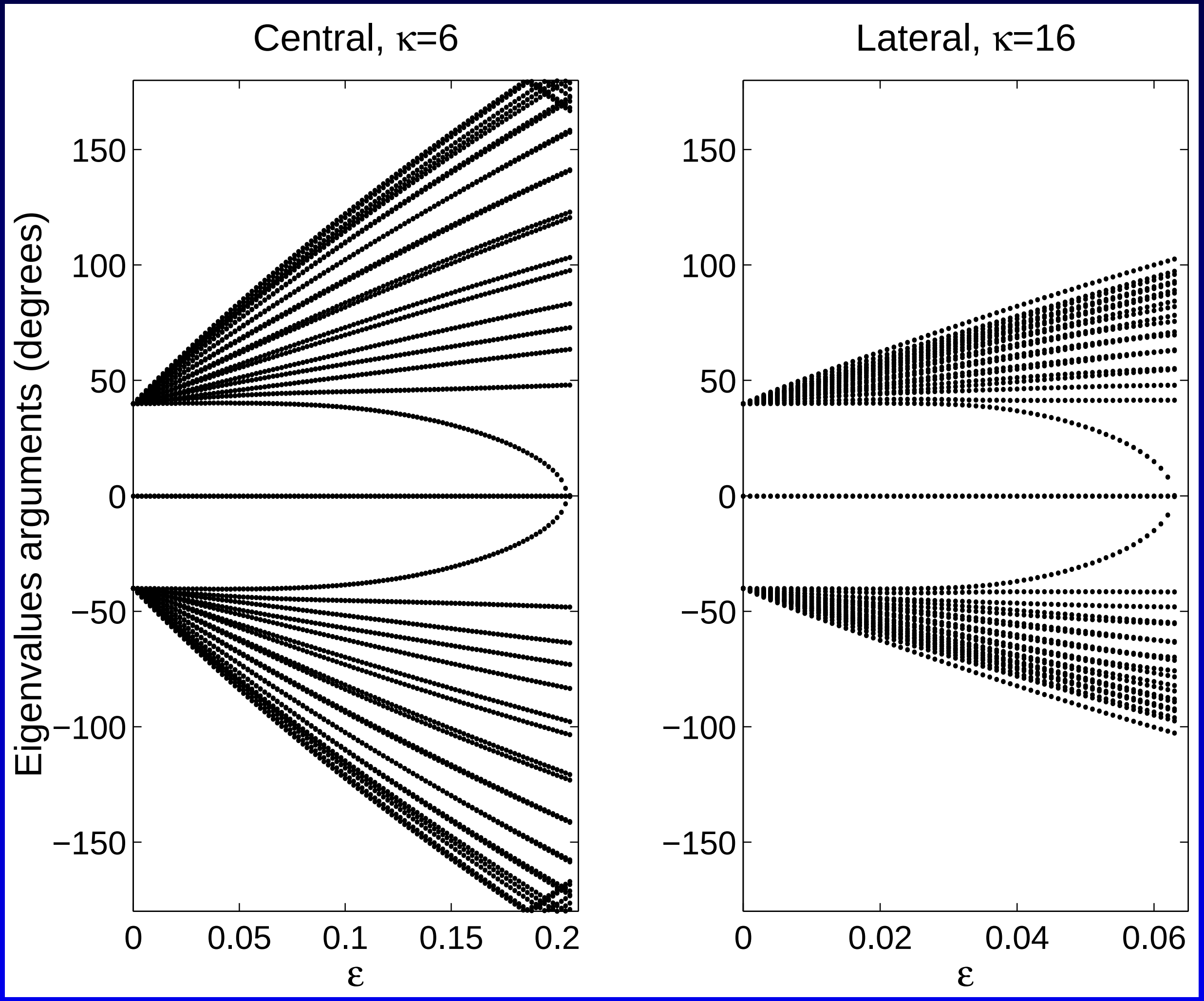


Highest frequency eigenvector

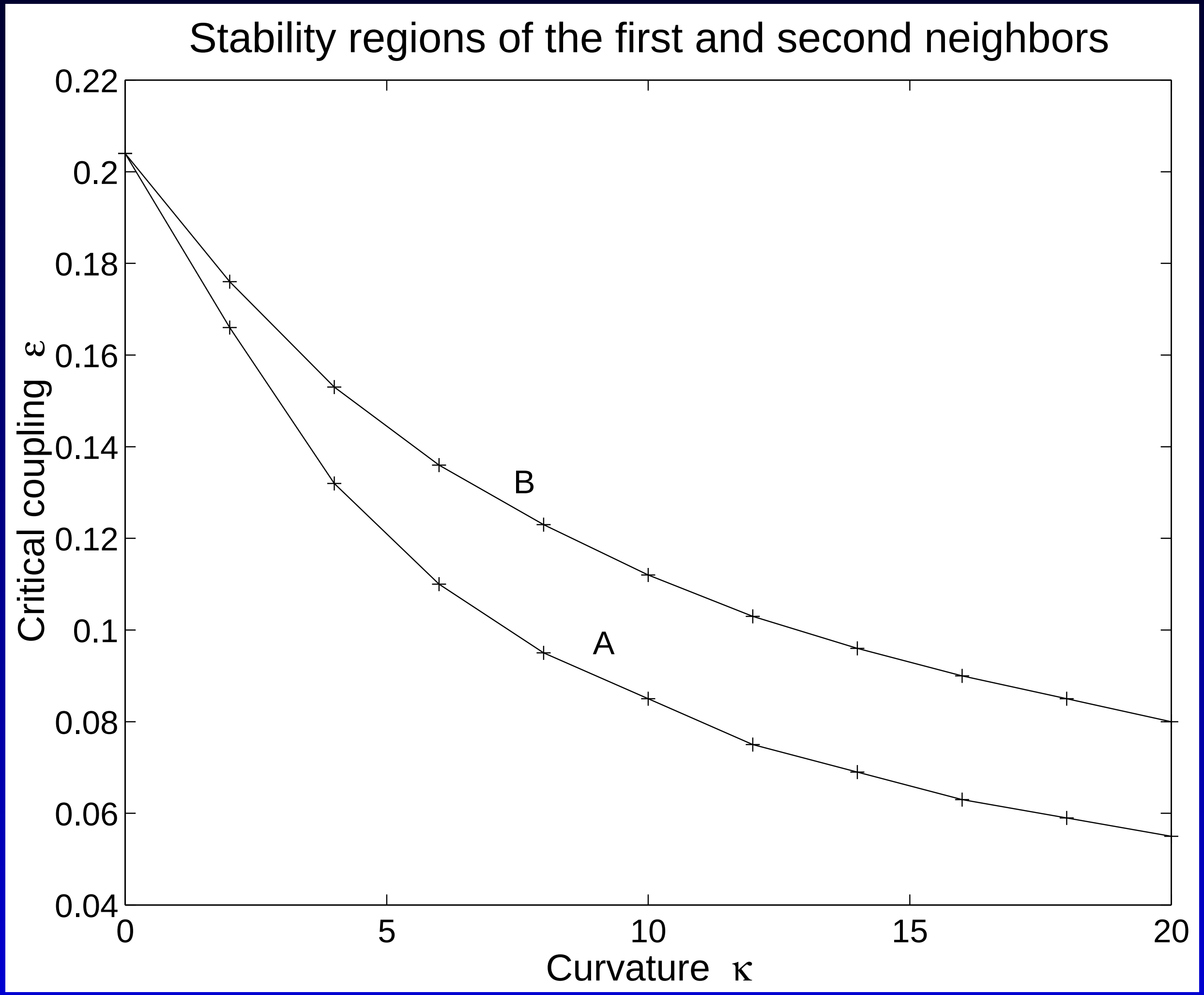


Floquet arguments

$$\theta_j \text{ in } \lambda_j = e^{\mathrm{i}\,\theta_j}$$



Stability regions

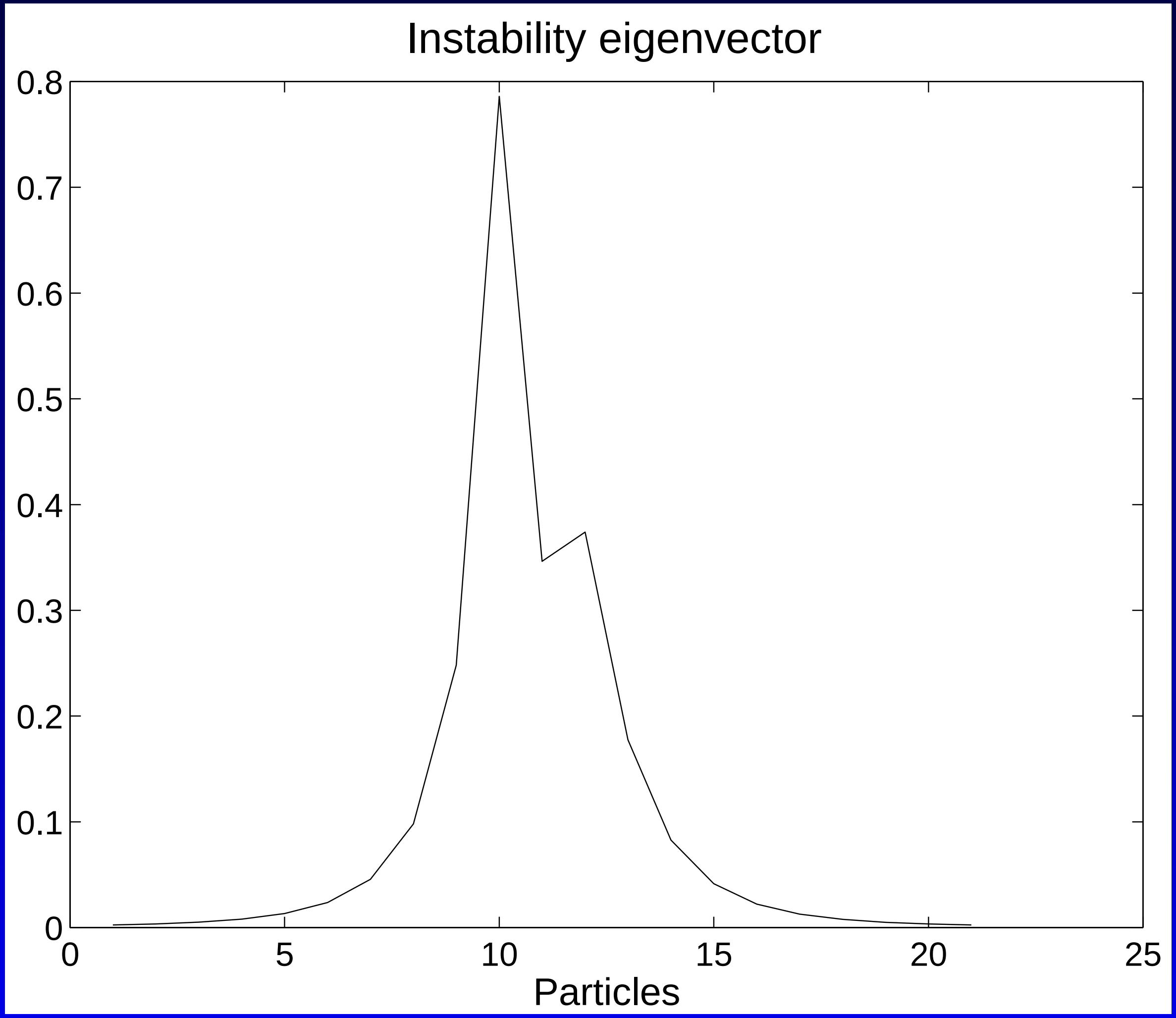


Bifurcation loci:

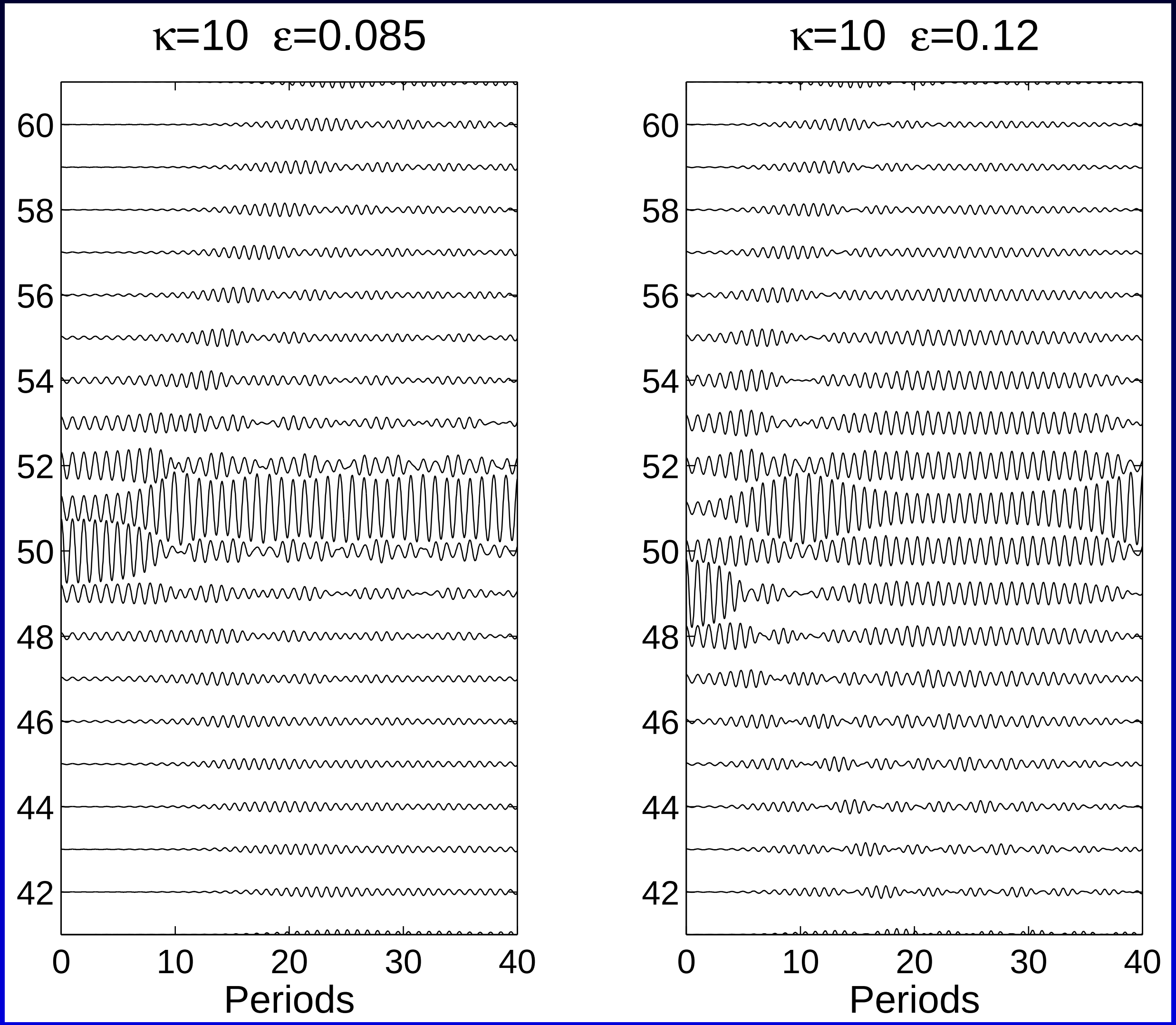
A: first neighbour breather; B: second neighbour breather

Instability eigenvector velocities

$$\kappa = 10, \varepsilon = 0.085$$



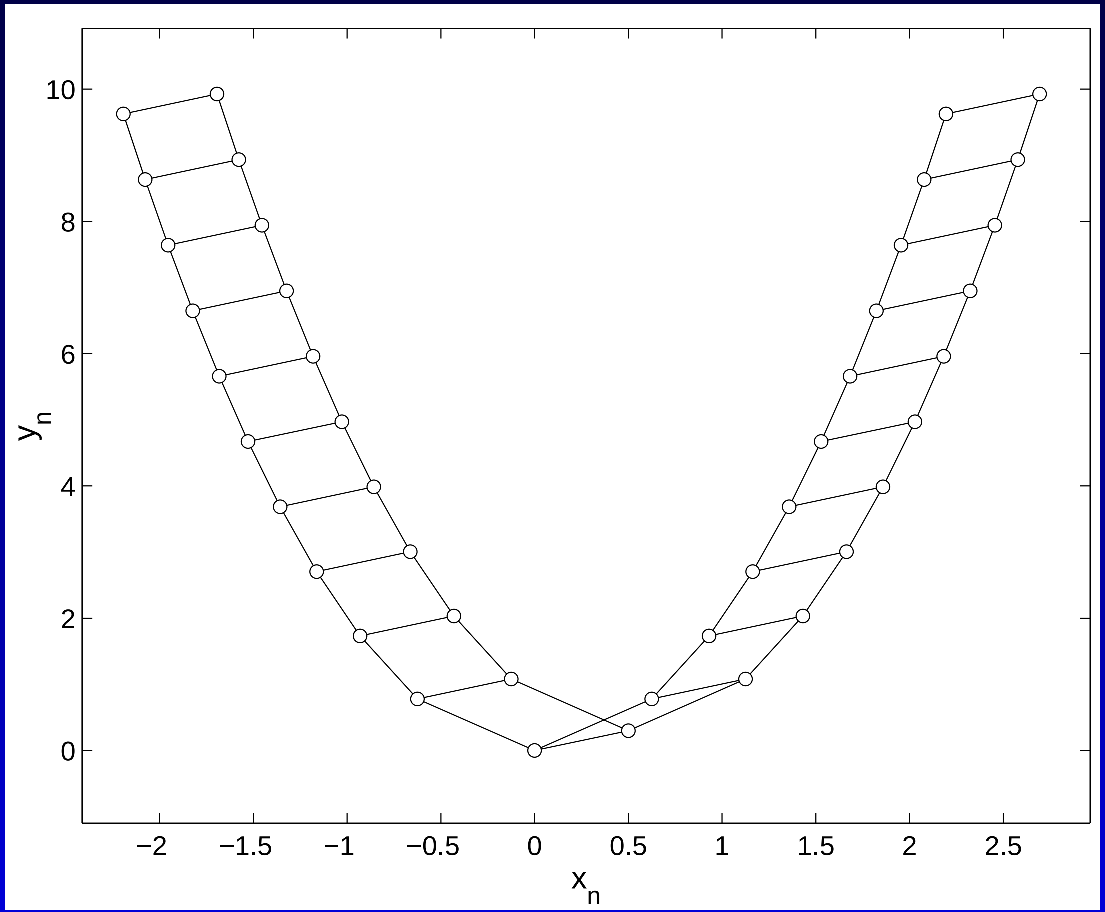
Position switching



Switching of the first and second neighbour breathers

Second model

Hard on–site potential and repulsive interaction



Hamiltonian

- Dipole interaction:

$$U_{\vec{p}_1\cdot\vec{p}_2} = \frac{\vec{p}_1\,\vec{p}_2}{|\vec{r}_{12}|^3} - \frac{3\,(\vec{p}_1\cdot\vec{r}_{12})(\vec{p}_2\cdot\vec{r}_{12})}{|\vec{r}_{12}|^5} = \frac{\vec{p}_1\cdot\vec{p}_2}{|\vec{r}_{12}|^3}$$

- Hamiltonian:

$$H = \sum_{n=1}^{N}\Big(\frac{1}{2}\,\dot{u}_n^2 \;+\frac{1}{2}\omega_0^2\,u_n^2 + \frac{1}{4}\,u_n^4 + \frac{1}{2}\,\varepsilon\sum_{m=1}^{N} J_{nm}u_n\,u_m\Big)$$

Equations

- Coupling coefficients:

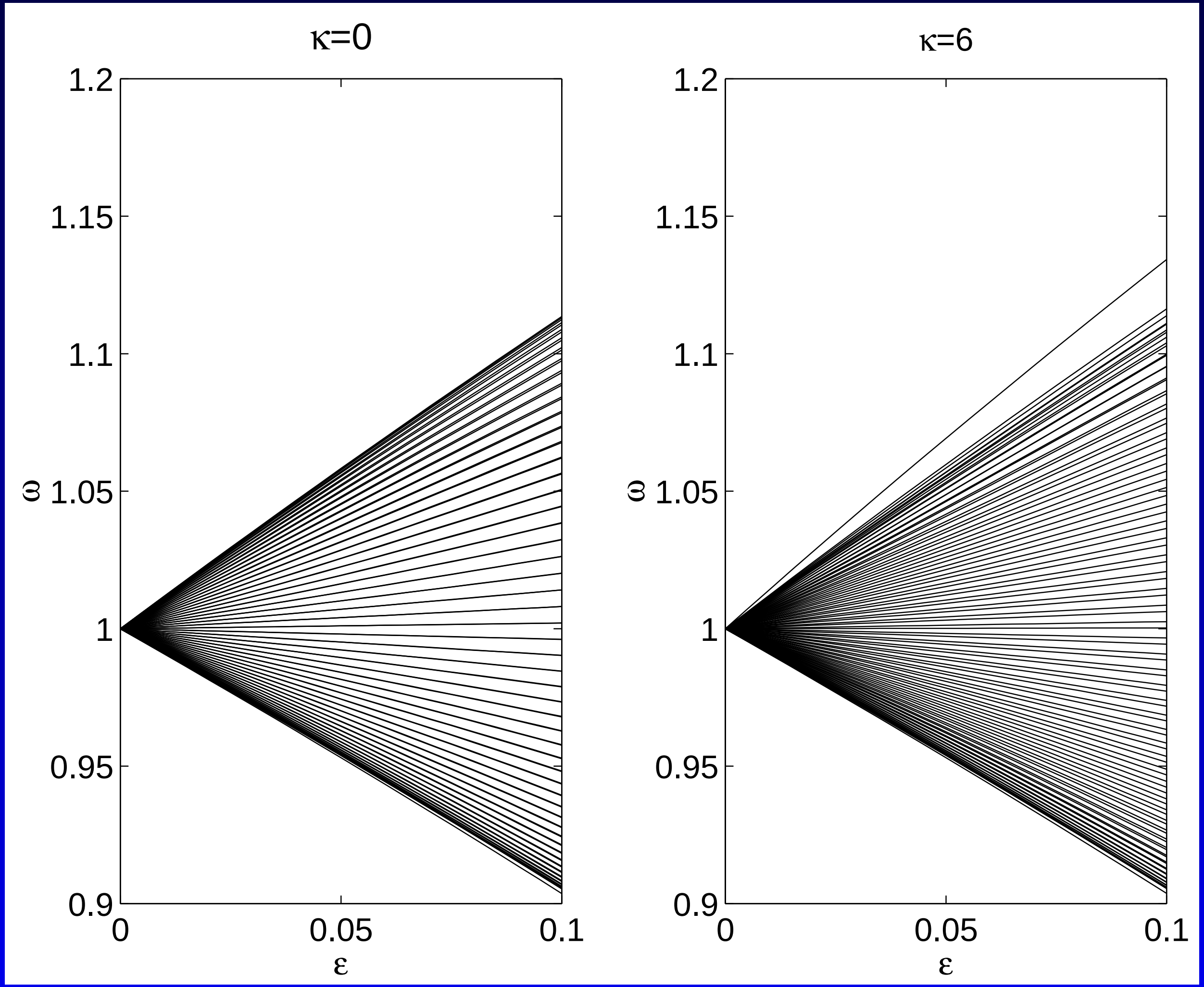
$$J_{n\,m} = \frac{1}{|\vec{r}_n - \vec{r}_m|^3} \quad n \neq m \quad ; \quad J_{n\,n} = 0$$

- Dynamical equations:

$$\ddot{u}_n + \omega_0^2\, u_n \,+\, u_n^3 + \varepsilon \sum_{m=1}^{N} J_{nm} u_m = 0$$

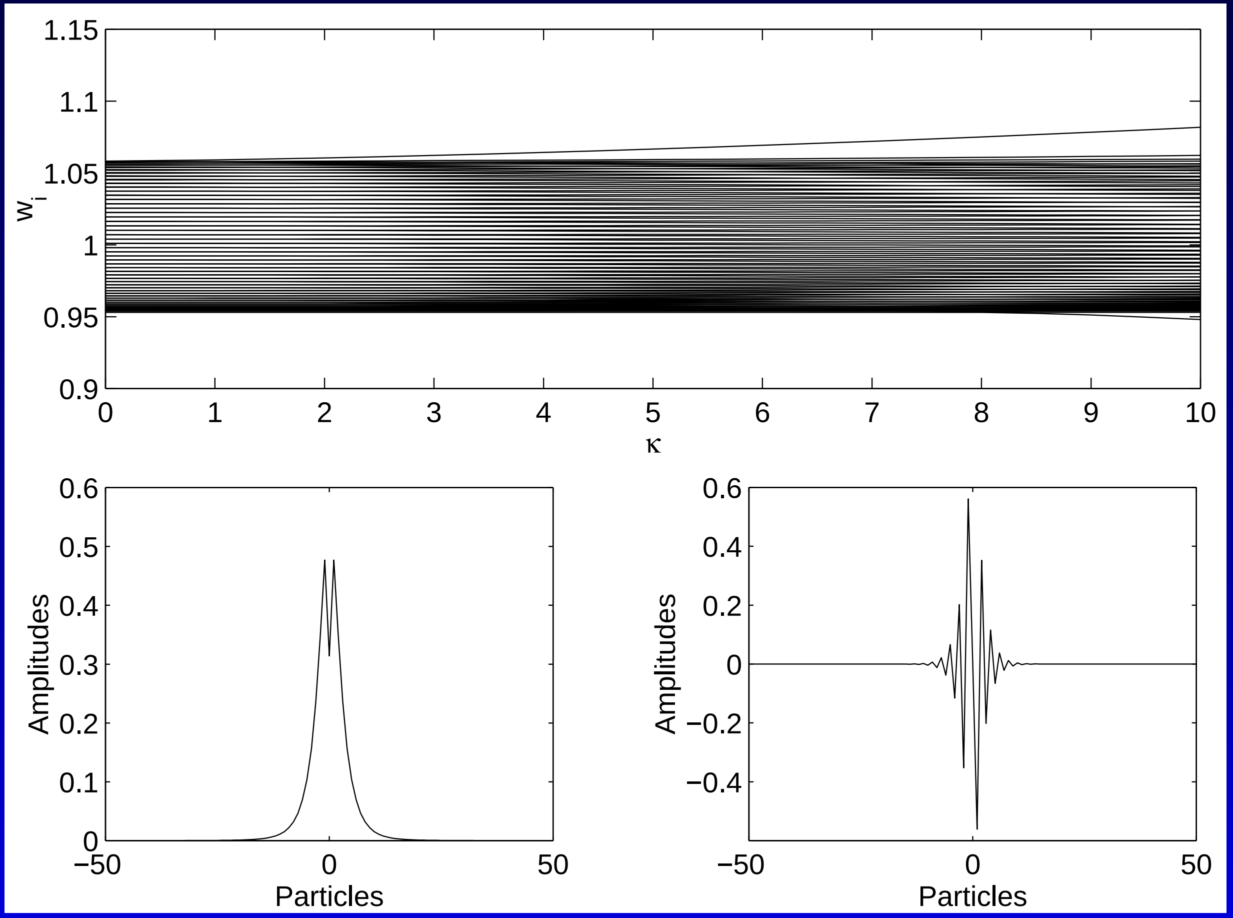
Linear spectrum I

Increasing the coupling parameter ε



Linear spectrum II

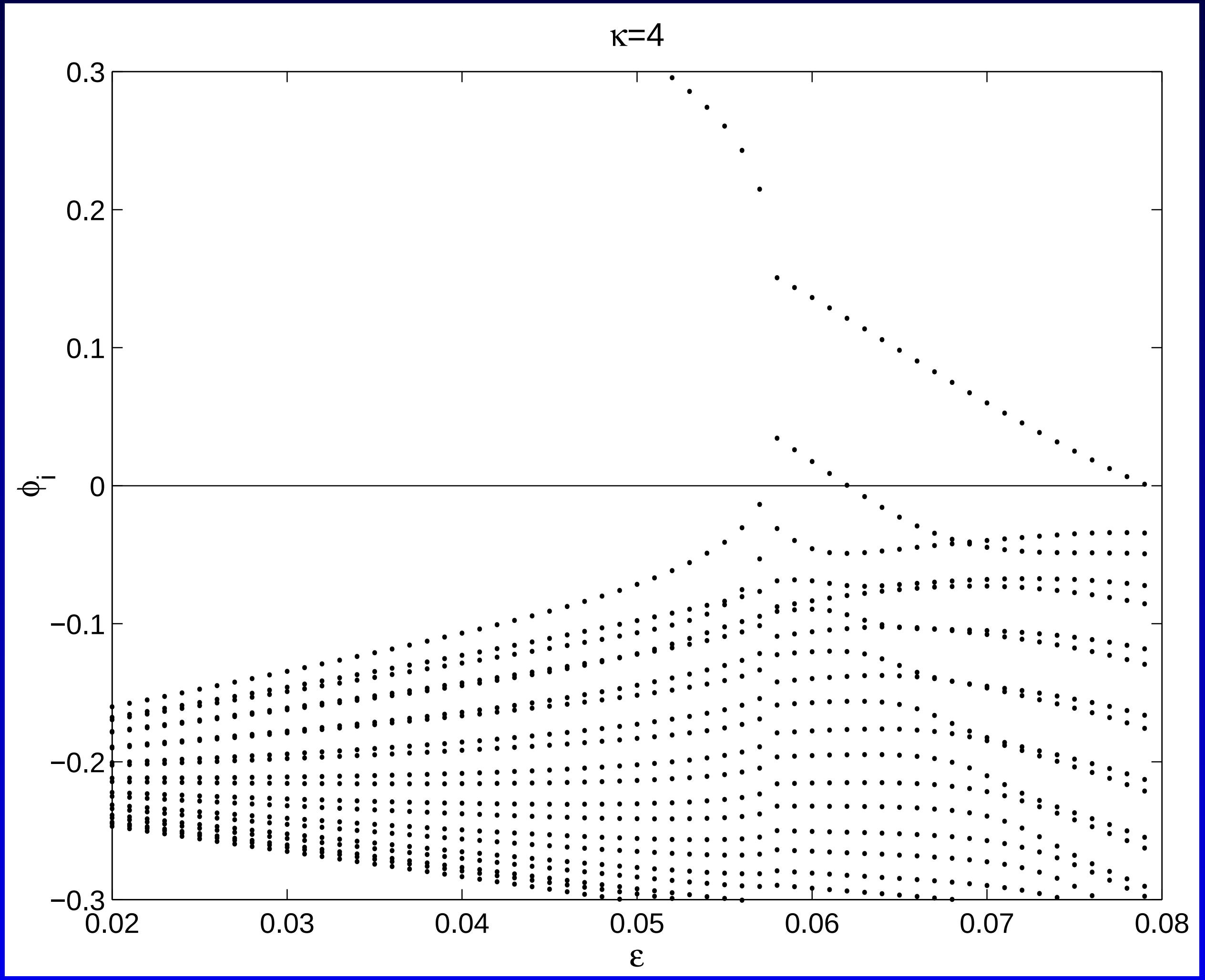
Increasing the curvature κ. Constant $\varepsilon = 0.05$



Modes of highest (double humped symmetric mode) and lowest frequency

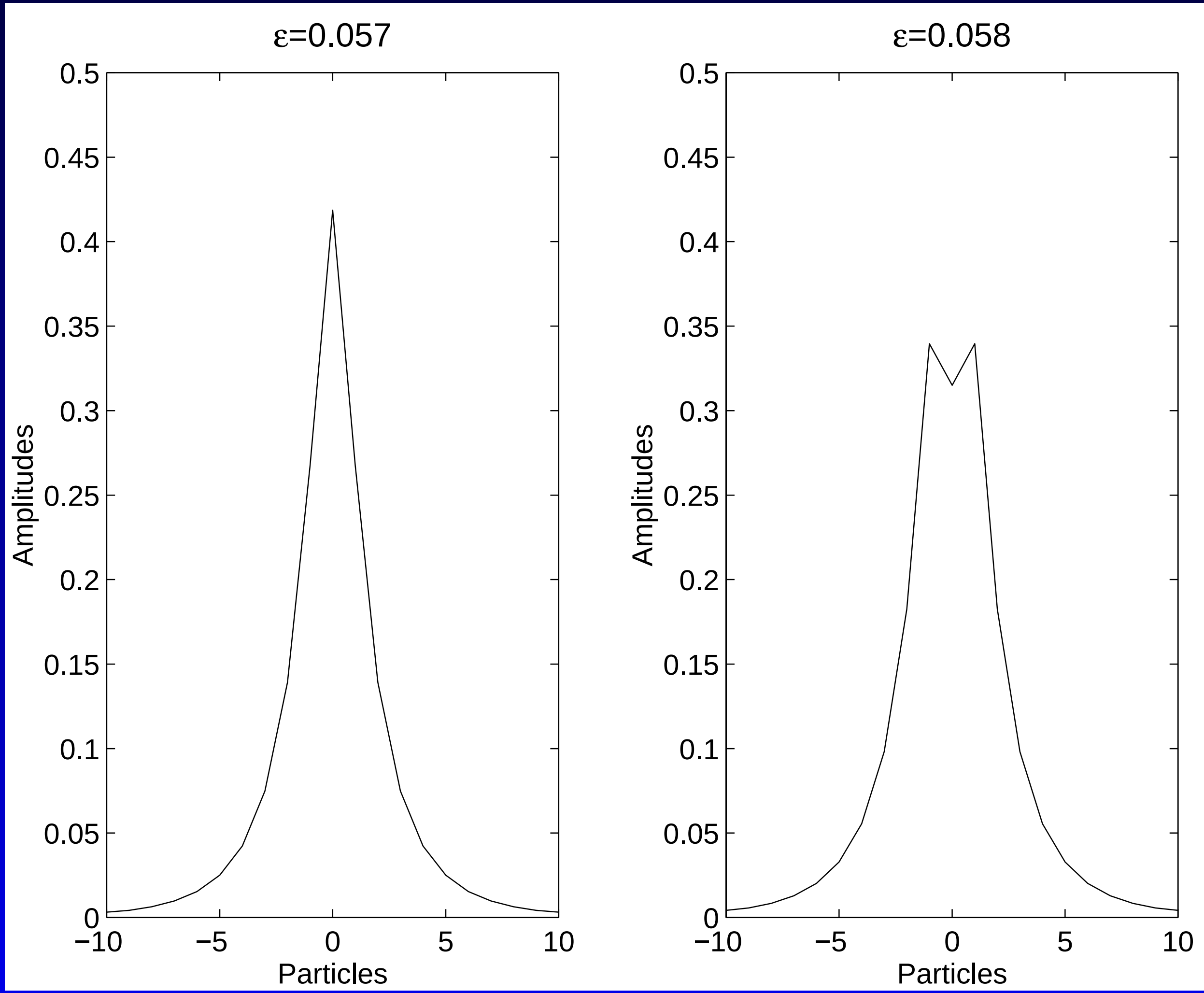
Jacobian eigenvalues

Central breather



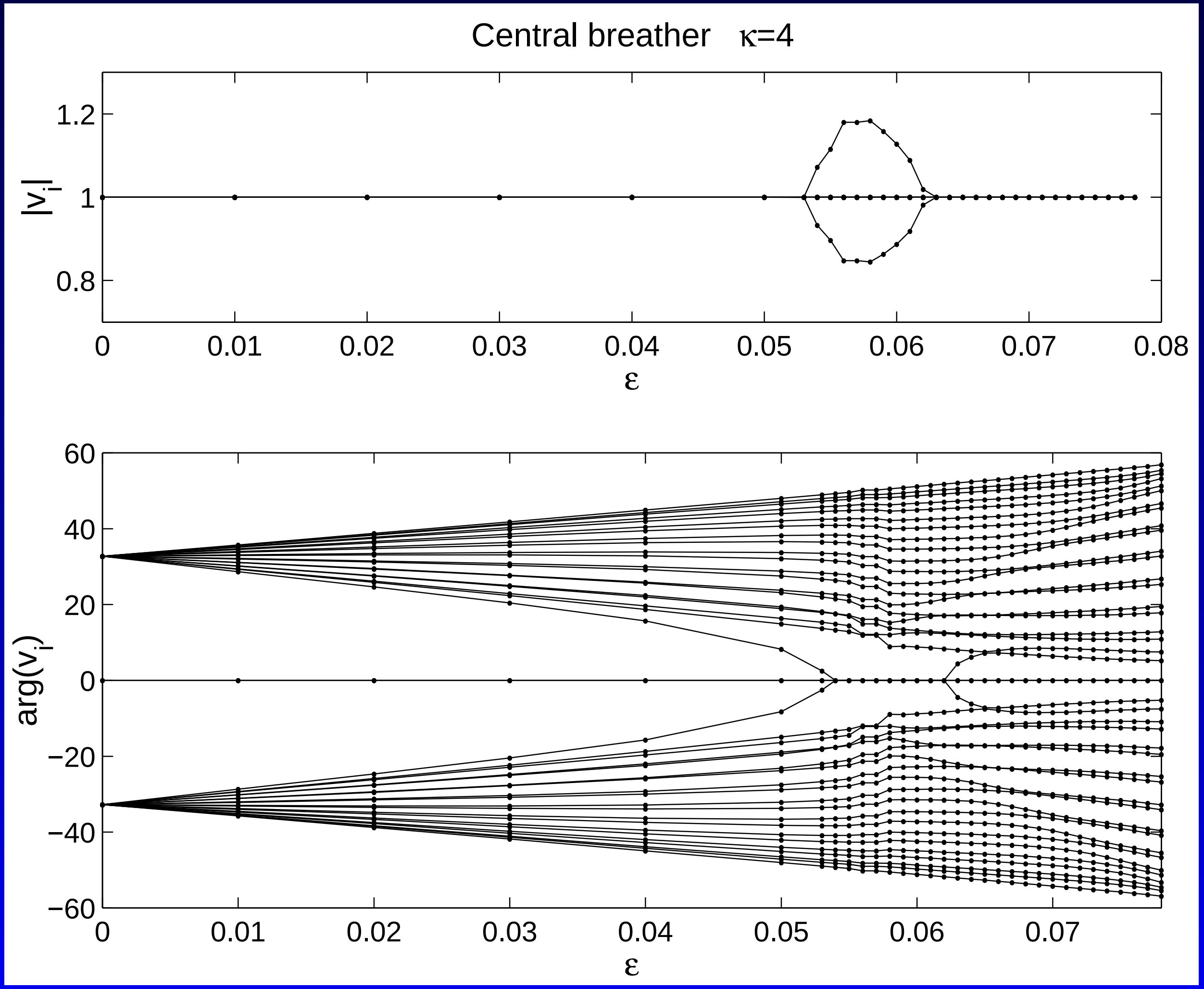
Central breather bifurcation

Curvature $\kappa = 4$

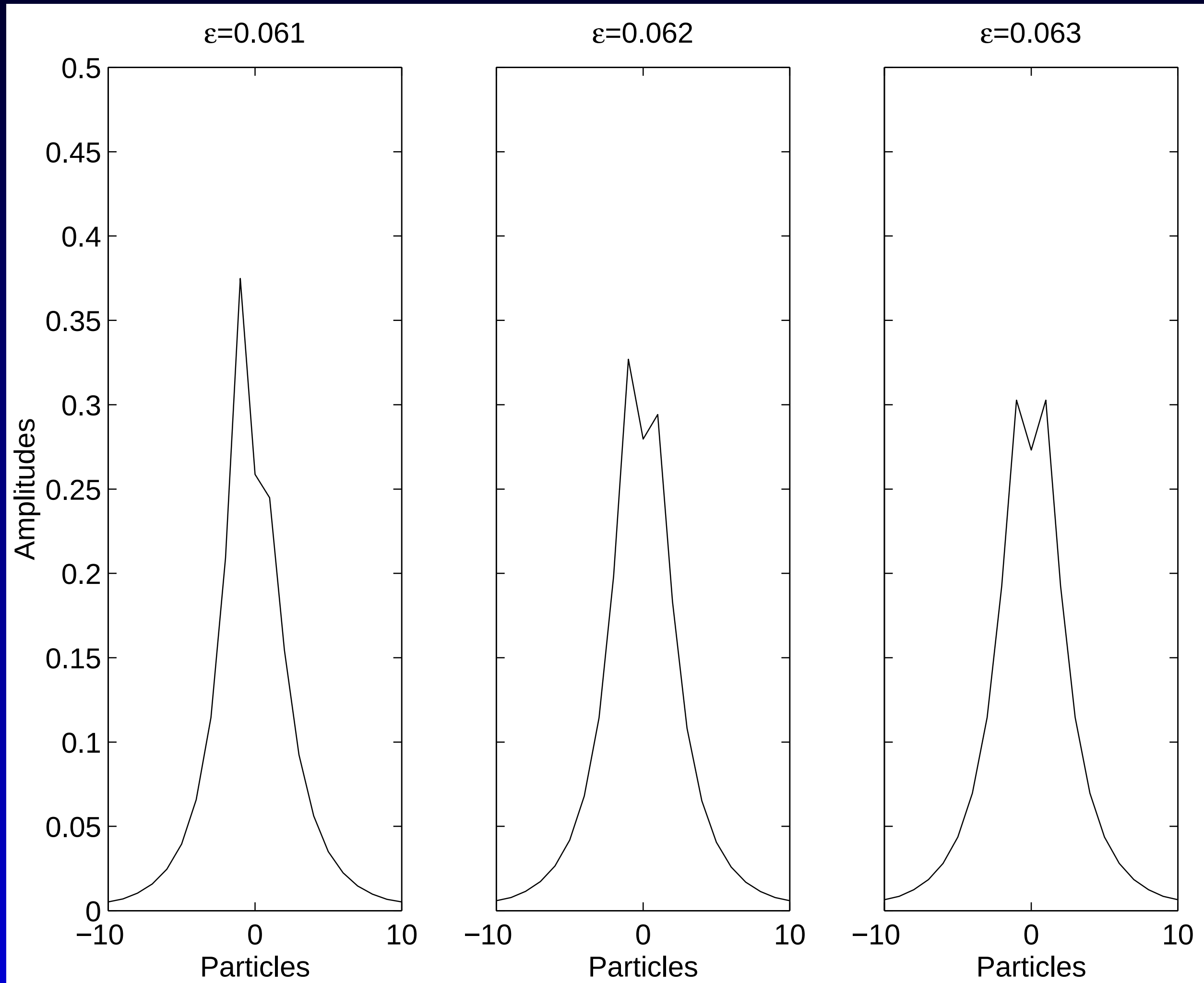


Central breather stability

Floquet arguments and moduli

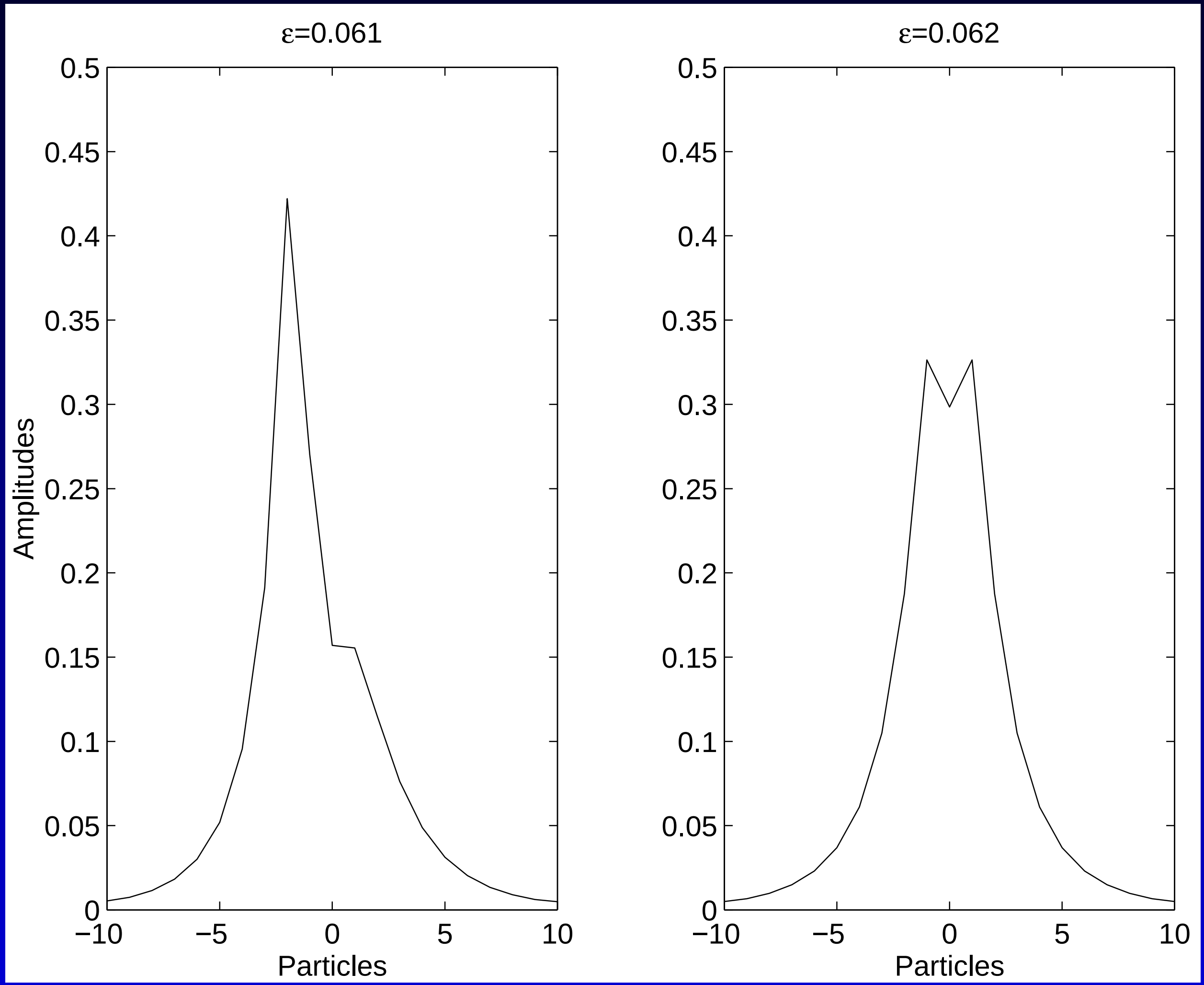


Lateral breather bifurcation



Inverse symmetry breaking. Curvature $\kappa = 4$

Second breather bifurcation



Inverse symmetry breaking. Curvature $\kappa = 4$

Coupling regimes

For $\kappa < \kappa_c \simeq 7$

- Low coupling: $\varepsilon \lesssim 0.3$
  The systems feels weakly the curvature
- Intermediate coupling: $0.3 \lesssim \varepsilon \lesssim 0.7$
  With increasing curvature bifurcation to the double humped mode, with inverse symmetry breaking bifurcations
- High coupling: $0.7 \lesssim \varepsilon$
  Soft transition to the double humped mode

The nonlinearity is able to maintain the asymmetry

Conclusions

The curvature of the systems brings about accumulation of energy at the bending points through different mechanisms:

- Soft on–site potential with attractive interaction:
  - Instability of the neighbours
  - Switching of position
- Hard on–site potential with repulsive interaction:
  - Bifurcations with inverse symmetry breaking
  - Soft transitions to symmetric breathers

References

- *Numerical study of breathers in a bent chain of oscillators with long range interaction*
  JFR Archilla, PL Christiansen, SF Mingaleev and Yu B Gaididei
  J Phys A-Math Gen 34 (33), 2001.
- *Interplay of nonlinearity and geometry in a DNA-related, Klein-Gordon model with long-range, dipole-dipole interaction*
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  Phys. Rev. E. 65(1), 2001.

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