

Theory and Numerics of Solitary Waves

- Hamiltonian structure of ODEs and PDEs -

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1 Finite Dimensional Differential Equations

- Poisson bracket, Hamiltonian
- Integrability of Hamiltonian ODEs
- Variational Calculus

2 Infinite Dimensional Differential Equations

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- Computational Considerations

Fin. dim. systems (ODEs): Poisson bracket, Hamiltonian

Hamiltonian function: $H(\mathbf{z}) : \mathbb{R}^n \rightarrow \mathbb{R}$

Poisson bracket: $\{\cdot, \cdot\} : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$ s.t.

- (i) $\{a\mathbf{z}_i + b\mathbf{z}_j, \mathbf{z}_k\} = a\{\mathbf{z}_i, \mathbf{z}_k\} + b\{\mathbf{z}_j, \mathbf{z}_k\}$ linearity
 - (ii) $\{\mathbf{z}_i, \mathbf{z}_j\} = -\{\mathbf{z}_j, \mathbf{z}_i\}$ antisymmetry
 - (iii) $\{\mathbf{z}_i\mathbf{z}_j, \mathbf{z}_k\} = \mathbf{z}_i\{\mathbf{z}_j, \mathbf{z}_k\} + \mathbf{z}_j\{\mathbf{z}_i, \mathbf{z}_k\}$ Leibniz property (chain rule)
 - (iv) $\{\mathbf{z}_i, \{\mathbf{z}_j, \mathbf{z}_k\}\} + \{\mathbf{z}_j, \{\mathbf{z}_i, \mathbf{z}_k\}\} + \{\mathbf{z}_k, \{\mathbf{z}_i, \mathbf{z}_j\}\} = 0$ Jacobi identity
- $\forall \mathbf{z}_i, \mathbf{z}_j, \mathbf{z}_k \in \mathbb{R}$

The Hamiltonian and the Poisson bracket define dynamics in time:

$$\frac{df}{dt} = \{f(\mathbf{z}), H(\mathbf{z})\}$$

Ex.: $f(\mathbf{z}(t)) = z_i(t)$; then $\frac{dz_i}{dt} = \{z_i, H(\mathbf{z})\}$

Remarks:

- $H(\mathbf{z})$ is constant in time b/c $dH/dt = \{H(\mathbf{z}), H(\mathbf{z})\} = 0$ by (ii)
- $\{z_i^m, g(\mathbf{z})\} = m z_i^{m-1} \{z_i, g(\mathbf{z})\}$ by (iii)

ODEs: Poisson bracket, Hamiltonian

For $f(z) : \mathbb{R}^n \rightarrow \mathbb{R}$ analytic with Taylor expansion

$$f(z) = \sum_{\alpha} \frac{D^{\alpha} f(0)}{\alpha!} z^{\alpha}, \quad \alpha = (\alpha_1, \dots, \alpha_n), \quad z^{\alpha} = z_1^{\alpha_1} z_2^{\alpha_2} \dots z_n^{\alpha_n}$$

this implies

$$\begin{aligned} \{f, g\} &= \sum_{\alpha} \frac{D^{\alpha} f(0)}{\alpha!} \{z_1^{\alpha_1} z_2^{\alpha_2} \dots z_n^{\alpha_n}, g\} &&= \alpha_j z_j^{\alpha_j - 1} \{z_j, g\} \\ &\stackrel{(iii)}{=} \sum_{\alpha} \frac{D^{\alpha} f(0)}{\alpha!} \sum_{j=1}^n z_1^{\alpha_1} z_2^{\alpha_2} \dots z_{j-1}^{\alpha_{j-1}} z_{j+1}^{\alpha_{j+1}} \dots z_n^{\alpha_n} \overbrace{\{z_j^{\alpha_j}, g\}} &&= \sum_{j=1}^n \frac{\partial f}{\partial z_j} \{z_j, g\} \end{aligned}$$

Performing the same also on g we get

$$\{f, g\} = \sum_{i,j=1}^n \frac{\partial f}{\partial z_i} \{z_i, z_j\} \frac{\partial g}{\partial z_j} = (\nabla f)^T \omega \nabla g, \quad \omega_{ij} = \{z_i, z_j\}$$

Therefore $\dot{z}_i = (\omega \nabla H)_i$ and $\dot{f}(z) = (\nabla f)^T \omega \nabla H$

$\omega \dots$ determines the Poisson structure

ODEs: Poisson bracket, Hamiltonian

Theorem (Darboux)

Given a Hamiltonian structure defined by ω and a Hamiltonian $H(z)$ it is always possible to find a transformation $z \xrightarrow{\phi} (q, p, C_1, \dots, C_r)$ with $q, p \in \mathbb{R}^N$ s.t. in the new variables

$$\hat{\omega} = \begin{pmatrix} 0 & I_N & 0 \\ -I_N & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad \text{canonical Poisson structure}$$

Then for $\hat{H} = H(\phi^{-1}(q, p, C_1, \dots, C_r))$

$$\dot{q}_i = (\hat{\omega} \nabla \hat{H})_i = \frac{\partial \hat{H}}{\partial p_i}, \quad \dot{p}_i = (\hat{\omega} \nabla \hat{H})_{i+N} = -\frac{\partial \hat{H}}{\partial q_i}, \quad i = 1, \dots, N.$$

In the new variables C_1, \dots, C_r (Casimirs) may be ignored. Then we get a $2N$ -dim. system with $\omega = \begin{pmatrix} 0 & I_N \\ -I_N & 0 \end{pmatrix}$. And

$$\{f, g\} = (\nabla f)^T \omega \nabla g = \sum_{j=1}^N \left(\frac{\partial f}{\partial q_j} \frac{\partial g}{\partial p_j} - \frac{\partial f}{\partial p_j} \frac{\partial g}{\partial q_j} \right).$$

ODEs: Poisson bracket, Hamiltonian, Integrability

Example: $H = \sum_{i=1}^N \frac{p_i^2}{2m_i} + V(q_1, \dots, q_N), \quad \omega = \begin{pmatrix} 0 & I_N \\ -I_N & 0 \end{pmatrix}$

$$\dot{q}_i = \frac{\partial H}{\partial p_i} = \frac{p_i}{m_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q_i} = -\frac{\partial V}{\partial q_i}$$

$$m_i \ddot{q}_i = -\frac{\partial V}{\partial q_i} \quad \text{Newton's equations of motion}$$

Canonical transformation: such a transformation $Z(z)$ of variables z of a Hamiltonian system with Poisson structure ω under which the Poisson structure is invariant

$$\{Z_i, Z_j\} = \{z_i, z_j\}, \quad i, j = 1, \dots, n.$$

Hamiltonian ODEs: Integrability

Assume we have canonical variables $q_1, \dots, q_N, p_1, \dots, p_N$.

Idea: find a canonical transformation to $Q_1, \dots, Q_N, P_1, \dots, P_N$ s.t. in these

$$\dot{P}_k = -\frac{\partial H}{\partial Q_k} = 0 \quad \text{for some } k \in \{1, \dots, N\}$$

Clearly for every P_k s.t. $\dot{P}_k = 0$ the conjugate variable Q_k satisfies

$$\dot{Q}_k = \frac{\partial H}{\partial P_k}(P_k) =: \Omega_k = \text{const.} \quad \Rightarrow \quad Q_k = \Omega_k t + Q_k(0)$$

i.e. **both equations** can be **easily integrated** (and $H = \sum_{k=1}^N \Omega_k P_k$)

Terminology: P_k **action** variables (usually J_k); Q_k **angle** variables (usually θ_k)

Conclusion: **to completely solve a Hamiltonian system** it suffices to find N (not $2N$) variables P_k s.t.

$$\dot{P}_k = -\frac{\partial H}{\partial Q_k} = 0 \quad \text{and} \quad \{P_i, P_k\} = 0, \quad i, k = 1, \dots, N.$$

The involution condition is due to the canon. condition on $q, p \rightarrow Q, P$ and the fact $\{p_i, p_k\} = 0$.

Hamiltonian ODEs: Integrability

Theorem (Liouville-Arnol'd)

If for a $2N$ -dim. Hamiltonian system defined by ω and a Hamiltonian H there are N functionally independent (gradients linearly independent everywhere) conserved quantities F_1, \dots, F_N mutually in involution

$$\{F_i, F_j\} = 0, \quad i, j = 1, \dots, N$$

then the Hamiltonian system is completely integrable.

Note: F_i need not be action variables.

Example: Harmonic oscillator with $H = \frac{p^2}{2m} + \frac{kq^2}{2}$ and canonical Poisson structure

$N = 1 \Rightarrow 1$ conserved quantity needed for integrability (take H)

$$\frac{d}{dt} \begin{pmatrix} q \\ p \end{pmatrix} = \begin{pmatrix} \frac{\partial H}{\partial p} \\ -\frac{\partial H}{\partial q} \end{pmatrix} = \begin{pmatrix} p/m \\ -kq \end{pmatrix} \Rightarrow \ddot{q} + \mu^2 q = 0, \quad \mu = \sqrt{k/m}$$

Easily solvable:

$$q = A \sin(\mu t + \phi_0), \quad p = A\sqrt{km} \cos(\mu t + \phi_0) \Rightarrow H = A^2 k/2$$

Hamiltonian ODEs: Integrability

Obvious action-angle variables:

$$\theta = \mu t + \phi_0, \quad \mathbf{J} = H/\dot{\theta} = H/\mu = \frac{A^2}{2} \sqrt{km}$$

The transformation reads:

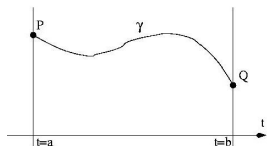
$$q = \sqrt{2J/\sqrt{km}} \sin(\theta), \quad p = \sqrt{2J\sqrt{km}} \cos(\theta)$$

and its inverse is

$$\mathbf{J} = (q^2 km + p^2)/(2\sqrt{km}), \quad \theta = \text{atan}(q\sqrt{km}/p)$$

Towards Hamiltonian PDEs - Variational Calculus

Because for PDEs we will need to replace derivatives with *functional derivatives*, let's review variational calculus.



Given $P, Q \in \mathbb{R}^N$ and a functional (“action functional”)

$$S[\gamma] = \int_a^b L(x, \dot{x}, \ddot{x}, \dots, x^{(m)}) dt \quad L \dots \text{Lagrangian}$$

find γ given by $x(t) = (x_1(t), \dots, x_N(t))$, $t \in [a, b]$ that extremizes S .

Theorem (Fundam. Theorem of Variational Calculus (FTVC))

$\gamma : t \in [a, b] \rightarrow x(t)$ is an extremum of S iff the Euler-Lagrange equations hold:

$$\frac{\delta S}{\delta x_i} := \frac{\partial L}{\partial x_i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}_i} + \frac{d^2}{dt^2} \frac{\partial L}{\partial \ddot{x}_i} + \dots + (-1)^m \frac{\partial L}{\partial x_i^{(m)}} = 0 \quad \forall i \in \{1, \dots, n\}$$

Variational Calculus

Proof:

$\mathbf{x}(t)$ is a c.p. iff $\frac{dS}{d\varepsilon} [\mathbf{x}(t) + \varepsilon \eta(t)] |_{\varepsilon=0} = \mathbf{0} \quad \forall \eta \in C^m(a, b), \eta(a) = \eta(b) = \mathbf{0}$

i.e. $\frac{dS}{d\varepsilon} [x_i(t) + \varepsilon \eta_i(t)] |_{\varepsilon=0} = 0 \quad i \in \{1, \dots, n\}$.

$$\frac{dS}{d\varepsilon} [x_i(t) + \varepsilon \eta_i(t)] = \frac{d}{d\varepsilon} \int_a^b L(x_i + \varepsilon \eta_i, \dot{x}_i + \varepsilon \dot{\eta}_i, \ddot{x}_i + \varepsilon \ddot{\eta}_i, \dots, x_i^{(m)} + \varepsilon \eta_i^{(m)}) dt$$

$$\frac{dS}{d\varepsilon} [x_i(t) + \varepsilon \eta_i(t)] |_{\varepsilon=0} = \int_a^b \frac{\partial L}{\partial x_i} \eta_i + \frac{\partial L}{\partial \dot{x}_i} \dot{\eta}_i + \frac{\partial L}{\partial \ddot{x}_i} \ddot{\eta}_i + \dots + \frac{\partial L}{\partial x_i^{(m)}} \eta_i^{(m)} dt$$

$$\stackrel{\text{by parts}}{=} \int_a^b \left(\frac{\partial L}{\partial x_i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}_i} + \frac{d^2}{dt^2} \frac{\partial L}{\partial \ddot{x}_i} + \dots + (-1)^m \frac{\partial L}{\partial x_i^{(m)}} \right) \eta_i dt$$

$$= \mathbf{0} \quad \forall i \in \{1, \dots, n\}.$$

where we write $\frac{\partial L}{\partial x_i^{(k)}} = \frac{\partial L}{\partial x_i^{(k)}}(x_i, \dot{x}_i, \dots, x_i^{(m)})$. As the last equ. holds for all $\eta_i \in C^m(a, b)$, we get the theorem statement (use of a continuity argument).

Variational Calculus

Example: Wave equation: $u_{tt} - c^2 u_{xx} = 0$, $t \in [a, b]$, $x \in \mathbb{R}$.

As a first order system ($v = u_t$)

$$u_t - v = 0, \quad v_t - c^2 u_{xx} = 0 \quad (1)$$

Now γ is a surface on $[a, b] \times \mathbb{R}$

$$\gamma : (t, x) \in [a, b] \times \mathbb{R} \rightarrow u(x, t), \quad S[\gamma] = \int_a^b \int_{\mathbb{R}} L dx dt$$

Using FTVC (proved via Green's theorem instead of integr. by parts) get L from the Euler-Lagrange equations (1):

$$L = \frac{1}{2} v^2 + \frac{c^2}{2} u_x^2 - u_t v$$

Check:

$$\frac{\delta S}{\delta u} = \frac{\partial L}{\partial u} - \partial_x \frac{\partial L}{\partial u_x} - \partial_t \frac{\partial L}{\partial u_t} = -c^2 u_{xx} + v_t = 0$$

$$\frac{\delta S}{\delta v} = \frac{\partial L}{\partial v} - \partial_x \frac{\partial L}{\partial v_x} - \partial_t \frac{\partial L}{\partial v_t} = v - u_t = 0$$

Hamiltonian PDEs

ODEs

1) Hamiltonian

$$H = H(z_1, \dots, z_n)$$

→ function

2) Poisson bracket

$$\{f(z), g(z)\} = (\nabla f)^T \omega \nabla g$$

ω ... antisym. matrix

3) Dynamics

$$\dot{f} = \{f, H\}$$

PDEs

$$H = \int_{\Omega} \mathcal{H}(u, D^{\alpha} u) dy, \quad y \in \Omega \subset \mathbb{R}^d$$

→ functional (\mathcal{H} ... Hamiltonian density)

α ... multiindex

$$\{F, G\} = \int_{\Omega} \frac{\delta F}{\delta u} B \frac{\delta G}{\delta u} dy$$

B ... antisym. operator

$$\frac{\partial K(u)}{\partial t} = \{K(u), H(u)\}$$

Dynamics of the coordinate functions u (or u_1, \dots, u_m):

$$u_t = \{u, H(u)\} = \int \frac{\delta u(x, t)}{\delta u(y, t)} B \frac{\delta H(u(x, t))}{\delta u(y, t)} dy = ?$$

Note:

$$u(x, t) = \int \delta(x - y) u(y, t) dy \Rightarrow \frac{\delta u(x, t)}{\delta u(y, t)} = \delta(x - y)$$

$$\Rightarrow u_t = \int \delta(x - y) B \frac{\delta H(u(x, t))}{\delta u(y, t)} dy = B \frac{\delta H(u(x, t))}{\delta u(x, t)} = B \frac{\delta H}{\delta u}$$

Hamiltonian PDEs

examples of B :

- $\begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$ (for $m = 2$)
- $\partial_x f$
- $u \partial_x f + \partial_x u$

Complete integrability of a Hamiltonian PDE:

- a necessary condition is the existence of infinitely many conserved quantities mutually in involution

Back to the Wave Equation

$$u_t - v = 0, \quad v_t - c^2 u_{xx} = 0, \quad t \in [a, b], x \in \mathbb{R}.$$

$$L = \frac{1}{2} v^2 + \frac{c^2}{2} u_x^2 - u_t v$$

Q: What is the corresponding Hamiltonian?

As shown above $\frac{\partial}{\partial t} \begin{pmatrix} u \\ v \end{pmatrix} = B \begin{pmatrix} \frac{\delta H}{\delta u} \\ \frac{\delta H}{\delta v} \end{pmatrix}$

For the canonical $B = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$ we can find H from the action defined via L (more precisely use of “Legendre transform” is needed)

$$H = \frac{1}{2} \int_{\mathbb{R}} v^2 + c^2 u_x^2 dx.$$

i.e. “ \mathcal{H} is L without the part that gives t -derivatives”

NLS as a Hamiltonian system

Euler-Lagrange equations:

$$iq_t = -\frac{1}{2}q_{xx} + \sigma|q|^2q$$

As a real system for $q = u + iv$

$$u_t = -\frac{1}{2}v_{xx} + \sigma(u^2 + v^2)v, \quad v_t = \frac{1}{2}u_{xx} - \sigma(u^2 + v^2)u$$

Lagrangian: $L = \frac{1}{2}(v_t u - u_t v) + \frac{1}{2}(u_x^2 + v_x^2) + \frac{\sigma}{4}(u^2 + v^2)^2$.

Hamiltonian structure:

$$B = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}, \quad H = \int_{\mathbb{R}} \frac{1}{2}(u_x^2 + v_x^2) + \frac{\sigma}{4}(u^2 + v^2)^2 dx$$

Check:

$$\frac{\delta H}{\delta u} = \frac{\partial \mathcal{H}}{\partial u} - \partial_x \frac{\partial \mathcal{H}}{\partial u_x} = \sigma(u^2 + v^2)u - \frac{1}{2}u_{xx} = -v_t$$

$$\frac{\delta H}{\delta v} = \frac{\partial \mathcal{H}}{\partial v} - \partial_x \frac{\partial \mathcal{H}}{\partial v_x} = \sigma(u^2 + v^2)v - \frac{1}{2}v_{xx} = u_t$$

NLS as a Hamiltonian system

Equivalently NLS can be written as a system for q and $p := q^*$:

$$iq_t = -\frac{1}{2}q_{xx} + \sigma q^2 p, \quad -ip_t = -\frac{1}{2}p_{xx} + \sigma p^2 q$$

Lagrangian: $L = \frac{i}{2}(p_t q - q_t p) + \frac{1}{2}q_x p_x + \frac{\sigma}{2}q^2 p^2$.

Hamiltonian structure

$$B = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad H = \int \frac{1}{2}q_x p_x + \frac{\sigma}{2}q^2 p^2 dx \quad \left(= \int \frac{1}{2}|q_x|^2 + \frac{\sigma}{2}|q|^4 dx \right)$$

Check:

$$\frac{\delta H}{\delta q} = \frac{\partial \mathcal{H}}{\partial q} - \partial_x \frac{\partial \mathcal{H}}{\partial q_x} = \sigma p^2 q - \frac{1}{2}p_{xx} = iq_t$$

$$\frac{\delta H}{\delta p} = \frac{\partial \mathcal{H}}{\partial p} - \partial_x \frac{\partial \mathcal{H}}{\partial p_x} = \sigma q^2 p - \frac{1}{2}q_{xx} = -ip_t$$

thus

$$i \begin{pmatrix} q_t \\ p_t \end{pmatrix} = B \begin{pmatrix} \frac{\delta H}{\delta q} \\ \frac{\delta H}{\delta p} \end{pmatrix}, \quad \text{usually written as } iq_t = \frac{\delta H}{\delta q^*}$$

KdV as a Hamiltonian system

Euler-Lagrange equations:

$$u_t + uu_x + u_{xxx} = 0$$

Hamiltonian structure:

$$B = \partial_x, \quad H = \int \frac{1}{2} u_x^2 - \frac{1}{6} u^3 dx$$

Check:

$$\frac{\delta H}{\delta u} = \frac{\partial \mathcal{H}}{\partial u} - \partial_x \frac{\partial \mathcal{H}}{\partial u_x} = -\frac{1}{2} u^2 - u_{xx}$$

thus, indeed,

$$u_t = B \frac{\delta H}{\delta u}.$$

Computational Considerations

(I) Conservation of H

- although spatial discretization of a Hamilt. PDE may not result in a Hamilt. system of ODEs, it is often “close to Hamiltonian” - i.e. almost preserves the corresp. quadrature of the Hamiltonian functional
- special discretization methods for preseving Hamiltonian structure exist [4]
- use symplectic time integration methods - e.g. implicit midpoint or symplectic split-step methods

(II) Computing stationary solutions

Recall: u solves the Euler-Lagrange equations (=the given PDE) iff $\frac{\delta S}{\delta u} = 0$

Idea: extremize the action functional S in a suitable finite dim. space

- expand u in a suitable complete orthogonal basis $(\phi_k(\mathbf{x}; \beta_1, \beta_2, \dots, \beta_p))_{k=1}^{\infty}$ with parameters β_j :

$$u \approx \sum_{k=1}^M a_k(t) \phi_k(\mathbf{x}) \quad \text{with } \phi_k \text{ satisfying the BC's}$$

$$S = \int_a^b \int_{\Omega} L(u, u_t, D^{\alpha} u) dx dt, \quad D^{\alpha} u \text{ denotes all the spatial derivatives of } u$$

Computational Considerations

$$\begin{aligned}
 S &= \int_a^b \int_{\Omega} L(u, u_t, D^{\alpha} u) dx dt, \\
 &\approx \int_a^b \int_{\Omega} L\left(\sum a_k \phi_k, \sum \dot{a}_k \phi_k, \sum a_k D^{\alpha} \phi_k\right) dx dt
 \end{aligned}$$

If $a_k(t) = b_k e^{-i\omega t}$, b_k constant, then need to extremize the reduced action

$$\begin{aligned}
 \tilde{S} &= \int_{\Omega} L\left(\sum b_k \phi_k, -i\omega \sum b_k \phi_k, \sum b_k D^{\alpha} \phi_k\right) dx \\
 &= [\phi_k, D^{\alpha} \phi_k \text{ known}] =: F(b_1, \dots, b_M, \beta_1, \dots, \beta_p)
 \end{aligned}$$

- often F is a polynomial (not for Sine-Gordon eq.).
- need to solve $\nabla F = 0$ (∇ is w.r.t. $(b_1, \dots, b_M, \beta_1, \dots, \beta_p)$)

Example: Cubic-quintic NLS

$$iu_t = -\frac{1}{2}u_{xx} + \sigma|u|^2u - \gamma|u|^4u, \quad x \in \mathbb{R}$$

Lagrangian density: $L = \frac{i}{2}(u_t^*u - u_tu^*) + \frac{1}{2}|u_x|^2 + \frac{\sigma}{2}|u|^4 - \frac{\gamma}{3}|u|^6$

For the solitary wave solutions $u = e^{-i\omega t}v(x)$, $v \in \mathbb{R}$ get

$$L = -\omega v^2 + \frac{1}{2}v_x^2 + \frac{\sigma}{2}v^4 - \frac{\gamma}{3}v^6$$

Orthogonal basis of test functions: $\phi_k = \operatorname{sech}(\mu x)P_k(\tanh(\mu x))$, where P_k is the k -th Legendre polynomial.

Using the expansion $v(x) \approx \sum_{k=1}^M b_k \phi_k(x; \mu)$ the reduced action functional is

$$\tilde{S} = -\omega \vec{b}^T D(\mu) \vec{b} + \vec{b}^T M(\mu) \vec{b} + G(\vec{b}, \mu) =: F(\vec{b}, \mu),$$

where

$$D_{ij} = \frac{2}{a(2j+1)} \delta_{i,j}, \quad M_{ij} = \frac{1}{2} \int_{\mathbb{R}} \phi_i' \phi_j' dx, \quad G = \int_{\mathbb{R}} \frac{\sigma}{2} \left(\sum b_k \phi_k \right)^4 - \frac{\gamma}{3} \left(\sum b_k \phi_k \right)^6 dx$$


Example: Cubic-quintic NLS


Thus


$$\nabla F = -\omega \left(\frac{2D(\mu)\vec{b}}{\vec{b}^T D'(\mu)\vec{b}} \right) + \left(\frac{2M(\mu)\vec{b}}{\vec{b}^T M'(\mu)\vec{b}} \right) + \left(\frac{\nabla_{\vec{b}} \mathbf{G}}{\frac{\partial \mathbf{G}}{\partial \mu}} \right)$$


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