Variational Approximations in Discrete Nonlinear Schrödinger Equations

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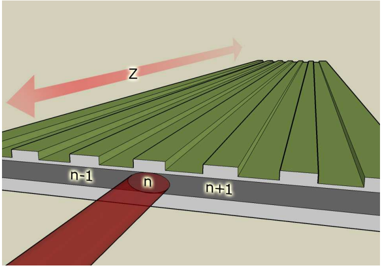
The Discrete Nonlinear Schrödinger Equation

The 1D DNLS equation is

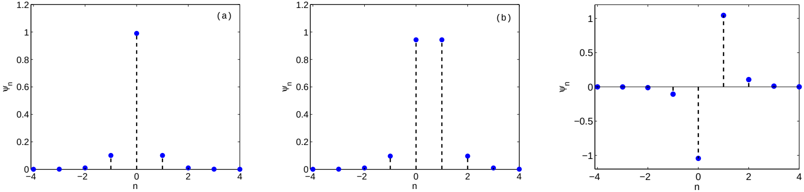
$$i\frac{d\psi_n}{dt} + \epsilon\left(\psi_{n+1} + \psi_{n-1} - 2\psi_n\right) + |\psi_n|^2\psi_n = 0,$$

where $\psi(t) = \{\psi_n(t)\}_{n\in\mathbb{Z}} : \mathbb{R} \to \mathbb{C}^{\mathbb{Z}}$ and $\epsilon \in \mathbb{R}$.



P.G. Kevrekidis, *The Discrete Nonlinear Schrödinger Equation* (Springer, 2009)

Discrete solitons (localized solutions)



Methods to establish existence of such localized solutions:

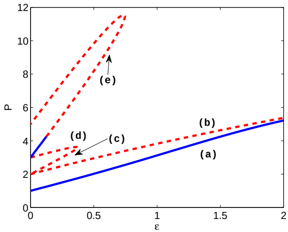
- Continuation from the anticontinuum ($\epsilon = 0$)
- Dynamical methods (discrete maps)
- Calculus of variations (energy functionals)

D.E. Pelinovsky, *Localization in Periodic Potentials: from Schrödinger operators to the Gross–Pitaevskii equation* (Cambridge University Press, 2011)

Continuation from the anticontinuum ($\epsilon = 0$)

Discrete solitons $\psi_n(t) = \phi_n e^{-it}$ are found from:

$$\epsilon \left(\phi_{n+1} + \phi_{n-1} - 2\phi_n\right) + (|\phi_n|^2 - 1)\phi_n = 0, \quad n \in \mathbb{Z}.$$



With $\epsilon = 0$ the steady-state solutions have the form,

$$\phi_n = e^{i\theta_n} \quad \text{or} \quad \phi_n = 0$$

where $\theta_n \in \mathbb{R}$ is a phase. In 1D: $\theta \in \{\pm\pi, 0\}$, hence $\phi \in \mathbb{R}$.

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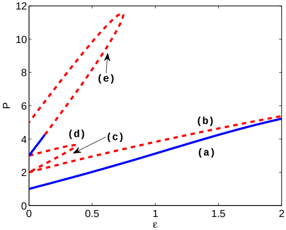

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Calculus of variations (energy functionals)

The stationary DNLS equation is the Euler–Lagrange equation for the energy functional:

$$H(\psi) = \sum_{n\in\mathbb{Z}} \epsilon \left(\bar{\psi}_n \psi_{n+1} + \psi_n \bar{\psi}_{n+1} - 2|\psi_n|^2\right) + \frac{1}{2}|\psi_n|^4.$$

- M. Weinstein (1999): minimization of $H(\psi)$ subject to the fixed $Q(\psi) = \sum_{n\in\mathbb{Z}} |\psi_n|^2$.
- A. Pankov (2005): linking theorems to guarantee existence of critical points of $H(\psi)$
- M. Hermann (2011): minimization of $H(\psi)$ for the class of on-site and off-site solitons:

$$\text{(on-site)} \quad \psi_n = \psi_{-n}; \quad \text{(off-site)} \quad \psi_n = \psi_{1-n}.$$

Variational Formulation of the DNLS

Consider the action functional $S(\psi)$,

$$S = \int_0^{t_0} \mathcal{L}\, dt,$$

with the Lagrangian:

$$\mathcal{L}(\psi) = \sum_{n\in\mathbb{Z}} \frac{i}{2}\left(\bar{\psi}_n \partial_t \psi_n - \psi_n \partial_t \bar{\psi}_n\right) + H(\psi),$$

where $H(\psi)$ is the DNLS energy functional.

The Euler-Lagrange equation recovers the DNLS equation:

$$i\frac{d\psi_n}{dt} + \epsilon\left(\psi_{n+1} + \psi_{n-1} - 2\psi_n\right) + |\psi_n|^2\psi_n = 0, \quad t \in [0, t_0].$$

Variational Approximation (VA)

Reduce degrees of freedom by using a *variational approximation* for a solution of the Euler–Lagrange equations.

We pose a trial configuration (ansatz),

$$\psi_n^{\text{ansatz}} = Ae^{i\alpha+i\beta(n-s)}e^{-\eta|n-s|}$$

with real parameters $A(t), \alpha(t), \beta(t), \eta(t), s(t)$.

The sums in the Lagrangian can be explicitly computed to define the "effective Lagrangian",

$$\mathcal{L}_{\text{eff}}(A, \alpha, \beta, \eta, s) := \mathcal{L}(\psi^{\text{ansatz}})$$

which produces reduced dynamical equations on $A, \alpha, \beta, \eta, s$.

References on Variational Approximation

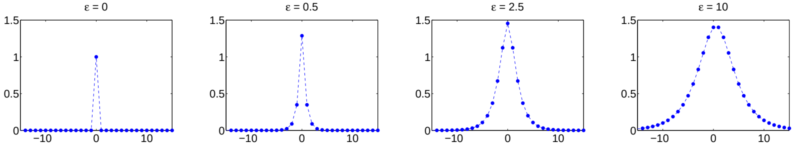
- Malomed (2002): review of variational methods in the context of nonlinear optics (pdes)
- Malomed & Weinstein (1996); Kaup (2005): applications of the VA to on-site and off-site solitons of the DNLS equation
- Carretero *et al.* (2006); Cuevas *et al.* (2009); Chong & P. (2011); Chong *et al.* (2011); Susanto & Matthews (2011) : applications of the VA to nonlinear lattice equations
- Kaup & Vogel (2007) : an attempt of "justification" of the VA for nonlinear pdes

C. Chong, D.E. Pelinovsky, and G. Schneider, On the validity of the variational approximation in discrete nonlinear Schrodinger equations, Physica D **241**, 115–124 (2012)

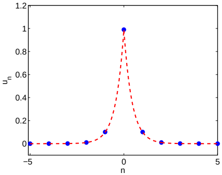
Validity of the Approximation

Heuristically, VA should be better for small ϵ:

$$\epsilon\left(\phi_{n+1}+\phi_{n-1}-2\phi_n\right)+(|\phi_n|^2-1)\phi_n=0,\quad n\in\mathbb{Z}.$$



DNLS solutions



Ansatz

VA: stationary DNLS equation

Consider steady-state solutions of the form $\psi_n = \phi_n e^{i(1-2\epsilon)t}$, where ϕ solves a stationary DNLS equation,

$$R_n(\phi) := \epsilon\left(\phi_{n+1} + \phi_{n-1}\right) + (\phi_n^2 - 1)\phi_n = 0, \quad n \in \mathbb{Z}.$$

The Lagrangian of this stationary DNLS equation is the energy:

$$H(\phi) = \sum_{n\in\mathbb{Z}} \left[\frac{1}{2}|\phi_n|^4 - |\phi_n|^2 + \epsilon(\bar{\phi}_n\phi_{n+1} + \phi_n\bar{\phi}_{n+1})\right].$$

Let ϕ_* be an approximate solution of the stationary DNLS equation such that

$$\|R(\phi_*)\|_{l^2} = \mathcal{O}(\epsilon^p) \quad \text{as} \quad \epsilon \to 0$$

for some $p > 0$.

Justification Result

Lemma: *Assume that there is a finite set* $S \subset \mathbb{Z}$ *and a binary set* $\{\sigma_n\}_{n\in S} \in \{+1,-1\}$ *such that*

$$\lim_{\epsilon\longrightarrow 0} \|\phi_* - \sum_{n\in S} \sigma_n e_n\|_{l^2} = 0,$$

Then, there are $\epsilon_0 > 0$, $C > 0$, *and a unique solution of the stationary DNLS equation with* $\epsilon \in (0,\epsilon_0)$ *such that*

$$\|\phi - \phi_*\|_{l^2} \leq C\epsilon^p.$$

Proof: After the substitution $\phi = \phi_* + \varphi$, we have

$$L\varphi = R(\phi_*) + N(\varphi),$$

where L is a bounded invertible operator on $l^2(\mathbb{Z})$ for small ϵ and $N(\varphi)$ is quadratic in φ.

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VA - Simple Example

Consider the ansatz,

$$\phi_n^{\text{ansatz}} = Ae^{-\eta|n|}$$

and define η from the tail analysis:

$$1 = \epsilon(e^{\eta} + e^{-\eta}) \quad \Rightarrow \quad \eta = \operatorname{arccosh}\left(\frac{1}{2\epsilon}\right)$$

The effective Lagrangian,

$$\begin{aligned}\mathcal{L}(\phi^{\text{ansatz}}) &= \frac{1}{2}A^4\coth(2\eta) - A^2\coth(\eta) \\ &\quad +2\epsilon A^2\left(\coth(\eta)\cosh(\eta) - \sinh(\eta)\right)\end{aligned}$$

yields the only equation:

$$A^2 = \left(1 - 2\epsilon e^{-\eta}\right)\tanh(2\eta) = 1 + \mathcal{O}(\epsilon^2).$$

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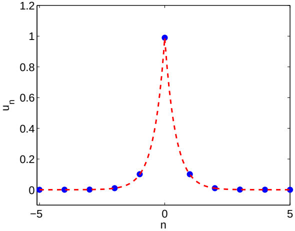
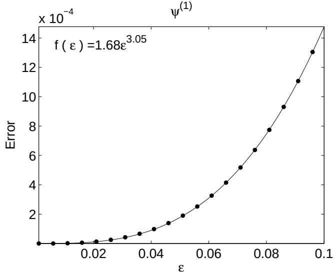
VA - Simple Example

Explicit computation shows that $R(\phi^{\text{ansatz}}) = \mathcal{O}(\epsilon^3)$ and hence

$$\|\phi - \phi^{\text{ansatz}}\|_{l^2} \leq C\epsilon^3.$$





This approximation is good for on-site solitons.

VA - Another Example

Consider the ansatz with two parameters A and B,

$$\phi_n^{\text{ansatz}} = \begin{cases} B & n = 0, \\ Ae^{-\eta(|n|-1)} & |n| \in \mathbb{N}, \end{cases}$$

The effective Lagrangian yields now two equations:

$$\frac{A^3}{1 - e^{-4\eta}} - A(1 - \epsilon e^{-\eta}) + \epsilon B = 0$$

and

$$(B^2 - 1)B + 2\epsilon A = 0.$$

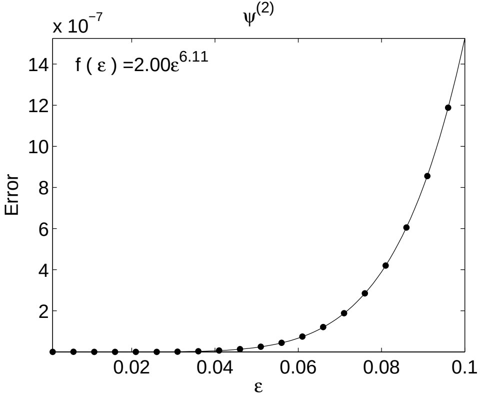
There exists solutions for A and B such that

$$A = \epsilon + \mathcal{O}(\epsilon^3) \quad \text{and} \quad B = 1 + \mathcal{O}(\epsilon^2).$$

VA - Another Example

Explicit computation shows that $R(\phi^{\text{ansatz}}) = \mathcal{O}(\epsilon^6)$ and hence

$$\|\phi - \phi^{\text{ansatz}}\|_{l^2} \leq C\epsilon^6.$$



Similar approximations can be constructed for off-site and twisted solitons (supported on two sites as $\epsilon \to 0$).

VA - Kaup's approximation

Consider the ansatz with two parameters A and s,

$$\phi_n^{\text{ansatz}} = Ae^{-\eta|n-s|}, \quad n \in \mathbb{Z}.$$

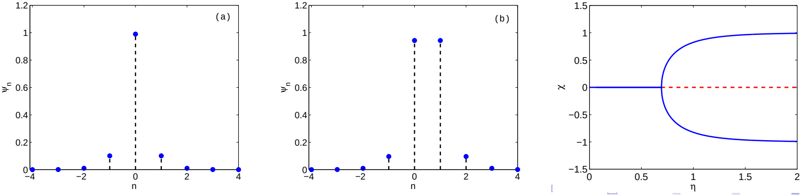
The effective Lagrangian yield two equations:

$$\text{either} \quad \chi = 0 \quad \text{or} \quad A^2 = \epsilon \frac{\sinh(2\eta)}{\cosh(\eta\chi)}$$

and

$$A^2 = 2\epsilon \frac{\sinh(2\eta)}{\cosh(2\eta\chi)} \left(\cosh(\eta\chi) - e^{-\eta}\right),$$

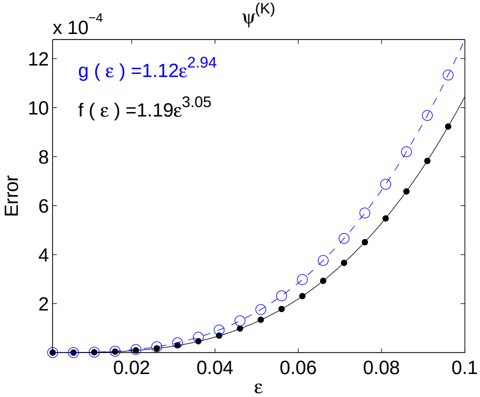
where $\chi = 2s - 1 \in [-1, 1]$ if $s \in [0, 1]$.



VA - Kaup's approximation

Explicit computation shows that $R(\phi^{\text{ansatz}}) = \mathcal{O}(\epsilon^3)$ and hence

$$\|\phi - \phi^{\text{ansatz}}\|_{l^2} \leq C\epsilon^3.$$



The coalescence point at $\eta \approx 0.69$ ($\epsilon \approx 0.4$) is an artefact of the VA for large values of ϵ.

Time-dependent VAs

Using the trial function,

$$\psi_n^{\text{ansatz}} = Ae^{i\alpha + i\beta(n-s)}e^{-\eta|n-s|}$$

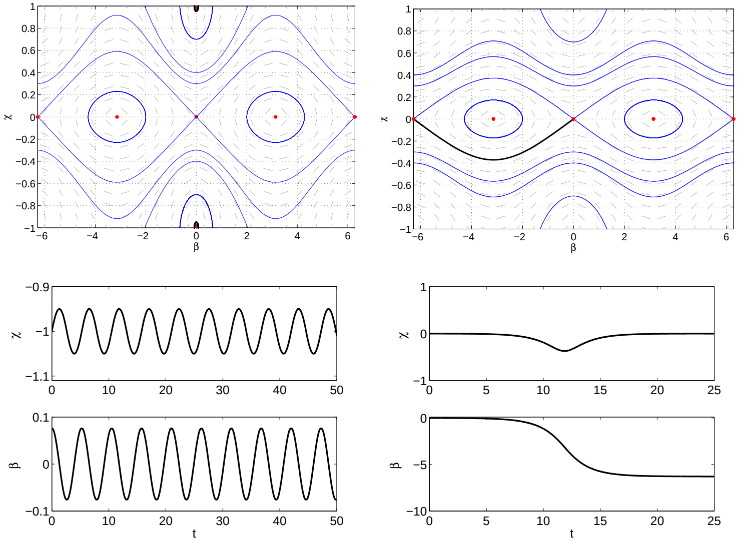
we obtain the effective Lagrangian

$$\mathcal{L}_{\text{eff}}(A, \alpha, \beta, \chi) := \mathcal{L}(\psi^{\text{ansatz}}),$$

which produces an integral of motion for A, an uncoupled equation for α, and a planar Hamiltonian system of equations for β and γ:

$$\frac{d\beta}{dt} = F(\beta, \chi), \quad \frac{d\chi}{dt} = G(\beta, \chi).$$

Time-dependent VAs



Time-dependent VAs

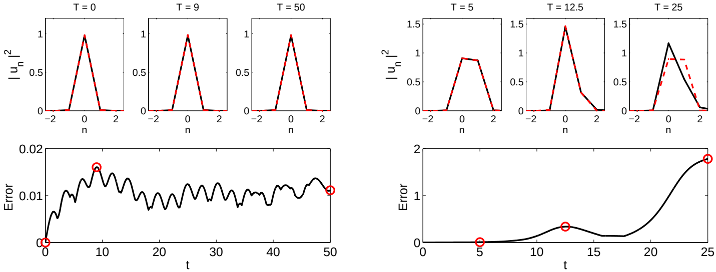


Figure: Comparison between the VA and the numerical solutions of the DNLS equation for the on-site (left) and off-site (right) solitons.

Justification of the time-dependent VAs

Theorem: *Fix* $\epsilon_0 > 0$ *and let* $(\beta, \chi) \in C(\mathbb{R}, \mathbb{R}^2)$ *be a family of periodic solutions of the planar system such that for all* $\epsilon \in (0, \epsilon_0)$, *there exists* $C_0 > 0$ *such that*

$$\sup_{t \in \mathbb{R}} \left(|\beta(t)| + \eta |\chi(t) + 1| \right) \leq C_0.$$

For all $\epsilon \in (0, \epsilon_0)$ *and a given* $T_0 > 0$, *there exists* T_0*-dependent constant* $C > 0$ *such that a time-dependent solution* ψ *of the DNLS equation with* $\psi|_{t=0} = \psi^{\text{ansatz}}|_{t=0}$ *satisfies*

$$\sup_{t \in [0, T_0]} \sup_{n \in \mathbb{Z}} |\psi_n(t) - \psi_n^{\text{ansatz}}(t)| \leq C\epsilon.$$

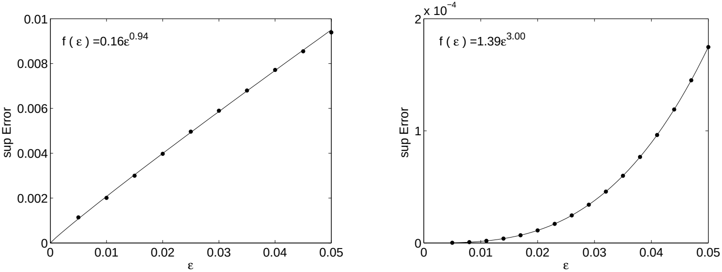
Improved result

Corollary: *Under the conditions of Theorem, if* $(\beta, \chi) \in C(\mathbb{R}, \mathbb{R}^2)$ *satisfies*

$$\sup_{t\in\mathbb{R}} \left(|\beta(t)| + \eta|\chi(t) + 1|\right) \le C_0 \epsilon^2,$$

then the VA satisfies the bound

$$\sup_{t\in[0,T_0]} \sup_{n\in\mathbb{Z}} |\psi_n(t) - \psi_n^{\text{ansatz}}(t)| \le C\epsilon^3.$$



Remarks

- Near the center point $(0, \chi_0) \approx (0, -1)$, the frequency of oscillations is near $\sqrt{2}$, which is different from the frequency of oscillations of linear oscillators $(= 1)$.
- The period of the periodic oscillations is $\mathcal{O}(1)$ as $\epsilon \to 0$, whereas $|\chi_0 + 1| = \mathcal{O}(\epsilon^2)$ as $\epsilon \to 0$.
- The proof is based on the decomposition $\psi = \psi^{\text{ansatz}} + U$:

$$i\dot{U} = F(U) + \text{Res}(\psi^{\text{ansatz}}),$$

where $\|\text{Res}(\psi^{\text{ansatz}})\|_{l^\infty} = \mathcal{O}(\epsilon)$ as $\epsilon \to 0$. By Gronwall's inequality, we have

$$\sup_{t\in[0,T_0]} \|U(t)\|_{l^\infty} \leq CT_0 \sup_{t\in[0,T_0]} \|\text{Res}(\psi^{\text{ansatz}})\|_{l^\infty}.$$

Cubic-Quintic DNLS Equations

The DNLS equation is:

$$i\frac{d\psi_n}{dt} + \epsilon\left(\psi_{n+1} + \psi_{n-1} - 2\psi_n\right) + 2|\psi_n|^2\psi_n - |\psi_n|^4\psi_n = 0,$$

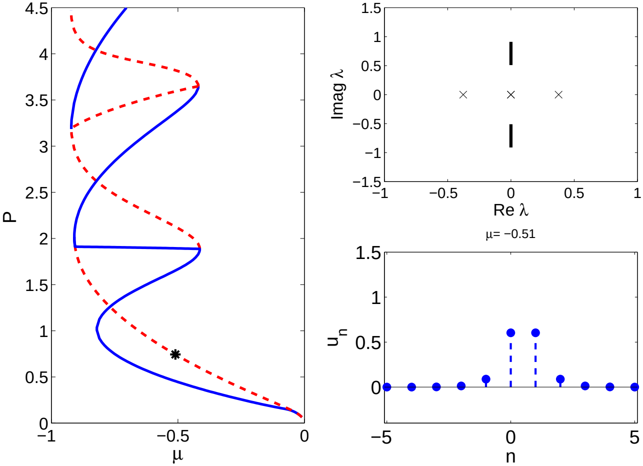
Same game: Start with steady states $\psi_n = \phi_n e^{-i\mu t}$ by using the ansatz

$$\phi_n^{\text{ansatz}}(t) = Ae^{i(\alpha+k(n-s)+\beta(n-s)^2)}e^{-\eta|n-s|}.$$

Note: two parameters (μ, ϵ) exist. Snaking behavior is obtained by fixing $\epsilon = 0.1$ in the plane (μ, P), where $P = \|\phi\|_{l^2}^2$.

R. Carretero-González, J.D. Talley, C. Chong and B.A. Malomed. Multistable solitons of the cubic-quintic discrete nonlinear Schrödinger equation *Physica D* **216** (2006) 77-89.

Cubic-Quintic DNLS Equations



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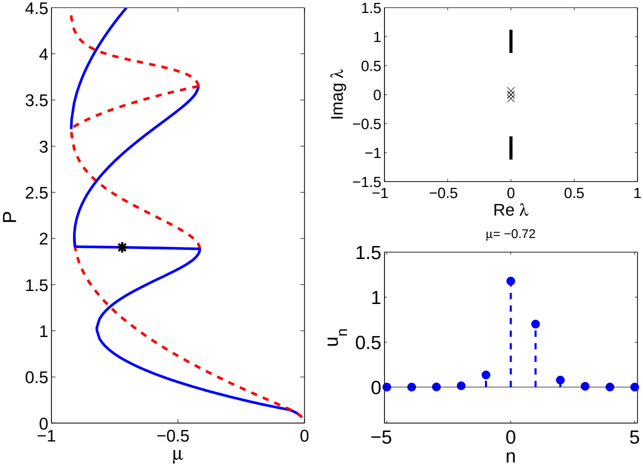

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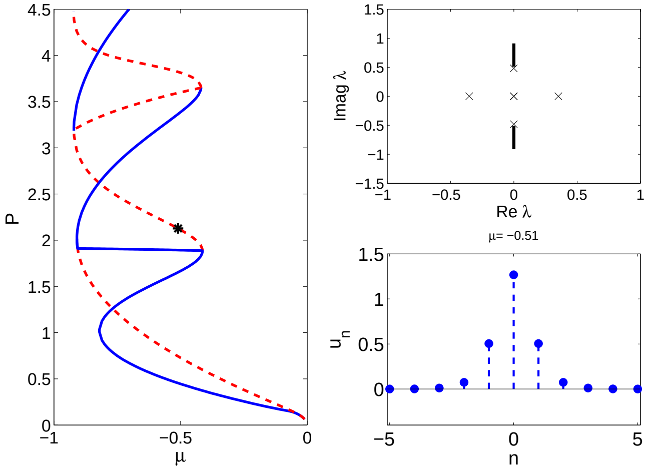
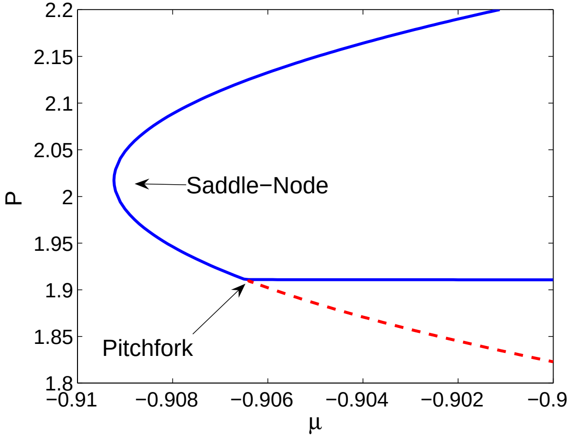


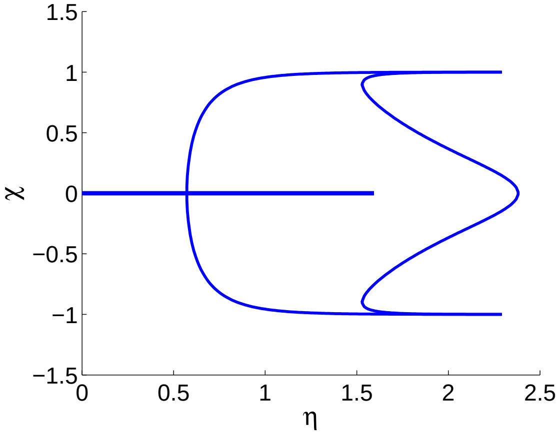
Cubic-Quintic DNLS Equations



Zoom of pitchfork bifurcation

VA for the CQ DNLS

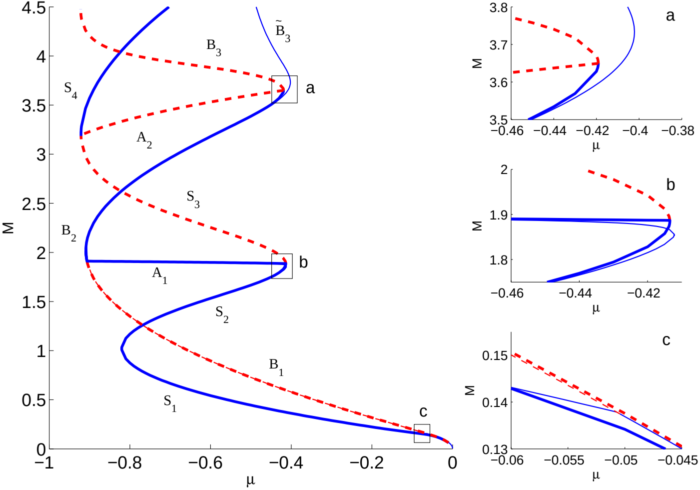
Using the VA, we find the solutions for parameters $\chi = 2s - 1$ and η:



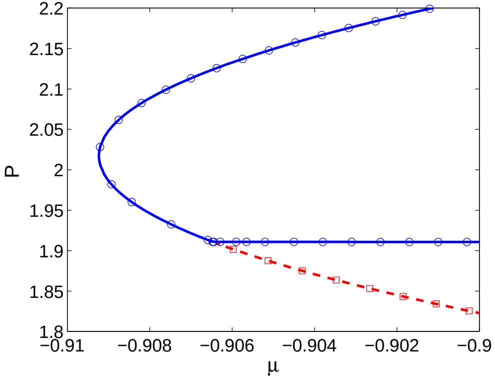
Solutions of the VA equations

VA for the CQ DNLS

All lower energy states are captured by the VA:



VA for the CQ DNLS



The saddle-node and pitchfork bifurcations are captured by the VA.

C. Chong and D.E. Pelinovsky. Variational approximations of bifurcations of asymmetric solitons in cubic-quintic nonlinear Schrödinger lattices. **DCDS S 4** 1019-1032 (2011)

Summary

In the context of DNLS equations, the variational approximation

- is simple,
- yields very good qualitative results,
- makes functional dependencies clear,
- can be used for a host of problems,
- has an Approximation Property

but the variational approximation

- gets complicated quickly
- is not always necessary if numerical approximations are easy and clear.