Long-time analysis of Hamiltonian partial differential equations and their discretizations

Ludwig Gauckler – Universität Tübingen
gauckler@na.uni-tuebingen.de

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A linear Schrödinger equation

Free Schrödinger equation

$$i\frac{\partial}{\partial t}\psi = -\Delta\psi, \quad \psi = \psi(x,t),$$

$$x \in \mathbb{T} = \mathbb{R}/(2\pi\mathbb{Z}) \quad \text{(periodic b. c.)}$$

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The same equation in terms of the Fourier coefficients

$$i\frac{d}{dt}\xi_j(t) = j^2\xi_j(t) \qquad (j \in \mathbb{Z})$$

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The same equation in terms of the Fourier coefficients

$$i\frac{d}{dt}\xi_j(t) = j^2\xi_j(t) = \frac{\partial H}{\partial \eta_j}(\xi(t),\overline{\xi(t)}) \qquad (j \in \mathbb{Z})$$

with $\xi = (\xi_j)_{j\in\mathbb{Z}}$ and the Hamiltonian function

$$H(\xi,\eta) = \sum_{j\in\mathbb{Z}} j^2\xi_j\eta_j$$

A nonlinear Schrödinger equation

Cubic nonlinear Schrödinger equation

$$i\frac{\partial}{\partial t}\psi = -\Delta\psi + |\psi|^2\psi, \quad \psi = \psi(x,t) = \sum_{j\in\mathbb{Z}} \xi_j(t) e^{ijx},$$

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The same equation in terms of the Fourier coefficients

$$i\frac{d}{dt}\xi_j(t) = j^2\xi_j(t) + \sum_{k_1+k_2-\ell_1=j} \xi_{k_1}(t)\xi_{k_2}(t)\overline{\xi_{\ell_1}(t)} = \frac{\partial H}{\partial \eta_j}(\xi(t),\overline{\xi(t)})$$

with $\xi = (\xi_j)_{j\in\mathbb{Z}}$ and the Hamiltonian function

$$H(\xi,\eta) = \sum_{j\in\mathbb{Z}} j^2\xi_j\eta_j + \frac{1}{2}\sum_{k_1+k_2-\ell_1-\ell_2=0} \xi_{k_1}\xi_{k_2}\eta_{\ell_1}\eta_{\ell_2}$$

Hamiltonian differential equations

A Hamiltonian differential equation ...

... is an equation of the form

$$i\frac{d}{dt}\xi_j(t) = \frac{\partial H}{\partial \eta_j}(\xi(t), \overline{\xi(t)}) \qquad (j \in \mathcal{N})$$

- $\xi = (\xi_j)_{j\in\mathcal{N}} \subseteq \mathbb{C}$ with a set of indices $\mathcal{N} \subseteq \mathbb{Z}^d$
- Hamiltonian function $H : \mathcal{U} \times \mathcal{U} \to \mathbb{C}$ defined on open subset of $l_s^2 \times l_s^2$ with

$$l_s^2 = \left\{ \xi = (\xi_j)_{j\in\mathcal{N}} : \|\xi\|_s = \Big(\sum_{j\in\mathcal{N}} |j|^{2s} |\xi_j|^2\Big)^{\frac{1}{2}} < \infty \right\},$$

where $|j|^2 = \max(1, j_1^2 + \cdots + j_d^2)$

Hamiltonian differential equations

With real variables

$$\xi_j = \frac{p_j + iq_j}{\sqrt{2}}$$

and Hamiltonian function

$$\widetilde{H}(q,p) = H(\xi,\overline{\xi})$$

we get

$$\frac{d}{dt}q_j(t) = \frac{\partial \widetilde{H}}{\partial p_j}(q(t),p(t))$$
$$\frac{d}{dt}p_j(t) = -\frac{\partial \widetilde{H}}{\partial q_j}(q(t),p(t))$$

Conserved quantities I

Conservation of energy

exact conservation of energy

$$H(\xi, \overline{\xi})$$

along solutions of Hamiltonian differential equations

Known: Long-time near-conservation of energy along symplectic discretizations of Hamiltonian ODEs

Question: Discretizations of Hamiltonian PDEs?

discretizations of HamPDEs	HamPDEs
long-time behaviour of energy?	exact conservation of energy

discretizations of HamPDEs	nonlinear HamPDEs	linear HamPDEs
long-time behaviour of energy?	exact conservation of energy	exact conservation of energy

Conserved quantities II

Conservation of actions

exact conservation of actions

$$I_j(\xi, \overline{\xi}) = |\xi_j|^2 \qquad (j \in \mathcal{N})$$

(only) along solutions of linear Hamiltonian differential equations

$$i \frac{d}{dt} \xi_j(t) = \frac{\partial H}{\partial \eta_j}(\xi(t), \overline{\xi(t)}) = \omega_j \xi_j(t)$$

with real frequencies ω_j and $H(\xi, \eta) = \sum_{j \in \mathcal{N}} \omega_j \xi_j \eta_j$

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Known: Long-time near-conservation of actions along weakly nonlinear Hamiltonian ODEs (perturbation theory)

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Question: Hamiltonian PDEs?

Question: discretizations of Hamiltonian PDEs?

discretizations of weakly nonlinear HamPDEs	weakly nonlinear HamPDEs	linear HamPDEs
long-time behaviour of energy?	exact conservation of energy	exact conservation of energy
long-time behaviour of actions?	long-time behaviour of actions?	exact conservation of actions

discretizations of weakly nonlinear HamPDEs	weakly nonlinear HamPDEs	linear HamPDEs
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Weakly nonlinear Hamiltonian PDEs

Nonlinear perturbation of linear Hamiltonian PDE

$$H(\xi,\eta)=\sum_{j\in\mathcal{N}}\omega_j\xi_j\eta_j+P(\xi,\eta)$$

with P (at least) cubic

$$i\frac{d}{dt}\xi_j(t)=\omega_j\xi_j(t)+\frac{\partial P}{\partial\eta_j}(\xi(t),\overline{\xi(t)})$$

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$$i\frac{d}{dt}\xi_j(t) = \omega_j \xi_j(t) + \frac{\partial P}{\partial \eta_j}(\xi(t),\overline{\xi(t)})$$

Nonlinear effects are small for small initial values

$$\|\xi(0)\|_s = \Big(\sum_{j\in\mathcal{N}} |j|^{2s} |\xi_j(0)|^2\Big)^{\frac{1}{2}} \le \varepsilon$$

Weakly nonlinear Hamiltonian PDEs

Nonlinear perturbation of linear Hamiltonian PDE

$$H(\xi,\eta) = \sum_{j\in\mathcal{N}} \omega_j \xi_j \eta_j + P(\xi,\eta)$$

with P (at least) cubic

$$i\varepsilon^{-1}\frac{d}{dt}\xi_j(t) = \omega_j\varepsilon^{-1}\xi_j(t) + \varepsilon^{-1}\frac{\partial P}{\partial \eta_j}(\xi(t),\overline{\xi(t)})$$

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$$H(\xi,\eta) = \sum_{j\in\mathcal{N}} \omega_j \xi_j \eta_j + P(\xi,\eta)$$

with P (at least) cubic

$$i\frac{d}{dt}\widetilde{\xi}_j(t) = \omega_j \widetilde{\xi}_j(t) + \varepsilon^{-1}\frac{\partial P}{\partial \eta_j}\big(\varepsilon\widetilde{\xi}_j(t), \overline{\varepsilon\widetilde{\xi}_j(t)}\big)$$

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Weakly nonlinear Hamiltonian PDEs

Nonlinear perturbation of linear Hamiltonian PDE

$$H(\xi,\eta) = \sum_{j\in\mathcal{N}} \omega_j \xi_j \eta_j + P(\xi,\eta)$$

with P (at least) cubic

$$i \frac{d}{dt}\widetilde{\xi}_j(t) = \omega_j \widetilde{\xi}_j(t) + O(\varepsilon)$$

Nonlinear effects are small for small initial values

$$\|\xi(0)\|_s = \Big(\sum_{j\in\mathcal{N}} |j|^{2s} |\xi_j(0)|^2\Big)^{\frac{1}{2}} \le \varepsilon$$

Long-time near-conservation of actions

Theorem

Fix N. Under assumptions of

- *small initial values* $\|\xi(0)\|_s \le \varepsilon$
- *regularity of the nonlinearity P*
- *non-resonance of the frequencies* ω_j
- *small dimension or zero momentum*

we have near-conservation of actions

$$\sum_{j \in \mathcal{N}} |j|^{2s} \frac{|I_j(\xi(t), \overline{\xi(t)}) - I_j(\xi(0), \overline{\xi(0)})|}{\varepsilon^2} \le C_N \varepsilon^{\frac{1}{2}}$$

over long times

$$0 \le t \le \varepsilon^{-N}$$

Related results: Bambusi, Grébert (2006), Cohen, Hairer, Lubich (NLW, 2008), G., Lubich (NLS, 2010)

Discussion of the assumptions

- small initial values $\longleftrightarrow$ small nonlinear effects
- non-resonance condition: fulfilled in many situations
  - not for $\omega_j = j^2$: $\quad i\partial_t\psi = -\Delta\psi + |\psi|^2\psi$
  - but for $\omega_j \approx j^2$: $\quad i\partial_t\psi = -\Delta\psi + V(x)(\cdot/*)\psi + |\psi|^2\psi$

Sketch of proof – Modulated Fourier Expansions

Solution of the linear equation $i\frac{\partial}{\partial t}\xi_j = \omega_j \xi_j$:

$$\xi_j(t) = e^{-i\omega_j t}\xi_j(0)$$

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Ansatz for solution of the nonlinear equation:

$$\xi_j(t) = \sum_{\mathbf{k}} \prod_{\ell} e^{-ik_\ell \omega_\ell t} z_j^{\mathbf{k}}$$

where $\mathbf{k} = (k_\ell)_{\ell \in \mathbb{Z}}$ sequ. of integers with finitely many entries $\neq 0$

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$$\xi_j(t) = \sum_{\mathbf{k}} e^{-i(\mathbf{k}\cdot\boldsymbol{\omega})t} z_j^{\mathbf{k}}$$

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Ansatz for solution of the nonlinear equation:

Modulated Fourier expansion (two-scale expansion)

$$\xi_j(t) = \sum_{\mathbf{k}} e^{-i(\mathbf{k}\cdot\boldsymbol{\omega})t} z_j^{\mathbf{k}}(\varepsilon t)$$

where $\mathbf{k} = (k_\ell)_{\ell\in\mathbb{Z}}$ sequ. of integers with finitely many entries $\neq 0$, $\quad \mathbf{k}\cdot\boldsymbol{\omega} = \sum_\ell k_\ell \omega_\ell$

HAIRER, LUBICH (2000)

Sketch of proof – Modulation system

Inserting modulated Fourier expansion in equations of motion:

Modulation system

$$i\varepsilon\dot{z}_j^{\mathbf{k}} + (\mathbf{k}\cdot\boldsymbol{\omega})z_j^{\mathbf{k}} = \omega_j z_j^{\mathbf{k}} + \text{nonlinear terms},$$

$$\sum_{\mathbf{k}} z_j^{\mathbf{k}}(0) = \xi_j(0).$$

Sketch of proof – Modulation system

Inserting modulated Fourier expansion in equations of motion:

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$$i\varepsilon\dot{z}_j^{\mathbf{k}} + (\mathbf{k}\cdot\omega)z_j^{\mathbf{k}} = \omega_j z_j^{\mathbf{k}} + \text{nonlinear terms},$$
$$\sum_{\mathbf{k}} z_j^{\mathbf{k}}(0) = \xi_j(0).$$

This is a Hamiltonian differential equation with invariants:

Formal invariants

$$\mathcal{I}_\ell(t) = \sum_{\mathbf{k},j} k_\ell |z_j^{\mathbf{k}}(\varepsilon t)|^2.$$

Sketch of proof – Iterative solution

Iterative construction of modulation functions $z_j^{\mathbf{k}}$ on $[0, \varepsilon^{-1}]$:

- need non-resonance condition on frequencies ω_j
- small defect: ε^{N+2}
- formal invariants $\mathcal{I}_\ell$ become almost invariants:

$$|\mathcal{I}_\ell(t) - \mathcal{I}_\ell(0)| \leq C\varepsilon^{N+2}$$

- almost invariants $\mathcal{I}_\ell$ are close to actions:

$$|\mathcal{I}_\ell(t) - I_\ell(t)| \leq C\varepsilon^{5/2}$$

Sketch of proof – Long time intervals

On $[0, \varepsilon^{-1}]$:

- almost invariants $\mathcal{I}_\ell$ (ε^{N+2}) close to actions I_ℓ ($\varepsilon^{5/2}$)

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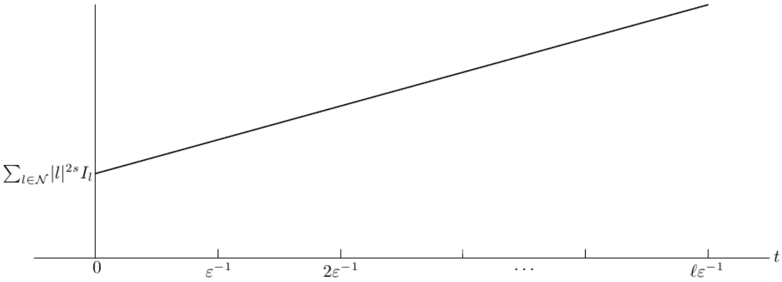

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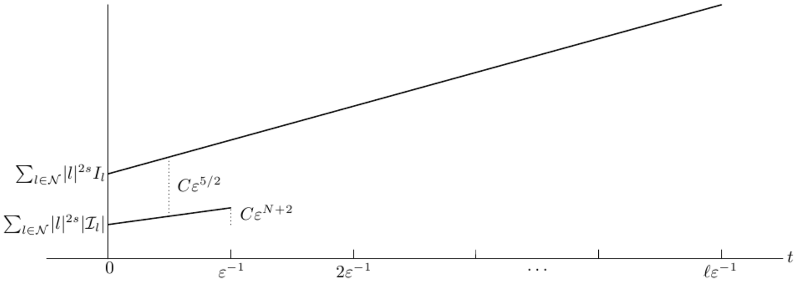

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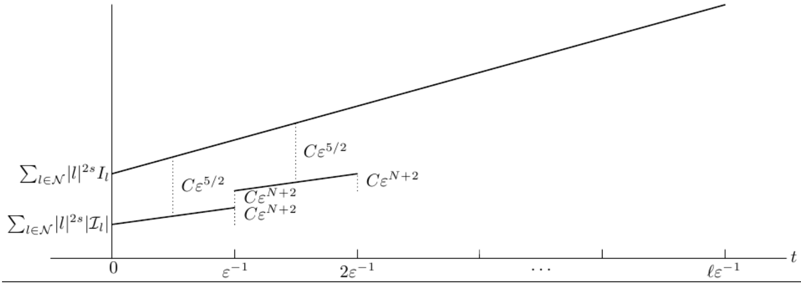

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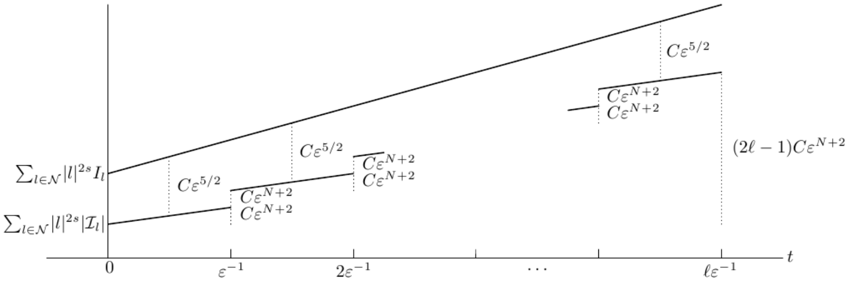

Patch short time intervals together to long time interval $[0, \varepsilon^{-N}]$

discretizations of weakly nonlinear HamPDEs	weakly nonlinear HamPDEs	linear HamPDEs
long-time behaviour of energy?	exact conservation of energy	exact conservation of energy
long-time behaviour of actions?	long-time near-cons. of actions	exact conservation of actions

Lie–Trotter splitting in time

Split differential equation

$$i\frac{d}{dt}\xi_j(t) = \omega_j\xi_j(t) + \frac{\partial P}{\partial \eta_j}(\xi(t), \overline{\xi(t)})$$

and solve separately

$$i\frac{d}{dt}\xi_j(t) = \omega_j\xi_j(t) \qquad\qquad i\frac{d}{dt}\xi_j(t) = \frac{\partial P}{\partial \eta_j}(\xi(t), \overline{\xi(t)})$$

Use flows of these equations for approximating $\xi^n \approx \xi(nh)$:

Lie–Trotter splitting

$$\xi^n = \Phi_h^{\text{linear}} \circ \Phi_h^P(\xi^{n-1})$$

Spectral collocation method in space (Example NLS)

- Ansatz

$$\psi^M(x,t) = \sum_{j \in \mathcal{N}_M} \xi_j(t) e^{ijx}$$

with finite set of indices

$$\mathcal{N}_M = \{-M, \ldots, M-1\}.$$

- Insert ψ^M in NLS and evaluate at collocation points

$$x_k = k\frac{\pi}{M}, \quad k \in \mathcal{N}_M$$

Spectral collocation method

$$i\frac{d}{dt}\psi^M(x_k,t) = (-\Delta\psi^M(\cdot,t))|_{x=x_k} + |\psi^M(x_k,t)|^2\psi^M(x_k,t)$$

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Long-time near-conservation of actions

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- *non-resonance of the frequencies* ω_j *and the step-size h*
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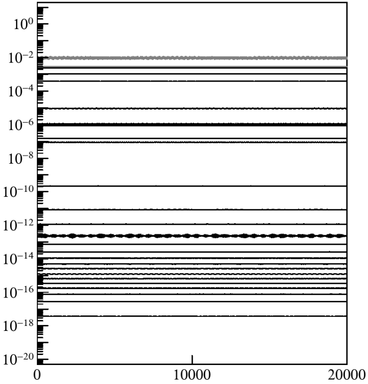
over long times

$$0 \le t_n = nh \le \varepsilon^{-N}$$

Related results: Cohen, Hairer, Lubich (NLW, 2008), G., Lubich (NLS, 2010), Faou, Grébert, Paturel (2010)

Numerical experiment I (NLS)



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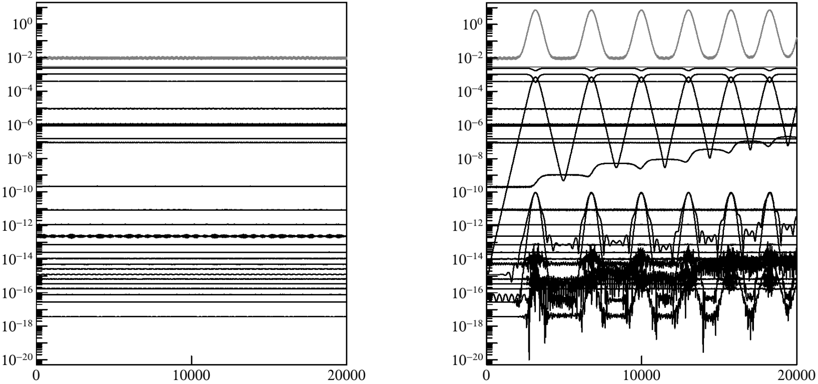
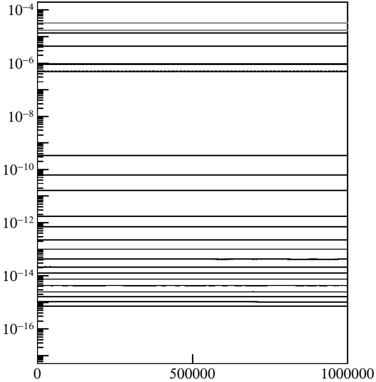
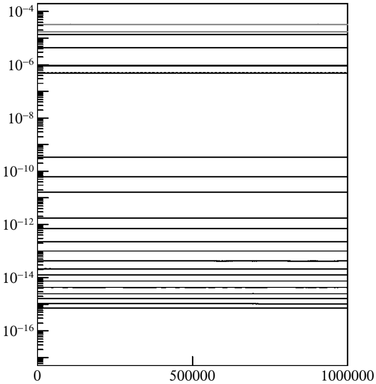


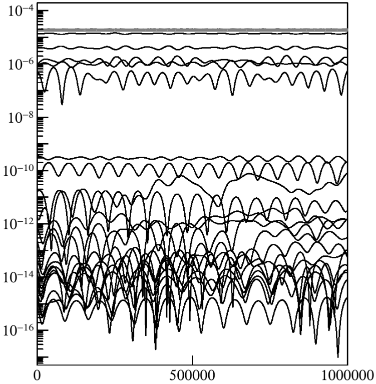
numerical resonance ($h = 2\pi/\omega_{-6}$)

Numerical experiment II (NLS)



Numerical experiment II (NLS)





physical resonance ($V = 0$)

Sketch of proof

Modulated Fourier expansion of the numerical solution:

Modulation system

$$e^{-i(\mathbf{k}\cdot\boldsymbol{\omega})h} z_j^{\mathbf{k}} + \sum_{\ell=1}^{\infty} \frac{(\varepsilon h)^{\ell}}{\ell!} (z_j^{\mathbf{k}})^{(\ell)} e^{-i(\mathbf{k}\cdot\boldsymbol{\omega})h} = e^{-i\omega_j h} z_j^{\mathbf{k}} + \text{nonlinear terms}$$

Recall modulation system for exact solution

$$(\mathbf{k}\cdot\omega) z_j^{\mathbf{k}} + i\varepsilon \dot{z}_j^{\mathbf{k}} = \omega_j z_j^{\mathbf{k}} + \text{nonlinear terms}$$

Similar analysis as for the exact solution!

discretizations of weakly nonlinear HamPDEs	weakly nonlinear HamPDEs	linear HamPDEs
long-time behaviour of energy?	exact conservation of energy	exact conservation of energy
long-time near-cons. of actions	long-time near-cons. of actions	exact conservation of actions

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we have near-conservation of energy

$$\frac{|H(\xi^n, \overline{\xi^n}) - H(\xi^0, \overline{\xi^0})|}{\varepsilon^2} \leq C_N \varepsilon^{\frac{1}{2}}$$

over long times

$$0 \leq t_n = nh \leq \varepsilon^{-N}$$

Related results: Cohen, Hairer, Lubich (NLW, 2008), G., Lubich (NLS, 2010)

Sketch of proof

Energy

$$H(\xi,\overline{\xi}) = \underbrace{\sum_{j\in\mathcal{N}_M} \omega_j I_j(\xi,\overline{\xi})}_{\text{long-time near-conservation}} + \underbrace{P(\xi,\overline{\xi})}_{O(\|\xi\|_s^3)=O(\varepsilon^3)}$$

discretizations of weakly nonlinear HamPDEs	weakly nonlinear HamPDEs	linear HamPDEs
long-time near-cons. of energy	exact conservation of energy	exact conservation of energy
↑		
long-time near-cons. of actions ←	long-time near-cons. of actions	exact conservation of actions