Searching for Time Periodic Solutions to the Cubic Non-Linear Schrödinger Equation

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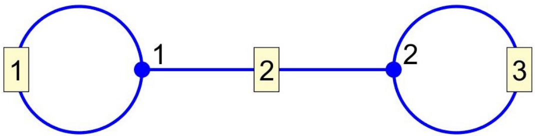
My Problem

Find time-periodic solutions to

$$iu_t = -u_{xx} - |u|^2 u$$

on

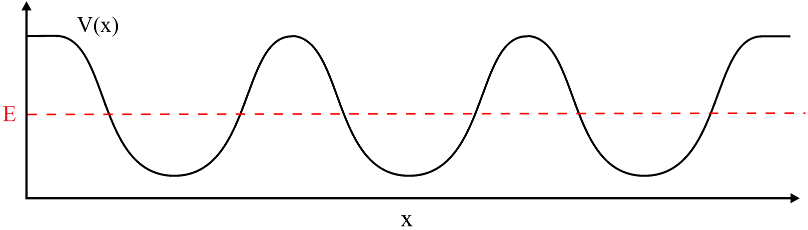


Why it is Interesting

The solutions on the dumbbell have been proven to have solutions that are spectrally similar to the triple-well problem:

$$iu_t = -u_{xx} + V(x)u - |u|^2 u$$

Where $V(x)$ is the triple-well potential:



Why We Think We Will Succeed

My Problem: Want time periodic solutions for an *infinite* dimensional Hamiltonian system.

Lyapunov Center Theorem: Time periodic solutions exist for *finite* dimensional Hamiltonian systems.

Goodman and Yang: Found *near* time periodic solutions for NLS on $\mathbb{R}$

Xu: Found time periodic solutions for NLS on a *torus*

Goals

Numerically

- ☐ Solve the spatial component with machine precision
  - ☐ Generalize our code so it works on *any* graph
- ☐ Find a time solver that compliments the precision of our spatial solver

Analytically

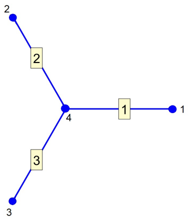
- ☐ Prove time periodic solutions exist on the dumbbell
- ☐ Find the neighborhood for the initial conditions of a periodic orbit

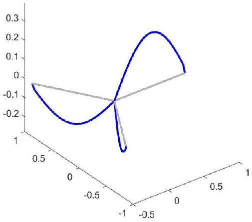
Graphs

- A **graph**, G, is a pair (V, E) where:
  - $V =$ set of vertices v_j
  - $E =$ set of edges e_j
- A **metric graph** has the additional condition:
  - each edge has a length $l_j \in (0, \infty)$
- A **quantum graph** is:
  - a metric graph
  - has a Schrödinger type operator on each edge
    - Schrödinger's Equation: $iu_t = \underset{\substack{\uparrow \\ \text{Schrödinger type} \\ \text{operator}}}{-u_{xx}} + f(u)$

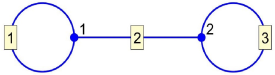
Example: Solutions on Graphs

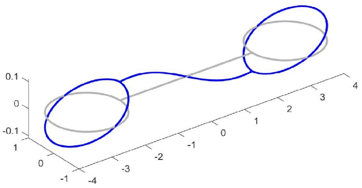
Star Graph





Dumbbell Graph





Vertex Conditions

Possible conditions at a vertex v:

1) Leaf Nodes (Incident to **exactly one** edge)

- Boundary Condition
  - Dirichlet: $u_j(v) = 0$
  - Neumann: $u_j'(v) = 0$
  - Robin: $\alpha_j u_j(v) + u_j'(v) = 0$

2) Internal Nodes (Incident to **more than one** edge)

- Matching Conditions
  - Continuity Condition: $u_j(v) = u_k(v)$
  - Current Conservation: $u_j'(v) + u_k'(v) = 0$
    - Kirchoff: $\sum_{j=1}^{d_v} u_j'(v) = \sigma u_1(v)$

Numerically Defining Operators

Goal: Define $\frac{d}{dx}$ numerically

Evaluate $f(x)$ at discrete points: $\{(x_j, f_j)\}_{j=1}^{n}$

Develop an interpolating polynomial: $f(x) \approx p(x) = \sum_{j=1}^{n} f_j l_j(x)$

Approximate the derivative: $f'(x) \approx p'(x) = \sum_{j=1}^{n} f_j l_j'(x)$

Defining $\mathbf{v}$ as $v_j = p(x_j)$ we can write: $\mathbf{v} = D\mathbf{f}$

where $D_{ij} = l_j'(x_i)$

Numerically Defining Operators: Line

Problem: Solve for u when $x \in [0, \ell]$ in:

$$u_{xx} = f(x), \quad u(0) = a, \;\; u(\ell) = b$$

Discretized Problem: $D^2\mathbf{u} = \mathbf{f}$

We know D^2 and $\mathbf{f}$ so we can solve for $\mathbf{u}$.

But how do we enforce the boundary conditions?

Numerically Defining Operators: BCs

Popular method: Row Replacement

- Remove top and bottom rows and replace with BC's

  $\Rightarrow$ Linear to quadratic convergence

Better method: Rectangular Collocation

- Project information from n points to $n-2$ points

  $\Rightarrow$ Spectral convergence - $e_n \sim (\frac{\ell}{n})^n$

(Driscoll and Hale 2016)

Rectangular Collocation

1. Start with:
   - n discretization points that we are currently evaluating at $\{x_k\}_{k=1}^{n}$
   - $n-2$ discretization points we'd like to be working on instead $\{y_k\}_{k=1}^{n-2}$

Rectangular Collocation

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2. Create an interpolating polynomial, $p_{n-1}(x)$, for the n points

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2. Create an interpolating polynomial, $p_{n-1}(x)$, for the n points
3. Evaluate that polynomial at new $n-2$ discretization points

$$p_{n-1}(\boldsymbol{y}) = P\ p_{n-1}(\boldsymbol{x})$$

Rectangular Collocation

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2. Create an interpolating polynomial, $p_{n-1}(x)$, for the n points
3. Evaluate that polynomial at new $n-2$ discretization points
4. Use vector multiplication to define the $n-2 \times n$ Barycentric Resampling Matrix: P

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3. Evaluate that polynomial at new $n-2$ discretization points
4. Use vector multiplication to define the $n-2 \times n$ Barycentric Resampling Matrix: P
5. Use P to create rectangular differentiation matrices

$$PD^2 = \text{Projected Second Derivative Matrix}$$

Numerically Defining Operators: Line

Problem: Solve for u when $x \in [0, \ell]$ in:

$$u_{xx} = f(x), \quad u(0) = a, \;\; u(\ell) = b$$

Discretized: $D^2\mathbf{u} = \mathbf{f}$ where D is the discretized version of $\frac{d}{dx}$

(*Still need to enforce the boundary conditions*)

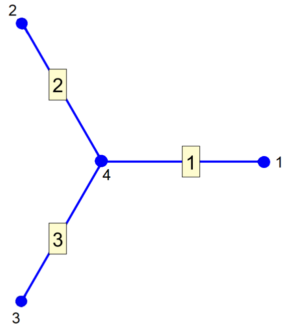
Numerically Defining Operators: Line

$$\underbrace{\begin{bmatrix} 1 & \dots & 0 \\ \begin{bmatrix} & & \\ & PD^2 & \\ & & \end{bmatrix} \\ 0 & \dots & 1 \end{bmatrix}}_{L} \underbrace{\begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_{n-1} \\ u_n \end{bmatrix}}_{\mathbf{u}} = \underbrace{\begin{bmatrix} a \\ f_2 \\ \vdots \\ f_{n-1} \\ b \end{bmatrix}}_{\mathbf{f}}$$

Now solve $L\mathbf{u} = \mathbf{f}$ for $\mathbf{u}$

Numerically Defining Operators: Graph

Problem: Solve $u_{xx} = f(x)$ when x is in:



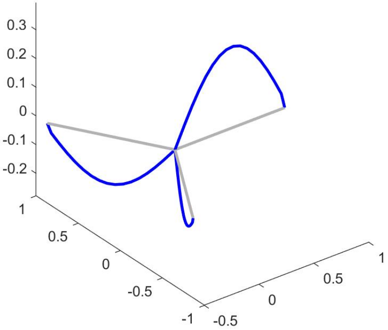
$$\begin{cases} u_1(l_1) = u_2(l_2) = u_3(l_3) = 0 & \text{Boundary Condition} \\ u_1(0) = u_2(0) = u_3(0) & \text{Continuity Condition} \\ u_1'(0) + u_2'(0) + u_3'(0) = 0 & \text{Current Conservation (Kirchoff Condition)} \end{cases}$$

Numerically Defining Operators: Graphs

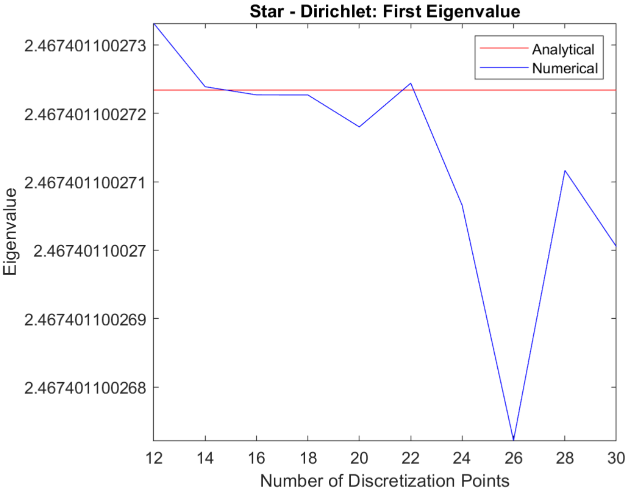
$$L = \begin{bmatrix} \begin{bmatrix} PD^2 & \dots & 0 \\ \vdots & PD^2 & \vdots \\ 0 & \dots & PD^2 \end{bmatrix} \\ \begin{bmatrix} & BC & \end{bmatrix} \\ \begin{bmatrix} & Continuity & \end{bmatrix} \\ \begin{bmatrix} & KC & \end{bmatrix} \end{bmatrix}$$

Numerically Defining Operators: Graphs

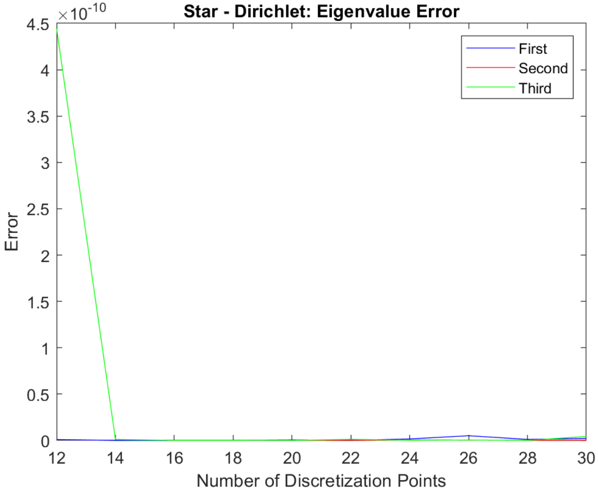
The solution to $L\mathbf{u} = \mathbf{f}$ when $f(x) = \begin{cases} -0.30 \sin x & \text{edge 1} \\ 0.15 \sin x & \text{edge 2} \\ 0.15 \sin x & \text{edge 3} \end{cases}$ is:



Convergence of Spatial Operator



Convergence of Spatial Operator



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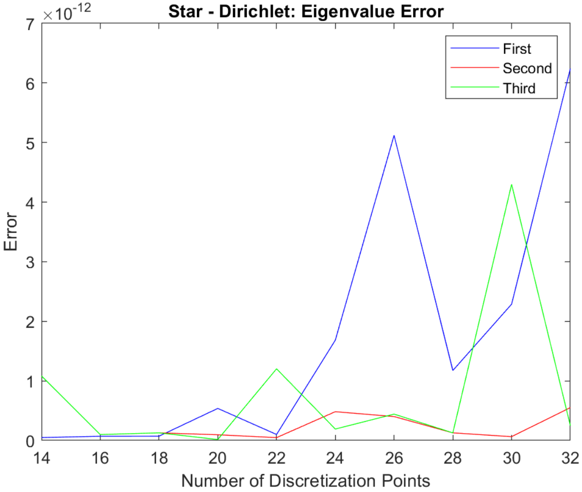
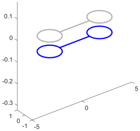
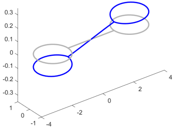


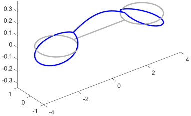
Spatial Operator's Eigenfunctions



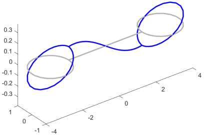
(a) $\lambda = 0.000$



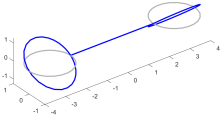
(b) $\lambda = 0.059$



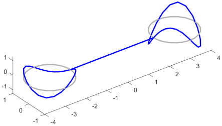
(c) $\lambda = 0.430$



(d) $\lambda = 1.000$



(e) $\lambda = 1.897$



(f) $\lambda = 4.000$

Adding the Nonlinear Component

Cubic NLS equation:

$$iu_t = -u_{xx} - |u|^2 u$$

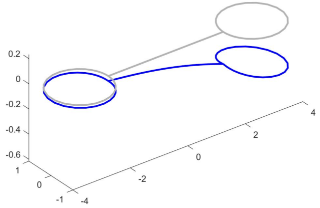
has stationary state solution:

$$u(x,t) = e^{i\mu t} u(x)$$

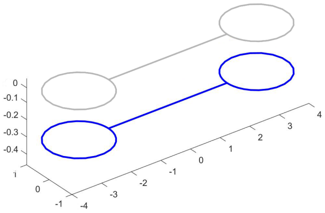
where $u(x)$ solves:

$$u''(x) - u^3(x) = \mu u(x)$$

Solutions for the Static NLS



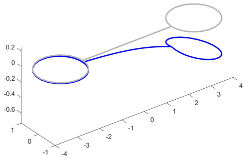
(a) Ground State: $\mu = -0.1781$



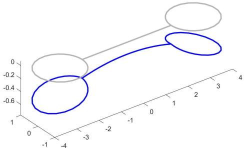
(b) Excited State: $\mu = -0.1786$

Figure: Possible solutions when μ is around -0.178

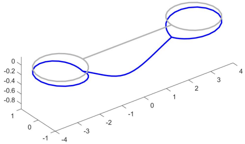
Solutions for the Static NLS



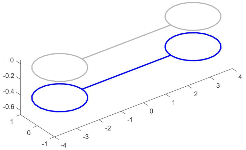
(a) Ground State: $\mu = -0.3370$



(b) Excited State: $\mu = -0.3374$



(c) Excited State: $\mu = -0.3369$

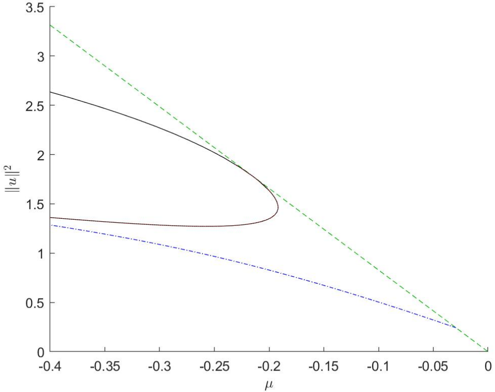


(d) Excited State: $\mu = -0.3273$

Figure: Possible solutions when μ is around -0.337

Bifurcations for the NLS

Bifurcation: A dramatic change in the solution's behavior when a parameter makes a small change



Linearization of the NLS Solution

Normal-mode perturbation:

$$u(x,t) = e^{i\mu t}\left[u(x) + f_1(x)e^{\lambda t} + \bar{f}_2(x)e^{\bar{\lambda} t}\right], \qquad f_1, f_2 \ll 1$$

Need f_1 and f_2 to satisfy the Spectral Problem:

$$J\mathcal{L}\begin{bmatrix} f_1 \\ f_2 \end{bmatrix} = \lambda \begin{bmatrix} f_1 \\ f_2 \end{bmatrix}$$

where

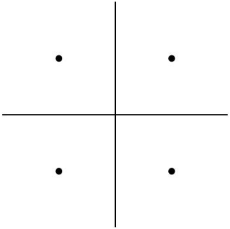
$$\mathcal{L} = \begin{bmatrix} \partial_{xx} - \mu - 2u^2(x) & u^2(x) \\ u^2(x) & \partial_{xx} - \mu - 2u^2(x) \end{bmatrix} \qquad J = -i\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Spectrum of $\mathcal{L}$

$$\sigma(\mathcal{L}) = \{\lambda \mid (\mathcal{L} - \lambda I) \text{ is singular}\}$$

Rephrased: the set of λ's such that $(\mathcal{L} - \lambda I)^{-1}$ does not exist.

Symmetry of $\mathcal{L}$ causes eigenvalues to occur in quadruplets.

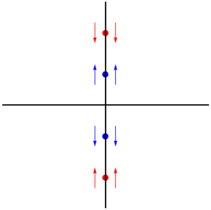


Spectrally Stable Solutions

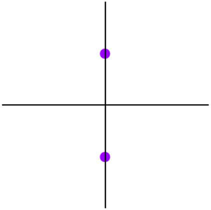
Our focus:

$$\mathrm{Re}(\lambda) = 0$$

Thus eigenvalues occur in $\lambda = \pm i\omega$ pairs



(a) The eigenvalues move as μ changes



(b) This could cause two eigenvalues to coalesce

Figure: Collision of eigenvalues

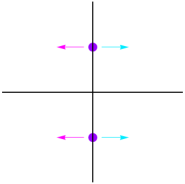
Krein Signature

The Krein signature of two eigenvalues before a collision determines their behavior after.

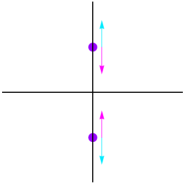
$$K_\lambda = \mathsf{sgn}(K(\lambda))$$

Where the Krein quantity is:

$$K(\lambda) = \langle \mathcal{L}v, v\rangle = \left(\omega \int_{\mathbb{R}} \left[|f_1(x)|^2 - |f_2(x)|^2\right] \, dx\right)$$



(a) Opposite



(b) Same

Figure: Eigenvalue behavior depending on the Krein signature

Hamilton-Hopf Bifurcations

Hamilton-Hopf Bifurcations: A bifurcation that occurs when two eigenvalues with opposite Krein signatures collide on the imaginary axis.

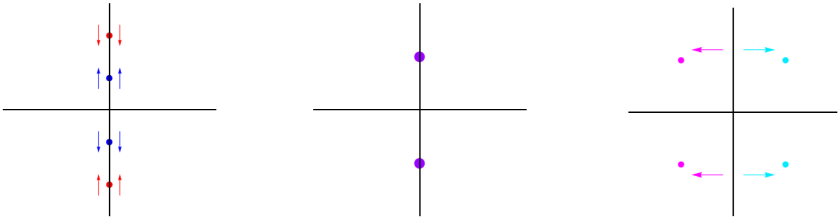


Figure: Conditions for a Hamilton-Hopf bifurcation

Hamilton-Hopf Bifurcations

Suppose we have a Hamilton-Hopf bifurcation at $\mu_0 > 0$ resulting in the eigenvalue pair $\lambda = \pm i\omega$

Then $i\omega$ is a double discrete eigenvalue of $J\mathcal{L}_0 = J\mathcal{L}\big|_{\mu=\mu_0}$

with corresponding real eigenfunction: $[\psi_1, \psi_2]^T$

Thus:

$$J\mathcal{L}_0 \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = i\omega \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix}$$

Because of symmetry, $-i\omega$ has the real eigenfunction: $[\psi_2, \psi_1]^T$

So:

$$J\mathcal{L}_0 \begin{bmatrix} \psi_2 \\ \psi_1 \end{bmatrix} = -i\omega \begin{bmatrix} \psi_2 \\ \psi_1 \end{bmatrix}$$

Normal Form Transformation

Normal Form:

- Make a polynomial change of variables to your DE
- Locally improves the nonlinear system
- Lets us more easily recognize the PDE's dynamics

Analytical goal: Prove periodic solutions exist

Numerical goal: Find the periodic orbit

Normal Form Transformation: Ansatz

Hamilton-Hopf bifurcation point: $\mu = \mu_0$

Solution's perturbation series:

$$u(x,t) = e^{i\theta}\left[u_0(x) + \varepsilon u_1(x,t,\tau) + \varepsilon^2 u_2(x,t,\tau) + ...\right]$$

where

$$\theta(t,\tau) = \mu_0 t + \varepsilon \int_0^{\tau} \mu_1(s)\, ds + \varepsilon^2 \int_0^{\tau} \mu_2(s)\, ds + ...$$

(J. Yang 2016)

Normal Form Transformation: $\mathcal{O}(1)$

Useful terms:

$$\begin{aligned} u_t &= i\theta_t e^{i\theta}\left[u_0 + \varepsilon u_1 + \varepsilon^2 u_2 + \dots\right] + e^{i\theta}\left[\varepsilon u_{1t} + \varepsilon^2 u_{1\tau} + \varepsilon^2 u_{2t} + \varepsilon^3 u_{2\tau} + \dots\right] \\ u_{xx} &= e^{i\theta}\left[u_{0xx} + \varepsilon u_{1xx} + \varepsilon^2 u_{2xx} + \dots\right] \\ \theta_t &= \mu_0 + \varepsilon^2 \mu_1(\tau) + \varepsilon^3 \mu_2(\tau) + \dots \end{aligned}$$

The simplified $\mathcal{O}(1)$ equation is:

$$u_{0xx} + |u_0|^2 u_0 = \mu_0 u_0$$

Normal Form Transformation: $\mathcal{O}(\varepsilon)$

The simplified $\mathcal{O}(\varepsilon)$ equation:

$$(i\partial_t + \partial_{xx} - \mu_0 + 2u_0^2)u_1 + u_0^2\bar{u}_1 = 0$$

Summarize our information for u_1 using the above and its complex conjugate:

$$(i\partial_t + J\mathcal{L}_0)\begin{bmatrix} u_1 \\ \bar{u}_1 \end{bmatrix} = 0$$

Normal Form Transformation: $\mathcal{O}(\varepsilon)$

Recall:

$$J\mathcal{L}_0 \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = i\omega \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix}$$

$$J\mathcal{L}_0 \begin{bmatrix} \psi_2 \\ \psi_1 \end{bmatrix} = -i\omega \begin{bmatrix} \psi_2 \\ \psi_1 \end{bmatrix}$$

Thus we can solve

$$(i\partial_t + J\mathcal{L}_0) \begin{bmatrix} u_1 \\ \bar{u}_1 \end{bmatrix} = 0$$

Solution:

$$u_1(x,t) = B(\tau)\psi_1(x)e^{i\omega t} + \bar{B}(\tau)\psi_2(x)e^{-i\omega t}$$

where $B(\tau)$ is a complex envelope function determined by $\mathcal{O}(\varepsilon^2)$.

Adjoint Continuation Method

Newton scheme that utilizes the normal form as an initial condition to land us on the periodic orbit by finding fixed points

It requires:

- Initial condition
  - The normal form: $\bar{u}_0(x) \approx e^{i\theta t}\big(u_0(x) + \varepsilon u_1(x,0)\big)$
- The Jacobian of the objective function
- Explicit information about time

Adjoint Continuation Method

Initial value problem:

$$u_t = F(u), \qquad u(x,0) = \bar{u}_0(x)$$

where $F(u) = i(u_{xx} + |u|^2 u)$.

To compute nontrivial time periodic solutions, define:

$$G_{\text{tot}} = G(\bar{u}_0, T) + G_{\text{pen}}(\bar{u}_0, T)$$

with

$$G(\bar{u}_0, T) = \frac{1}{2}\int_0^{2\pi} \Big(u(x,T) - \bar{u}_0(x)\Big)^2 \, dx$$

and $G_{\text{pen}}(\bar{u}_0, T)$ is a nonnegative penalty function.

(Ambrose & Wilkening 2010)

Adjoint Continuation Method

$G_{\text{tot}}(\bar{u}_0, T) = 0$ implies u has time period T.

Goal: Numerically minimize G_{tot}

Need to compute the variational derivative:

$$\dot{G} = \frac{d}{d\varepsilon}\Big|_{\varepsilon=0} G(\bar{u}_0 + \varepsilon\dot{\bar{u}}_0,\, T) = \int_0^{2\pi} \left(u(x,T) - \bar{u}_0(x)\right)\left(\dot{u}(x,T) - \dot{\bar{u}}_0\right) dx$$

Adjoint Continuation Method

Necessary components to calculate $\dot{G}$:

$$G_T = \int_0^{2\pi} (u(x,T) - u_0(x))(u_t(x,T))\,dx$$

$$G_{u_0}(x) = Q(x,T) - Q(x,0)$$

where $Q(x,0) = (u(x,T) - u_0(x))$ is the auxiliary quantity.

Next we need a time solver to compute G

Time Evolution

What we need: A solver with enough accuracy to converge to the fixed point of the objective function

Challenges:

- Finding a time-stepper that matches the accuracy of our spatial solver
- Accounting for encoded boundary conditions in our spatial solver
- Coping with the non-linearity

Possible Schemes:

- 8^{th} Order Runge-Kutta
  - Very accurate
  - Hasn't been adapted to DAEs
- Splitting Scheme
  - Preserves energy
  - Lower accuracy

Time Evolution: Runge-Kutta

Big Idea: A Newton solve on something sensitive

Dormand-Prince 8

- Simultaneously executes two Runge-Kutta schemes
- Incurs minimal computation cost
- Actively selects step-size to minimize truncation error

Once we have this, we'll be able to numerically find periodic orbits!

Conclusion

- Developing tools to model Quantum Graphs is essential
- Rectangular Collocation is a superior method for solving PDE's with Schrödinger type operators
- The nonlinear component introduces instabilities into the static problem, but with that, we get the initial conditions to time period solutions
- Evolving NLS through time comes with two challenges
  1. Finding a scheme accurate enough to go with our sensitive spatial data
  2. Finding such a scheme that works specifically with DAEs
- Will be ready to find periodic orbit solutions soon!

Thanks!

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Questions?