Isaac Newton Institute, 6 July 2007

High oscillations versus parasitic solutions

Ernst Hairer, Geneva

Joint work with Christian Lubich

Aim of the talk

Ideas of a theory – modulated Fourier expansion – that permits to treat the long-time behaviour of

- analytic (and numerical) solutions of highly oscillatory differential equations
- numerical solution of linear multistep methods

Outline of the talk

I) Results on the long-time behaviour of
highly oscillatory differential equations

$$\ddot{q} + \omega^2 q = -\nabla U(q)$$

II) Long-time behaviour of
linear multistep methods for $\ddot{q} = -\nabla U(q)$

III) **modulated Fourier expansion**
combined long-time error analysis

IV) **numerical illustration**

I. Highly oscillatory problems

Problem: $\ddot{q} + \omega^2 q = -\nabla U(q)$ with large ω.

- **Total energy** $$H(t) = \frac{1}{2}\dot{q}^T\dot{q} + \frac{\omega^2}{2}q^Tq + U(q)$$

  satisfies $H(t) = \textit{const}$ along solutions.

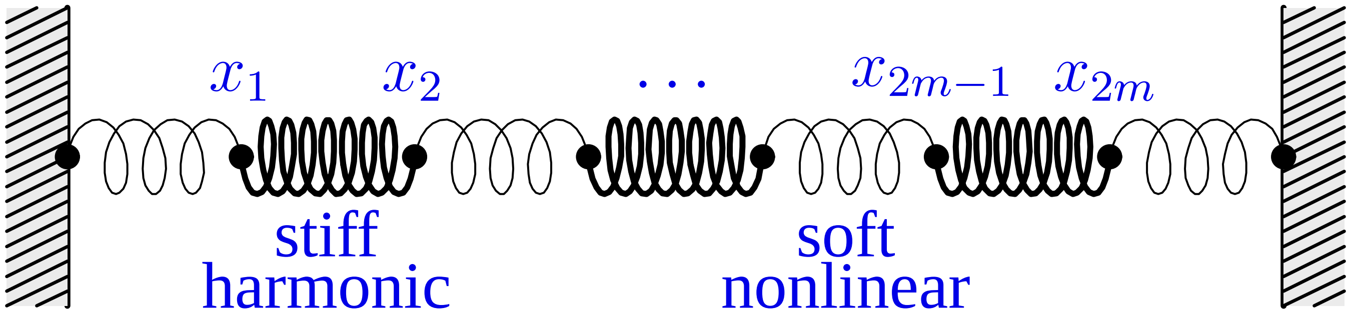
- **Harmonic energy** $$I(t) = \frac{1}{2}\dot{q}^T\dot{q} + \frac{\omega^2}{2}q^Tq$$

  satisfies $I(t) = \textit{const} + \mathcal{O}(\omega^{-1})$ along solutions

  on intervals of length $t \le T = \mathcal{O}(e^{\gamma\omega})$.

  (Benettin, Galgani & Giorgilli, 1987)

Example: FPU type problem



With the change of coordinates

$$q_{0,j} = \frac{1}{\sqrt{2}}(x_{2j} + x_{2j-1}), \qquad q_{1,j} = \frac{1}{\sqrt{2}}(x_{2j} - x_{2j-1})$$

the differential equation becomes

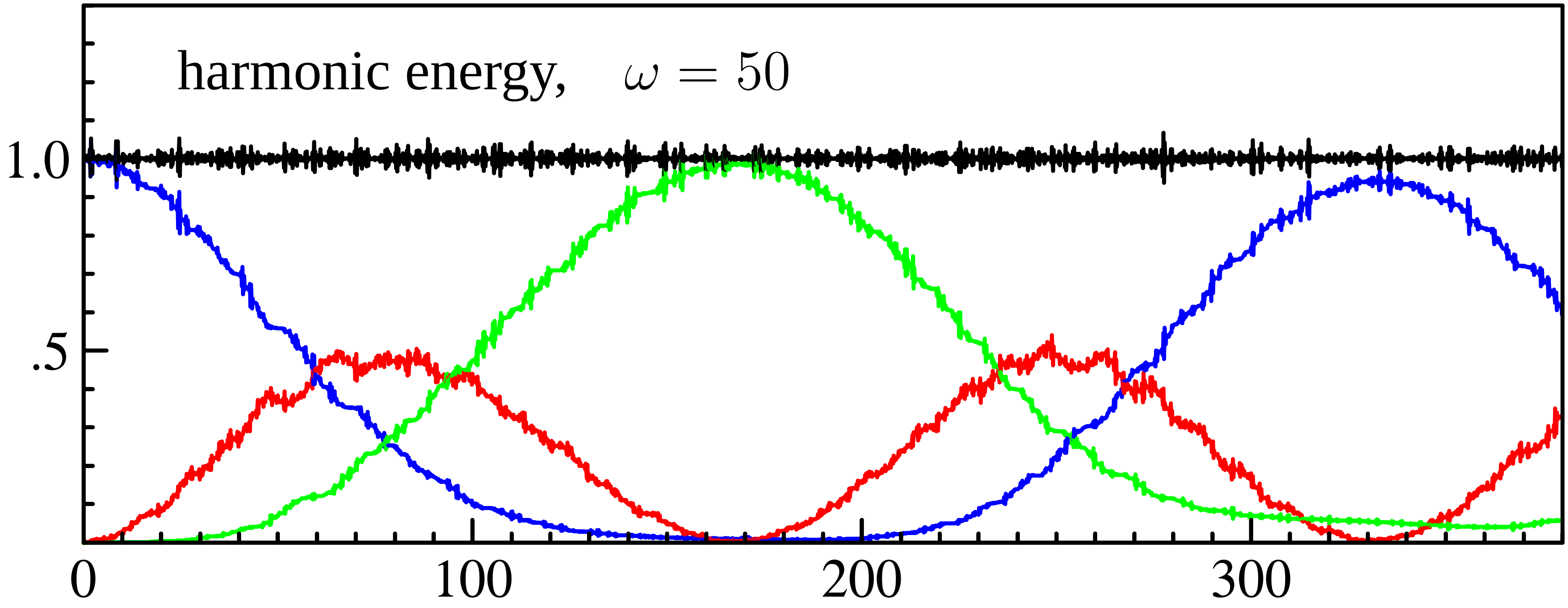
$$\boxed{\begin{aligned} \ddot{q}_0 \qquad\qquad &= -\nabla_{q_0} U(q_0, q_1) \\ \ddot{q}_1 + \omega^2 q_1 &= -\nabla_{q_1} U(q_0, q_1) \end{aligned}}$$

$q_0 \in \mathbb{R}^3 \; \dots$ displacements from the position of rest of the stiff springs,

$q_1 \in \mathbb{R}^3 \; \dots$ expansion/compression of the stiff springs.

Example: FPU type problem (cont.)

Harmonic energies I_1, I_2, I_3, and $I = I_1 + I_2 + I_3$.



II. Linear multistep methods

Problem: $\ddot{q} = f(q)$ with $f(q) = -\nabla U(q)$

Multistep method: $$\sum_{j=0}^{k} \alpha_j \, q_{n+j} \;=\; h^2 \sum_{j=0}^{k} \beta_j \, f(q_{n+j})$$

- **Total energy** $$\boxed{H(t) \;=\; \frac{1}{2}\,\dot{q}^T \dot{q} + U(q)}$$

  does it remain nearly constant along numerical solutions?

- **Harmonic energy ?**

  what is its analogue in this situation ?

Numerical experiment

Multistep method:
$$\sum_{i=0}^{k} \alpha_i \, q_{n+i} \;=\; h^2 \sum_{i=0}^{k} \beta_i \, f(q_{n+i})$$

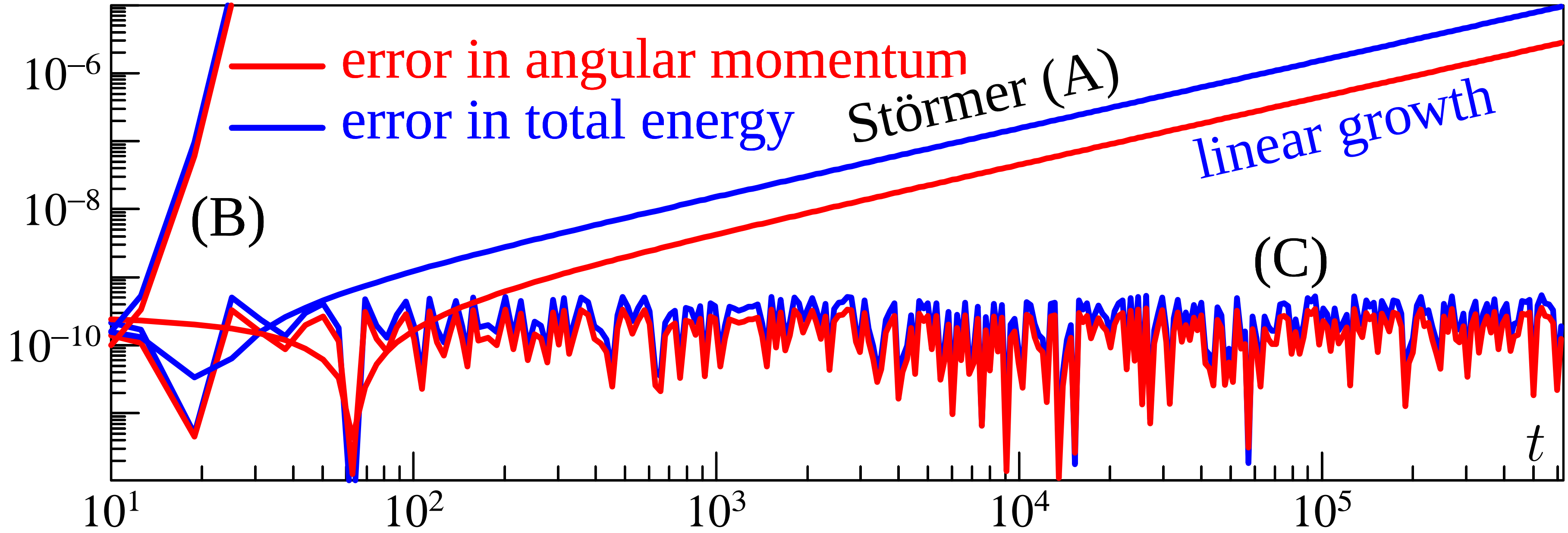
Char. polynomials: $\rho(\zeta) = \sum_{i=0}^k \alpha_i \zeta^i, \;\; \sigma(\zeta) = \sum_{i=0}^k \beta_i \zeta^i$

Methods used for the numerical experiment:

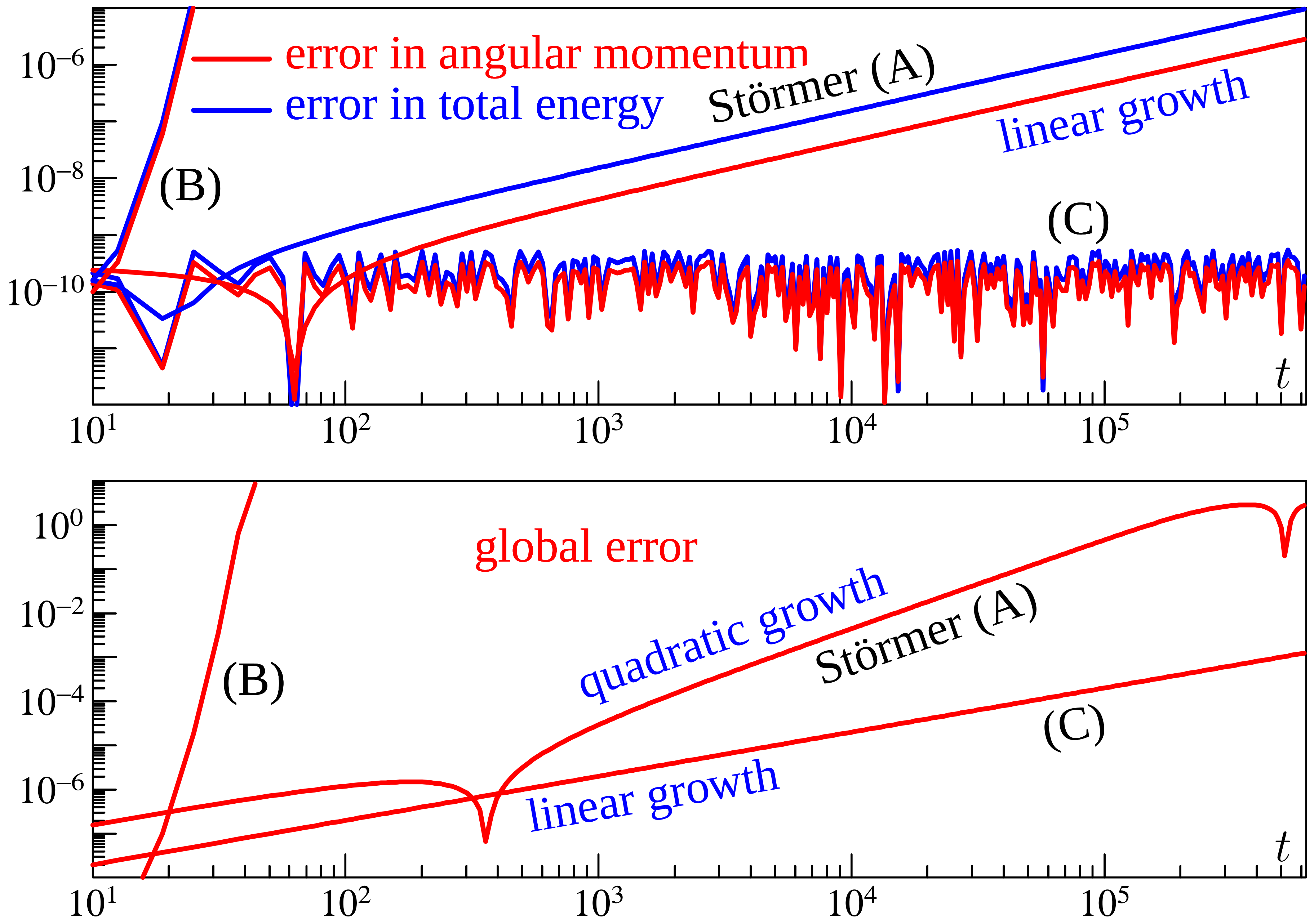
(A)	$\rho(\zeta) = (\zeta - 1)^2 \zeta^6$	(Störmer)
(B)	$\rho(\zeta) = (\zeta^4 - 1)^2$	(symmetric)
(C)	$\rho(\zeta) = (\zeta - 1)(\zeta^7 - 1)$	(symmetric, s-stable)

with $\sigma(\zeta)$ such that the methods are explicit and of order 8.

Numerical experiment: Kepler problem ($e = 0.2$)



Numerical experiment: Kepler problem   ($e = 0.2$)



Theorem.

Consider a linear multistep method that is

s-stable, symmetric, of order p

with sufficiently accurate starting approximations. Then,

$$H(q_n, \dot{q}_n) = H(q_0, \dot{q}_0) + \mathcal{O}(h^p) \quad \textit{for} \quad nh \leq \mathcal{O}(h^{-p-2})$$

Theorem.

Consider a linear multistep method that is

s-stable,   symmetric,   of order p

with sufficiently accurate starting approximations. Then,

$$H(q_n, \dot{q}_n) = H(q_0, \dot{q}_0) + \mathcal{O}(h^p) \quad \textit{for} \quad nh \leq \mathcal{O}(h^{-p-2})$$

A similar statement holds for

- angular momentum in N-body problems
- all action variables in nearly integrable systems

III. Modulated Fourier expansion

for

highly oscillatory problems (HOP)

and

linear multistep methods (LMM)

Two time scales (HOP)

In the equation $\frac{d^2q}{dt^2} + \omega^2 q = -\nabla U(q)$ there are

- **fast time** ωt , oscillations $e^{\pm i\omega t}$
- **slow time** t due to non-linearity (which is small)

Two time scales (HOP)

In the equation $\frac{d^2q}{dt^2} + \omega^2 q = -\nabla U(q)$ there are

- **fast time** ωt, oscillations $e^{\pm i\omega t}$
- **slow time** t due to non-linearity (which is small)

For the linear problem (absence of $U(q)$)

$$q(t) = c_{-1}e^{-i\omega t} + c_1 e^{i\omega t}$$

Ansatz for the general situation

$$q(t) = \sum_{|j|\le 2N} z_j(t)\, e^{ij\omega t}$$

with smooth functions $z_j(t)$, such that the defect is $\mathcal{O}(\omega^{-N})$.

Two time scales (LMM)

In the method $\sum_{i=0}^{k} \alpha_i \, q_{n+i} = h^2 \sum_{i=0}^{k} \beta_i \, f(q_{n+i})$ there are

- **fast time** t/h parasitic solutions $\zeta_j^n = \zeta_j^{t/h}$, $\quad \rho(\zeta_j) = 0$
- **slow time** t dynamics of the differential equation

Two time scales (LMM)

In the method $\sum_{i=0}^{k} \alpha_i \, q_{n+i} = h^2 \sum_{i=0}^{k} \beta_i \, f(q_{n+i})$ there are

- **fast time** t/h parasitic solutions $\zeta_j^n = \zeta_j^{t/h}$, $\quad \rho(\zeta_j) = 0$
- **slow time** t dynamics of the differential equation

For the linear difference equation (absence of $f(q)$)

$$q_n = c_0 + c_{0,1} n + c_{-1} \zeta_{-1}^n + c_1 \zeta_1^n + \ldots$$

Ansatz for the general situation

$$q_n = q(nh), \quad q(t) = \sum_{j \in \mathcal{I}} z_j(t) \, \zeta_j^{t/h}$$

with smooth functions $z_k(t)$, such that the defect is $\mathcal{O}(h^N)$.

Step 1: Existence of smooth coefficient functions

HOP: insert $q(t) = \sum_j z_j(t)\, e^{ij\omega t}$ into $\ddot{q} + \omega^2 q = -\nabla U(q)$ and compare the coefficients of $e^{ij\omega t}$

$$(1 - j^2)\,\omega^2\, z_j + 2\, ij\,\omega\, \dot{z}_j + \ddot{z}_j + \ldots = 0$$

Step 1: Existence of smooth coefficient functions

HOP: insert $q(t) = \sum_j z_j(t)\, e^{ij\omega t}$ into $\ddot{q} + \omega^2 q = -\nabla U(q)$

and compare the coefficients of $e^{ij\omega t}$

$$(1 - j^2)\,\omega^2\, z_j + 2\, ij\, \omega\, \dot{z}_j + \ddot{z}_j + \ldots = 0$$

LMM: insert $q_n = \sum_j z_j(t_n)\, \zeta_j^n$ into

$$\sum_{i=0}^k \alpha_i\, q_{n+i} \;=\; h^2 \sum_{i=0}^k \beta_i\, f(q_{n+i})$$

and compare the coefficients of ζ_j^n

$$\rho(\zeta_j\, e^{hD})\, z_j = h^2 \sigma(\zeta_j\, e^{hD})\, \ldots$$

This yields

$$\left(\frac{\rho}{\sigma}\right)(\zeta_j)\, z_j + \left(\frac{\rho}{\sigma}\right)'(\zeta_j)\, \zeta_j h\, \dot{z}_j + c_{j,2} h^2\, \ddot{z}_j + \ldots = 0$$

Step 2: Hamiltonian structure for coefficient functions

$$\mathcal{U}(\vec{z}) \;=\; U(z_0) + \sum_{m\geq 1} \frac{1}{m!} \sum_{j_1,\ldots,j_m} U^{(m)}(z_0)(z_{j_1}, \ldots, z_{j_m})$$

HOP: coefficients of $q(t) = \sum_j z_j(t)\, e^{ij\omega t}$ satisfy

$$(1 - j^2)\,\omega^2\, z_j + 2\, ij\,\omega\, \dot{z}_j + \ddot{z}_j + \nabla_{z_{-j}}\mathcal{U}(\vec{z}) = 0$$

Step 2: Hamiltonian structure for coefficient functions

$$\mathcal{U}(\vec{z}) = U(z_0) + \sum_{m\geq 1} \frac{1}{m!} \sum_{j_1,\ldots,j_m} U^{(m)}(z_0)(z_{j_1},\ldots,z_{j_m})$$

HOP: coefficients of $q(t) = \sum_j z_j(t)\, e^{ij\omega t}$ satisfy

$$(1-j^2)\,\omega^2\, z_j + 2\, ij\, \omega\, \dot{z}_j + \ddot{z}_j + \nabla_{z_{-j}}\mathcal{U}(\vec{z}) = 0$$

LMM: coefficients of $q_n = \sum_j z_j(t_n)\, \zeta_j^n$ satisfy

$$c_{j,0}\, z_j + c_{j,1} h\, \dot{z}_j + c_{j,2} h^2 \ddot{z}_j + \ldots + h^2 \nabla_{z_{-j}}\mathcal{U}(\vec{z}) = 0$$

where

$$c_{j,0} + c_{j,1} x + c_{j,2} x^2 + \ldots = \left(\frac{\rho}{\sigma}\right)(\zeta_j e^{ix})$$

Step 3 . . . etc.

HOP:

- Existence of formal invariants $\mathcal{H}(t)$ and $\mathcal{I}(t)$ in the system for the coefficient functions $z_j(t)$
- Closeness of the formal invariants to the Hamiltonian and the harmonic energy

Step 3 . . . etc.

HOP:

- Existence of formal invariants $\mathcal{H}(t)$ and $\mathcal{I}(t)$ in the system for the coefficient functions $z_j(t)$
- Closeness of the formal invariants to the Hamiltonian and the harmonic energy

---

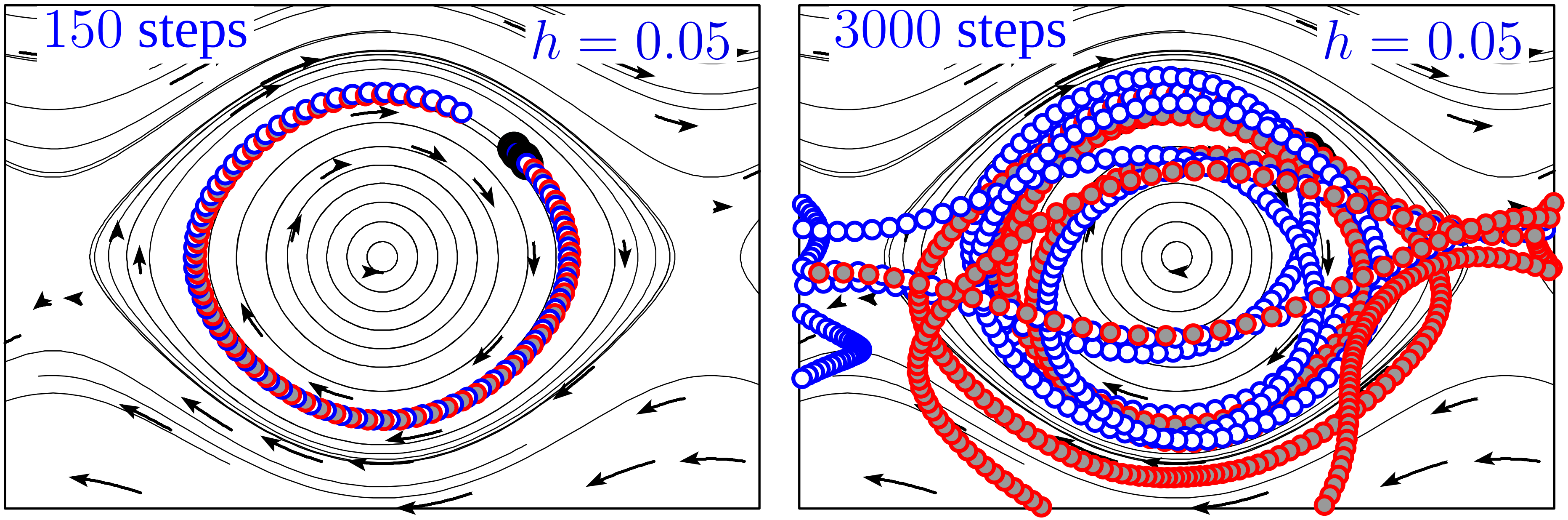
LMM:

- Existence of a formal invariant $\mathcal{H}(t)$ and of near-invariants $\mathcal{I}_\ell(t)$ (derivative of size $\mathcal{O}(h\delta^3)$) in the system for the coefficient functions $z_j(t)$
- Closeness of $\mathcal{H}(t)$ to the Hamilonian and of $\mathcal{I}_\ell(t)$ to the ℓ-th parasitic solution.

IV. Numerical illustration

Unstable propagation of perturbations in the starting values

$$\rho(\zeta) = (\zeta - 1)^2(\zeta + 1)^2, \qquad \sigma(\zeta) = \frac{4}{3}(\zeta + \zeta^2 + \zeta^3)$$

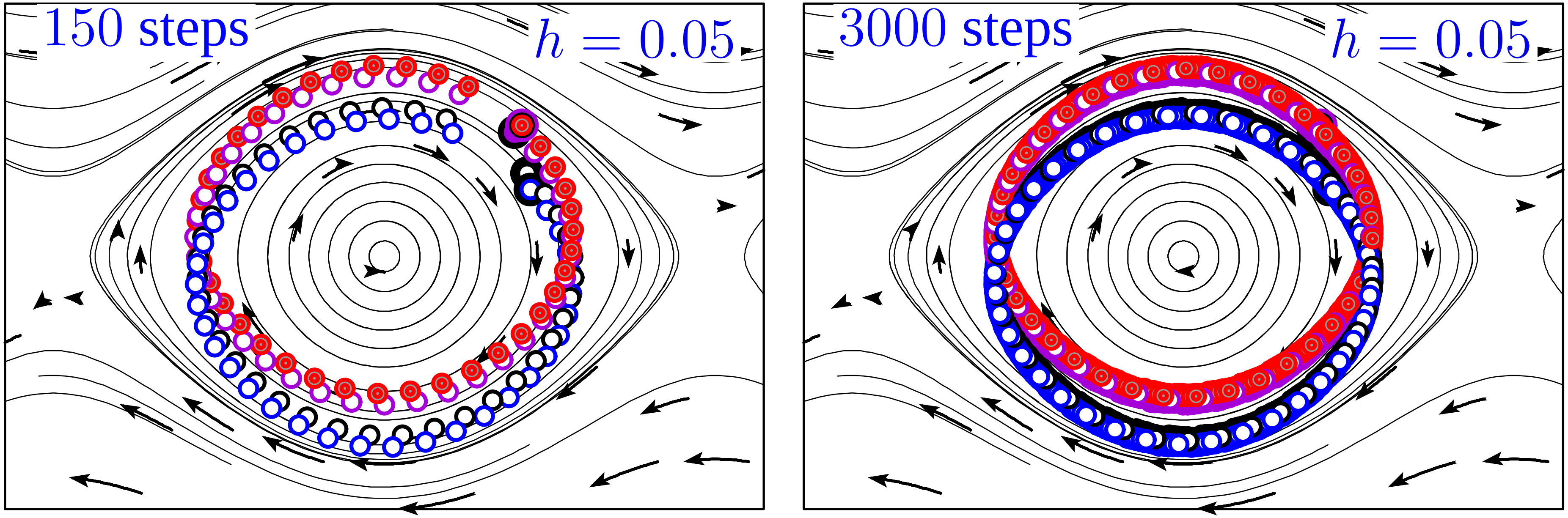


Numerical solution can be written as

$$q_n = y(nh) + (-1)^n z(nh)$$

Stable propagation of perturbations in the starting values

$$\rho(\zeta) = (\zeta - 1)^2(\zeta^2 + 1), \qquad \sigma(\zeta) = \frac{1}{6}(7\zeta - 2\zeta^2 + 7\zeta^3)$$

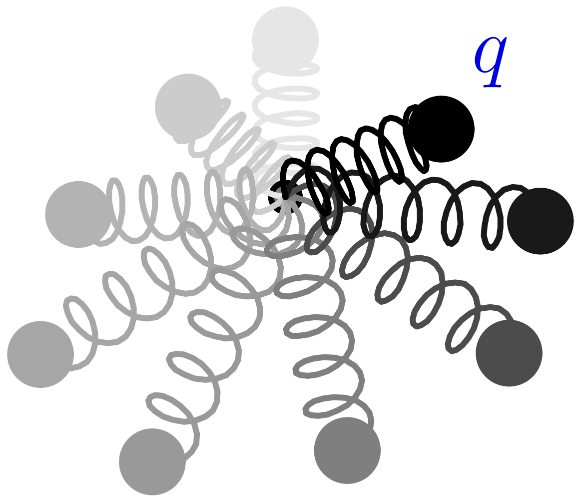


Numerical solution can be written as

$$q_n = y(nh) + i^n z_1(nh) + (-i)^n \overline{z_1(nh)} + (-1)^n z_2(nh)$$

Example: spring pendulum with gravity and attraction

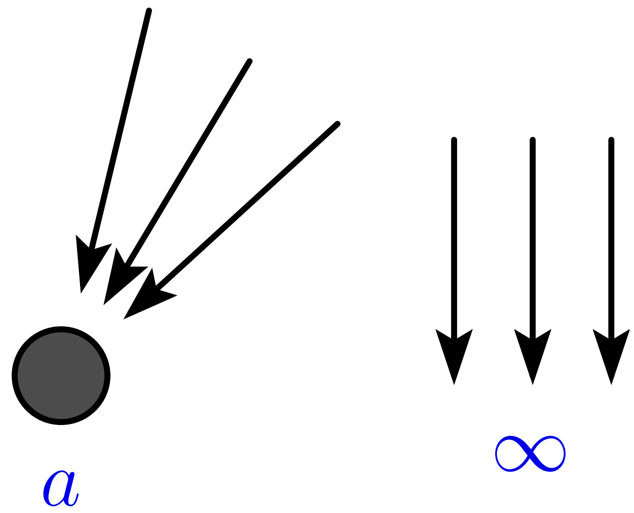
Two degrees of freedom $q = (q_1, q_2)^T$



$$U(q) = \frac{\omega^2}{2}\Big(\|q\| - 1\Big)^2 + q_2 - \frac{1}{\|q - a\|}$$

where $\omega = 2$,

and $a = (-3, -5)^T$



Numerical comparison (methods of order 4)