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Pulse propagation in discrete lattices

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- Introduction
- The microscopic model: an oscillator chain
- Dispersive evolution of a single pulse
- Three-wave interaction
- Justification: Method of proof
- Summary

Motivation:

Given a microscopic system of evolution equations, we want to derive and justify a macroscopic equation describing the evolution of macroscopic modulations of microscopic initial data directly.

Justification: Does the approximation that we obtain from the modulation equation stay close to the original solution for some macroscopic time?

Here: Microscopic system = an oscillator chain.
Two examples:

1. Dispersive evolution of a single pulse

G., MIELKE 2004 *Nonlinearity*, 2005 *submitted*

2. Three-wave interaction

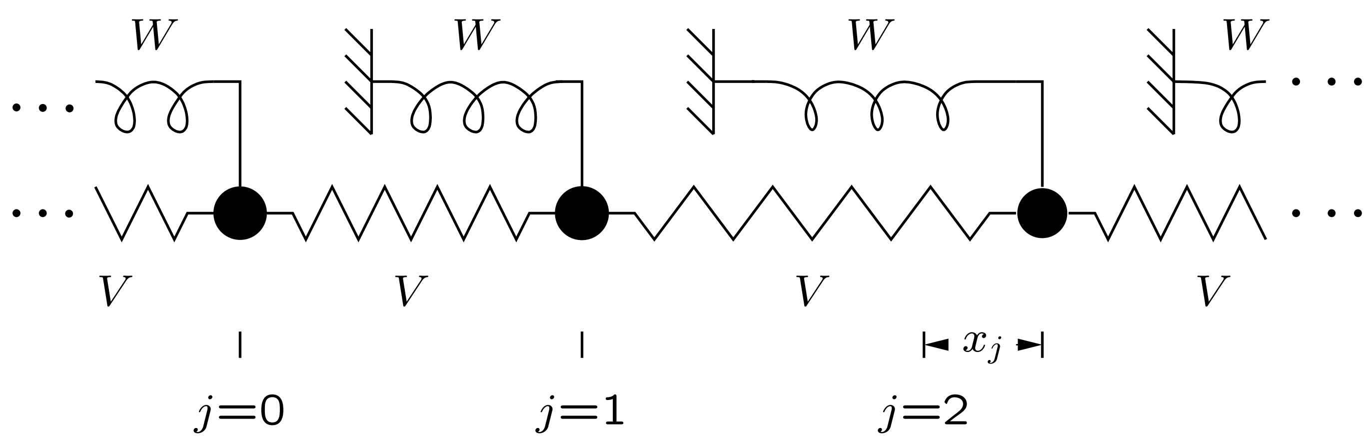
G., MIELKE 2005, *work in progress*

(cf. also SPOHN, The Phonon Boltzmann Equation, Properties and Link to Weakly Anharmonic Lattice Dynamics, April 2005)

$$\ddot{x}_\gamma = \sum_{m=1}^{M} [V'_m(x_{\gamma+m}-x_\gamma) - V'_m(x_\gamma-x_{\gamma-m})] - W'(x_\gamma) \quad (\gamma \in \mathbb{Z}) \tag{OC}$$

$$V_m(d) = \frac{\alpha_{m,1}}{2}d^2 + \frac{\alpha_{m,2}}{3}d^3 + \frac{\alpha_{m,3}}{4}d^4 + \mathcal{O}(d^5)$$ interaction potentials

$$W(y) = \frac{\beta_1}{2}y^2 + \frac{\beta_2}{3}y^3 + \frac{\beta_3}{4}y^4 + \mathcal{O}(y^5)$$ external potential



$$\ddot{x}_\gamma = \sum_{m=1}^{M} \alpha_{m,1}\,(x_{\gamma+m} - 2x_\gamma + x_{\gamma-m}) - \beta_1 x_\gamma$$

Exact (space–time–)periodic solutions

$$x_\gamma(t) = \mathbf{E}(t,\gamma) + \text{c.c.} \quad \text{with} \quad \mathbf{E}(t,\gamma) := \mathrm{e}^{\mathrm{i}(\omega(\vartheta)t + \vartheta\gamma)}$$

if and only if the dispersion relation holds

$$\omega^2(\vartheta) := 2\sum_{m=1}^{M} \alpha_{m,1}[1 - \cos(m\vartheta)] + \beta_1$$

Dispersion: (group velocity) $\omega'(\vartheta) \neq \dfrac{\omega(\vartheta)}{\vartheta}$ (phase velocity)

Stability condition (SC): $\omega^2(\vartheta) > 0$ for all $\vartheta \in (-\pi, \pi]$

Notation: $\mathbf{E}_j(t,\gamma) := \mathrm{e}^{\mathrm{i}(\omega_j t + \vartheta_j \gamma)}$ for fixed ϑ_j, $\omega_j^2 = \omega^2(\vartheta_j)$

Modulation ansatz: We consider solutions x of (OC) of the form

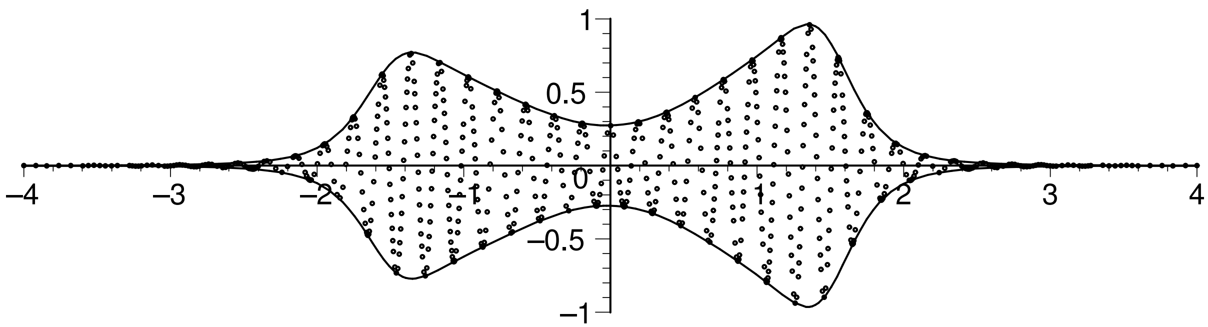
$$x = X_\varepsilon^A + \mathcal{O}(\varepsilon^2) \quad \text{with} \quad (X_\varepsilon^A)_\gamma(t) := \varepsilon A(\tau,\xi)\mathbf{E}_0(t,\gamma) + \text{c.c.}$$

$\mathbf{E}_0(t,\gamma) = \mathrm{e}^{\mathrm{i}(\omega_0 t + \vartheta_0 \gamma)}$: basic microscopic pattern

$\varepsilon A : [0,\tau_0] \times \mathbb{R} \to \mathbb{C}$: modulation (or amplitude) function (coefficient ε: weakly nonlinear case)

$\tau = \varepsilon^2 t$: macroscopic (slow) time variable

$\xi = \varepsilon(\gamma + \omega_0' t)$: macroscopic (long) space variable, coordinate system moving with the group velocity ω_0'



Note: Only this long time scale enables us to observe the effects of dispersion.

Formal derivation:

1. Insert in (OC) the multiscale ansatz ("improved approximation")

$$(Y_\varepsilon^A)_\gamma(t) := (X_\varepsilon^A)_\gamma(t) + \sum_{k=2}^{p} \varepsilon^k \sum_{n=-k}^{k} A_{k,n}(\tau,\xi)\mathbf{E}_0(t,\gamma)^n$$

with $X_\varepsilon^A = \varepsilon A \mathbf{E}_0 + \text{c.c.}, \quad A_{k,-n} = \overline{A}_{k,n}, \quad \tau = \varepsilon^2 t, \quad \xi = \varepsilon(\gamma + \omega_0' t).$

2. Equate for each term $\varepsilon^k \mathbf{E}_0^n$ its coefficient on the left to that on the right.

Result: From $\varepsilon^3 \mathbf{E}_0^1$ we obtain the nonlinear Schrödinger equation (NLS)

$$\mathrm{i}\partial_\tau A = \frac{1}{2}\omega_0''\partial_\xi^2 A + \rho|A|^2 A \quad \text{with} \quad \rho = \rho(\omega_0, \vartheta_0, \alpha_{m,i}, \beta_i)$$

p=3: $A_{2,1}$ undetermined $\Rightarrow$ Set $A_{2,1} \equiv 0$; p=4: From $\varepsilon^4 \mathbf{E}_0^1$ we obtain (A21):

$$\mathrm{i}\partial_\tau A_{2,1} = \frac{1}{2}\omega_0''\partial_\xi^2 A_{2,1} + \rho(2|A|^2 A_{2,1} + A^2 \bar{A}_{2,1}) + c_1\partial_\tau\partial_\xi A + c_2\partial_\xi^3 A + c_3|A|^2\partial_\xi A$$

Nonresonance conditions: $k^2\omega^2(\vartheta_0) - \omega^2(k\vartheta_0) \neq 0$ for $k = 0, 2, \ldots, p$.

Residuum: $[\mathrm{res}(Y_\varepsilon^A)]_\gamma := [\ddot{Y}_\varepsilon^A - LY_\varepsilon^A - N(Y_\varepsilon^A)]_\gamma = \mathcal{O}(\varepsilon^{p+1})$

Justification:

a) If $V_m, W \in \mathrm{C}^5(\mathbb{R})$ and the uniform nonresonance condition (uNR) holds

$$\inf_{s,t=1,2;\ \vartheta,\theta\in(-\pi,\pi]} \Big|\omega(\vartheta)+(-1)^s\omega(\theta)+(-1)^t\omega(\vartheta-\theta)\Big| \geq C_{\mathrm{uNR}} > 0,$$

then for $X_\varepsilon^A = \varepsilon A \mathbf{E}_0 + \text{c.c.}$, $A{:}[0,\tau_0]\times\mathbb{R}\to\mathbb{C}$ solving (NLS) with $A(0,\cdot)\in\mathrm{H}^6(\mathbb{R})$:

$\forall\ c>0\ \exists\ \varepsilon_0, C>0:\ \forall\ \varepsilon\in(0,\varepsilon_0)$ and for any solution x of (OC):

$$\|(x(0),\dot{x}(0)) - (X_\varepsilon^A(0),\dot{X}_\varepsilon^A(0))\|_{\ell^2\times\ell^2} \leq c\,\varepsilon^{3/2} \quad \Rightarrow$$
$$\|(x(t),\dot{x}(t)) - (X_\varepsilon^A(t),\dot{X}_\varepsilon^A(t))\|_{\ell^2\times\ell^2} \leq C\,\varepsilon^{3/2} \quad \text{for} \quad t\in[0,\tau_0/\varepsilon^2]. \qquad \text{(J)}$$

b) If $V_m,\ W \in \mathrm{C}^6(\mathbb{R})$ and the nonresonance condition (NR) holds

$$\inf_{s,t=1,2;\ \theta\in(-\pi,\pi]} \Big|\omega(\vartheta_0)+(-1)^s\omega(\theta)+(-1)^t\omega(\vartheta_0-\theta)\Big| \geq C_{\mathrm{NR}} > 0,$$

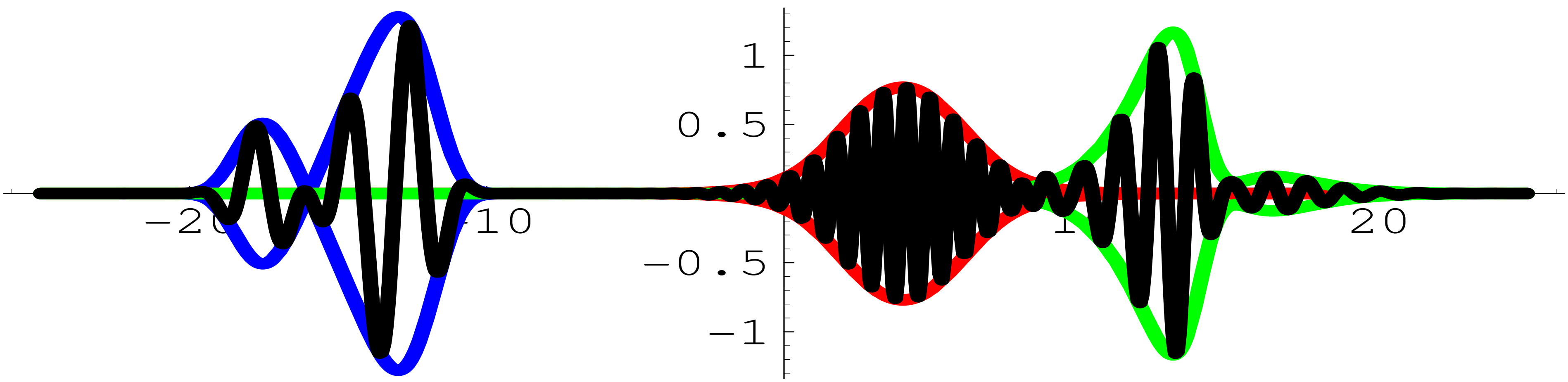
then (J) holds with $X_\varepsilon^{A,2} := \varepsilon A\mathbf{E}_0 + \varepsilon^2(a_1|A|^2 + A_{2,1}\mathbf{E}_0 + a_2A^2\mathbf{E}_0^2) + \text{c.c.}$, where $A, A_{2,1}{:}[0,\tau_0]\times\mathbb{R}\to\mathbb{C}$ solve (NLS),(A21) with $A(0,\cdot)\in\mathrm{H}^7(\mathbb{R})$, $A_{2,1}(0,\cdot)\in\mathrm{H}^6(\mathbb{R})$, and $\varepsilon^{3/2}$ replaced by ε^β with $\beta\in(2,5/2]$.

Modulation ansatz: We consider solutions x of (OC) of the form

$$x = X_\varepsilon^B + \mathcal{O}(\varepsilon^2), \quad (X_\varepsilon^B)_\gamma(t) := \varepsilon \sum_{j=1}^{3} B_j(\tau,\xi)\mathbf{E}_j(t,\gamma) + \text{c.c.}$$

with $\varepsilon B_j : [0,\tau_0]\times\mathbb{R}\to\mathbb{C}$, $\tau = \varepsilon t$, $\xi = \varepsilon\gamma$ (fixed coordinate system)
and $\mathbf{E}_j(t,\gamma) = \mathrm{e}^{\mathrm{i}(\omega_j t + \vartheta_j\gamma)}$ with $\omega_j^2 = \omega^2(\vartheta_j)$ and

$$\vartheta_1 + \vartheta_2 + \vartheta_3 = 0, \quad \omega_1 + \omega_2 + \omega_3 = 0$$



Aim: Derivation and justification of a system of macroscopic equations describing the amplitudes B_j of the three interacting pulses $j=1,2,3$

Formal derivation:

1. Insert in (OC) the multiscale ansatz (“improved approximation”)

$$(Y_\varepsilon)_\gamma(t) := (X_\varepsilon^B)_\gamma(t) + \varepsilon^2 \sum_{k,\ell=-3,\ k,\ell\neq 0}^{3} B_{k\ell}(\tau,\xi)\mathbf{E}_k(t,\gamma)\mathbf{E}_\ell(t,\gamma)$$

with $X_\varepsilon^B = \varepsilon \sum_{j=1}^{3} B_j \mathbf{E}_j + \text{c.c.}, \quad \mathbf{E}_j(t,\gamma) = \mathrm{e}^{\mathrm{i}(\omega_j t + \vartheta_j \gamma)}, \quad \omega_j^2 = \omega^2(\vartheta_j)$

and $B_{k\ell} = B_{\ell k} = \overline{B}_{-k,-\ell}, \quad \tau = \varepsilon t, \quad \xi = \varepsilon\gamma, \quad \omega_{-j} = -\omega_j, \quad \vartheta_{-j} = -\vartheta_j$

2. Expand the left- and right-hand side in terms of $\varepsilon^n \mathbf{E}_j$ and $\varepsilon^n \mathbf{E}_k \mathbf{E}_\ell$ for $n = 1, 2$

Result from $\varepsilon^2 \mathbf{E}_k \mathbf{E}_\ell$:

If $\overline{\mathbf{E}}_k \overline{\mathbf{E}}_\ell = \mathbf{E}_j$ ($\Leftrightarrow \omega_k + \omega_\ell + \omega_j = 0,\ \vartheta_k + \vartheta_\ell + \vartheta_j = 0$):

$$2\mathrm{i}\omega_j \partial_\tau B_j = 2\mathrm{i}\omega(\vartheta_j)\omega'(\vartheta_j)\partial_\xi B_j + 2\overline{c}_{jk}\overline{B}_k\overline{B}_\ell + 2\underbrace{[(\omega_k+\omega_\ell)^2 - \omega^2(\vartheta_k+\vartheta_\ell)]}_{=0}\overline{B}_{k\ell}$$

If $\mathbf{E}_k\mathbf{E}_\ell \neq \mathbf{E}_i, \overline{\mathbf{E}}_i$ for $i = 1, 2, 3$: $0 = 0 + 2c_{k\ell}B_k B_\ell + 2\underbrace{[(\omega_k+\omega_\ell)^2 - \omega^2(\vartheta_k+\vartheta_\ell)]}_{\neq 0 \text{ (required !)}} B_{k\ell}$

$\Rightarrow$ For $\omega_1+\omega_2+\omega_3=0$, $\vartheta_1+\vartheta_2+\vartheta_3=0$ and the nonresonance conditions

$(\omega_k+\omega_\ell)^2-\omega^2(\vartheta_k+\vartheta_\ell)\neq 0$ for $k,\ell=1,2,3$ with $\vee\ k=\ell\ \vee\ k\neq\ell,\ k\ell<0$

we obtain

$$\boxed{\begin{cases}\partial_\tau B_1=\omega_1'\partial_\xi B_1+\mathrm{i}(c/\omega_1)\overline{B}_2\overline{B}_3,\\ \partial_\tau B_2=\omega_2'\partial_\xi B_2+\mathrm{i}(c/\omega_2)\overline{B}_1\overline{B}_3,\\ \partial_\tau B_3=\omega_3'\partial_\xi B_3+\mathrm{i}(c/\omega_3)\overline{B}_1\overline{B}_2\end{cases}} \tag{3WI}$$

with $c:=\beta_2-2\mathrm{i}\sum_{m=1}^{M}\alpha_{m,2}\sum_{j=1}^{3}\sin(m\vartheta_j)$

$\Rightarrow$ Residuum $[\mathrm{res}(Y_\varepsilon)]_\gamma:=[\ddot{Y}_\varepsilon-LY_\varepsilon-N(Y_\varepsilon)]_\gamma=\mathcal{O}(\varepsilon^3)$

Justification: For $X_\varepsilon^B=\varepsilon\sum_{j=1}^{3}B_j\mathbf{E}_j+\text{c.c.}$,

where $B_j{:}[0,\tau_0]\times\mathbb{R}\to\mathbb{C}$ ($j=1,2,3$) solve (3WI) with $B_j(0,\cdot)\in\mathrm{H}^3(\mathbb{R})$

$\forall\ c>0\ \exists\ \varepsilon_0,C>0:\ \forall\ \varepsilon\in(0,\varepsilon_0)$ and for any solution x of (OC):

$$\|(x(0),\dot{x}(0))-(X_\varepsilon^B(0),\dot{X}_\varepsilon^B(0))\|_{\ell^2\times\ell^2}\leq c\,\varepsilon^{3/2}\quad\Rightarrow$$

$$\|(x(t),\dot{x}(t))-(X_\varepsilon^B(t),\dot{X}_\varepsilon^B(t))\|_{\ell^2\times\ell^2}\leq C\,\varepsilon^{3/2}\quad\text{for}\quad t\in[0,\tau_0/\varepsilon].$$

1. Write (OC) as a first-order Hamiltonian system in $\ell^2 \times \ell^2$ equipped with the energy norm $\| \cdot \| \sim \| \cdot \|_{\ell^2 \times \ell^2}$ under (SC) $\omega^2(\vartheta) > 0 \;\forall\, \vartheta \in (-\pi, \pi]$:

$$\dot{x} = Lx + N(x) \quad \text{with} \quad N(x) = Q(x,x) + M(x) \qquad \text{(OC')}$$

L linear, Q quadratic, M cubic and higher order terms

$\Rightarrow$ To show for a solution x of (OC') and the approximation X_ε

$$\|x(0) - X_\varepsilon(0)\| \leq c\varepsilon^\beta \quad \Rightarrow \quad \|x(t) - X_\varepsilon(t)\| \leq C\varepsilon^\beta \quad \text{for } \varepsilon \leq \varepsilon_0,\ \varepsilon^\alpha t \in [0, \tau_0]$$

Let the “improved approximation” Y_ε satisfy $(X_\varepsilon - Y_\varepsilon)_\gamma(t) = \mathcal{O}(\varepsilon^{\beta+1/2})$, i.e. $\|X_\varepsilon - Y_\varepsilon\|(t) = \mathcal{O}(\varepsilon^\beta)$

$\Rightarrow$ To show for the error $R_\varepsilon := \varepsilon^{-\beta}(x - Y_\varepsilon)$

$$\|R_\varepsilon(0)\| \leq d \quad \Rightarrow \quad \|R_\varepsilon(t)\| \leq D \quad \text{for } \varepsilon \leq \varepsilon_0,\ \varepsilon^\alpha t \in [0, \tau_0]$$

2. Insert $R_\varepsilon = \varepsilon^{-\beta}(x - Y_\varepsilon)$ into (OC') $\dot{x} = Lx + N(x)$

$$\dot{R}_\varepsilon = LR_\varepsilon + \varepsilon^{-\beta}[N(\varepsilon^\beta R_\varepsilon + Y_\varepsilon) - N(Y_\varepsilon) - \mathrm{res}(Y_\varepsilon)]$$

with residuum $[\mathrm{res}(Y_\varepsilon)]_\gamma := [\dot{Y}_\varepsilon - LY_\varepsilon - N(Y_\varepsilon)]_\gamma = \mathcal{O}(\varepsilon^{p+1}) = \mathcal{O}(\varepsilon^{\alpha+\beta+1/2})$,

i.e. $\|\mathrm{res}(Y_\varepsilon)\| \le \varepsilon^{\alpha+\beta} C_r$ for $\varepsilon \le \varepsilon_0$, $\varepsilon^\alpha t \in [0, \tau_0]$.

If

$$\|N(\varepsilon^\beta R_\varepsilon + Y_\varepsilon) - N(Y_\varepsilon)\| \le C_N \|Y_\varepsilon\|_\infty^\alpha \|\varepsilon^\beta R_\varepsilon\| \quad \text{for } \varepsilon \le \varepsilon_0,\ \varepsilon^\alpha t \le \tau_0,\ \|R_\varepsilon\| \le D$$

then by $\|Y_\varepsilon\|_\infty = \mathcal{O}(\varepsilon)$ the variation of constants formula yields

$$\begin{aligned}
\|R_\varepsilon(t)\| &\le \|R_\varepsilon(0)\| + \varepsilon^{-\beta} \int_0^t (\|N(\varepsilon^\beta R_\varepsilon + Y_\varepsilon) - N(Y_\varepsilon)\| + \|\mathrm{res}(Y_\varepsilon)\|)\, \mathrm{d}s \\
&\le d + \varepsilon^\alpha C_N \int_0^t \|R_\varepsilon(s)\|\, \mathrm{d}s + \varepsilon^\alpha t C_r \\
&\le (d + \varepsilon^\alpha t C_r) \mathrm{e}^{\varepsilon^\alpha t C_N} \qquad \text{(GRONWALL)} \\
&\le (d + \tau_0 C_r) \mathrm{e}^{\tau_0 C_N} =: D \qquad \text{for } \varepsilon \le \varepsilon_0,\ \varepsilon^\alpha t \le \tau_0
\end{aligned}$$

3. To show:

$$\|N(\varepsilon^\beta R_\varepsilon + Y_\varepsilon) - N(Y_\varepsilon)\| \leq C_N \|Y_\varepsilon\|_\infty^\alpha \|\varepsilon^\beta R_\varepsilon\| \quad \text{for } \varepsilon \leq \varepsilon_0,\ \varepsilon^\alpha t \leq \tau_0,\ \|R_\varepsilon\| \leq D$$

By mean value theorem:

Case 1: Dispersive evolution of a single pulse ($\alpha = 2$)

$Q = 0 \Rightarrow N = M$ (cubic) $\Rightarrow \|N(\varepsilon^\beta R + Y_\varepsilon) - N(Y_\varepsilon)\| \leq C_N \|Y_\varepsilon\|_\infty^2 \|\varepsilon^\beta R\|$

$Q \neq 0$ and (uNR): normal form transformation $y = x + B(x, x)$ of (OC') to $\dot{y} = Ly + N(y)$ with B such that $N(y) = M(y)$ (cubic)

$Q \neq 0$ and (NR): normal form transformation yields $N(y) = S(x, x) + M(y)$:

$$\begin{aligned} \|S(\varepsilon^\beta R_\varepsilon + Y_\varepsilon, \varepsilon^\beta R_\varepsilon + Y_\varepsilon) - S(Y_\varepsilon, Y_\varepsilon)\| &\leq \|S(\varepsilon^\beta R_\varepsilon, \varepsilon^\beta R_\varepsilon)\| + 2\|S(Y_\varepsilon, \varepsilon^\beta R_\varepsilon)\| \\ &\leq C_S \|\varepsilon^\beta R_\varepsilon\|_\infty \|\varepsilon^\beta R_\varepsilon\| + C_P \varepsilon^2 \|\varepsilon^\beta R_\varepsilon\| \end{aligned}$$

$\Rightarrow$ We need $\beta > \alpha = 2$ and for $p = 4$: $\beta \leq 5/2$

Case 2: Three-wave interaction ($\alpha = 1$)

$N = Q + M$ (quadratic) $\Rightarrow \|N(\varepsilon^\beta R + Y_\varepsilon) - N(Y_\varepsilon)\| \leq C_N \|Y_\varepsilon\|_\infty \|\varepsilon^\beta R\|$

For a microscopic nonlinear oscillator chain we derived and justified macroscopic modulation equations describing

1. the dispersive evolution of a single pulse
2. the interaction of three pulses under quadratic resonance

The mathematical justification relies on the same method.

The transfer of this method to the multidimensional case is expected to be straightforward.