Stationary States on Metric Graphs in the limit of large mass

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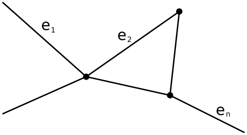
Nonlinear Schrödinger equation on metric graphs

Cubic nonlinear Schrödinger (NLS) equation on a graph Γ:

$$i\Psi_t = -\Delta\Psi - 2|\Psi|^2\Psi, \quad x \in \Gamma, \tag{1}$$

where Δ is the graph Laplacian and $\Psi(t,x)$ is defined componentwise on edges subject to boundary conditions at vertices.

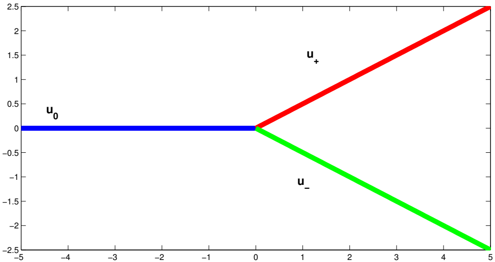


A metric graph $\Gamma = \{E, V\}$ is given by the sets of edges and vertices, with a metric structure on each edge. Proper boundary conditions are needed on the vertices to ensure that Δ is self-adjoint in $L^2(\Gamma)$.

Graph models are widely used in the modeling of quantum dynamics of thin graph-like structures (quantum wires, nanotechnology, large molecules, periodic arrays in solids, photonic crystals...).

Example: a star graph

A star graph is the union of N half-lines (edges) connected at a vertex. For $N = 2$, the graph is the line $\mathbb{R}$. For $N = 3$, the graph is a Y-junction.



Natural (Kirchhoff) boundary conditions:

- Components are continuous across the vertex.
- The sum of fluxes (signed derivatives of functions) is zero at the vertex.

Laplacian on the star graph

The Laplacian operator on the star graph Γ is defined by

$$\Delta\Psi = (\psi_1'', \psi_2'', \cdots, \psi_N'')$$

acting on functions in $L^2(\Gamma) = \oplus_{j=1}^N L^2(\mathbb{R}^+)$.

Weak formulation of Δ on Γ is in

$$H^1_\Gamma := \{\Psi \in H^1(\Gamma) : \quad \psi_1(0) = \psi_2(0) = \cdots = \psi_N(0)\},$$

Strong formulation of Δ on Γ is in

$$H^2_\Gamma := \left\{\Psi \in H^2(\Gamma) : \quad \psi_1(0) = \psi_2(0) = \cdots = \psi_N(0), \quad \sum_{j=1}^N \psi_j'(0) = 0\right\}.$$

Lemma

The graph Laplacian $\Delta : H^2_\Gamma \subset L^2(\Gamma) \to L^2(\Gamma)$ is self-adjoint.

NLS on the metric graph Γ

Nonlinear Schrödinger (NLS) equation can be defined on the metric graph Γ:

$$i\partial_t \Psi + \Delta \Psi + 2|\Psi|^2 \Psi = 0, \quad x \in \Gamma, \quad t \in \mathbb{R},$$

where both the linear term $\Delta\Psi$ and the nonlinear term $|\Psi|^2\Psi$ are defined in the componentwise sense coupled at vertices V of Γ.

The mass functional

$$Q(\Psi) = \|\Psi\|^2_{L^2(\Gamma)}$$

is constant in time t (related to the phase rotation).

The energy functional

$$E(\Psi) = \|\partial_x \Psi\|^2_{L^2(\Gamma)} - \|\Psi\|^4_{L^4(\Gamma)}$$

is constant in time t (related to the time translation).

Ground state

Ground state is a standing wave of smallest energy E at fixed mass Q,

$$\mathcal{E}_\mu = \inf\{E(\Psi) : \quad \Psi \in H^1_\Gamma, \quad Q(\Psi) = \mu\}.$$

Euler–Lagrange equation for the constrained variational problem is

$$-\Delta\Phi - 2|\Phi|^2\Phi = \Lambda\Phi \qquad \Phi \in H^2_\Gamma$$

where $\Lambda \in \mathbb{R}$ defines $\Psi(t,x) = \Phi(x)e^{-i\Lambda t}$.

Infimum $\mathcal{E}_\mu$ exists due to Gagliardo–Nirenberg inequality in 1D:

$$\|\Psi\|^4_{L^4(\Gamma)} \leq C_\Gamma \|\partial_x \Psi\|_{L^2(\Gamma)} \|\Psi\|^3_{L^2(\Gamma)},$$

for some Γ-specific C_Γ.

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for some Γ-specific C_Γ.

Bounded graphs: $\mathcal{E}_\mu$ is achieved at one of the standing waves.
Unbounded graphs: $\mathcal{E}_\mu$ may not be achieved at one of the standing waves.

Existence theorem for ground state

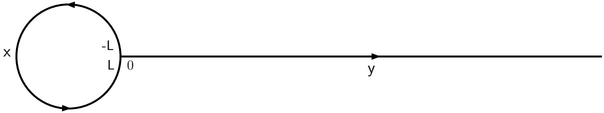
Adami–Serra–Tilli (2015, 2016): If Γ is unbounded and contains at least one half-line, then

$$\min_{u \in H^1(\mathbb{R}^+)} E(u;\mathbb{R}^+) \leq \mathcal{E}_\mu \leq \min_{u \in H^1(\mathbb{R})} E(u;\mathbb{R})$$

If Γ consists of either one half-line or two half-lines connected at a vertex with a bounded edge (pendant), then

$$\mathcal{E}_\mu < \min_{u \in H^1(\mathbb{R})} E(u;\mathbb{R})$$

and the infimum is achieved (ground state exists).



Nonexistence theorem for ground state

Adami–Serra–Tilli (2016): If Γ consists of more than two half-lines and is *connective to infinity*, then

$$\mathcal{E}_\mu = \min_{u \in H^1(\mathbb{R})} E(u; \mathbb{R})$$

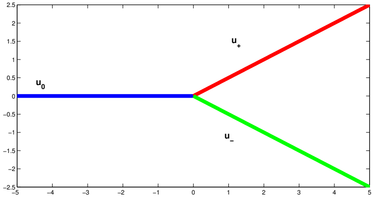
and the infimum is not achieved (ground state does not exist).

The reason is topological. By the symmetry rearrangements,

$$E(\Psi; \Gamma) > E(\hat{\Psi}; \mathbb{R}) \geq \min_{u \in H^1(\mathbb{R})} E(u; \mathbb{R}) = \mathcal{E}_\mu.$$

At the same time, a sequence of solitary waves escaping to infinity along one edge yields a function sequence that minimizes $E(\Psi; \Gamma)$ until it reaches $\mathcal{E}_\mu$.

Standing waves on the star graph



No ground state exists.

There exists the half-soliton state to the Euler–Lagrange equation:

$$-\Delta\Phi - 2|\Phi|^2\Phi = \Lambda\Phi \qquad \phi \in H^2_\Gamma,$$

in the form $\Phi = (\phi, \phi, \ldots, \phi)^T$ with $\phi(x) = \sqrt{|\Lambda|}\text{sech}(\sqrt{|\Lambda|}x)$, $x > 0$.

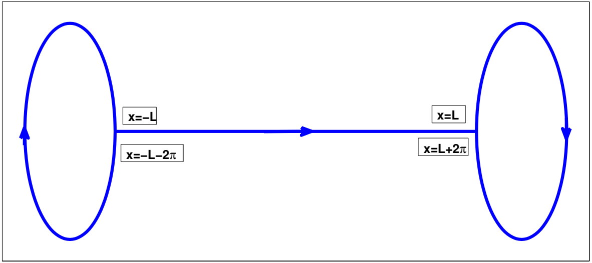
Half-soliton is a saddle point of energy E at fixed mass Q.
(Adami *et al.*, 2012) (Kairzhan–P, 2018)

Main goals of our project:

- Understand standing waves of NLS on a general metric graph Γ in the limit of large mass Q in connection to existence or non-existence of *a ground state* of energy.
- Develop new analytical tools to approximate standing waves of NLS in the limit of large mass Q.

- J. Marzuola and D.E. Pelinovsky, "Ground states on the dumbbell graph", Applied Mathematics Research Express **2016**, 98–145 (2016).
- G. Berkolaiko, J. Marzuola, and D.E. Pelinovsky, "Stationary states in the limit of large mass", in preparation (2018).

Dumbbell Graph



The PDE problem can be formulated in terms of components:

$$\Psi = \left[\begin{array}{ll} \psi_-(x), & x \in I_- := [-L-2\pi, -L], \\ \psi_0(x), & x \in I_0 := [-L, L], \\ \psi_+(x), & x \in I_+ := [L, L+2\pi], \end{array} \right],$$

where L is half-length of the central edge and π is half-length of the loop.

Spectrum of the Laplacian on Γ

The linear problem is

$$-\Delta u = \lambda u \qquad u \in H^2_\Gamma.$$

Since Γ is compact, the spectrum of $-\Delta$ consist of isolated eigenvalues λ. Eigenfunction can be constructed explicitly with parametrization $\lambda = \omega^2$:

$$\begin{cases} u_0(x) = c_0 \cos(\omega x) + d_0 \sin(\omega x), & x \in I_0, \\ u_\pm(x) = c_\pm \cos(\omega x) + d_\pm \sin(\omega x), & x \in I_\pm. \end{cases}$$

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- Double eigenvalues $\{n^2\}_{n\in\mathbb{N}}$ with functions supported in each ring.
- Simple eigenvalues $\{\omega_n^2\}_{n\in\mathbb{N}}$ with symmetric eigenfunctions.
- Simple eigenvalues $\{\Omega_n^2\}_{n\in\mathbb{N}}$ with anti-symmetric eigenfunctions.
- Zero eigenvalue with constant eigenfunction.

Stationary states for small mass

The eigenvalues are ordered as:

$$0 < \Omega_1 < \omega_1 < 1 < \Omega_2 < \dots$$

- 0 is the lowest eigenvalue λ with the constant eigenfunction.

  There exists the constant state of $-\Delta\Phi - 2|\Phi|^2\Phi = \Lambda\Phi$:

  $$\Phi(x) = p, \quad \Lambda = -2p^2, \quad p > 0.$$

  The constant state exists for every $\Lambda < 0$.

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- Ω_1 gives the next eigenvalue $\lambda = \Omega_1^2$ with the odd eigenfunction.

  When the odd eigenfunction is superposed on the constant solution, it leads to an asymmetric state of $-\Delta\Phi - 2|\Phi|^2\Phi = \Lambda\Phi$.

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  When the odd eigenfunction is superposed on the constant solution, it leads to an asymmetric state of $-\Delta\Phi - 2|\Phi|^2\Phi = \Lambda\Phi$.

- ω_1 gives a larger eigenvalue $\lambda = \omega_1^2$ with the even eigenfunction.

  When the even eigenfunction is superposed on the constant solution, it leads to a symmetric state of $-\Delta\Phi - 2|\Phi|^2\Phi = \Lambda\Phi$.

Bifurcation diagram: small mass $Q(\Psi) = \mu$

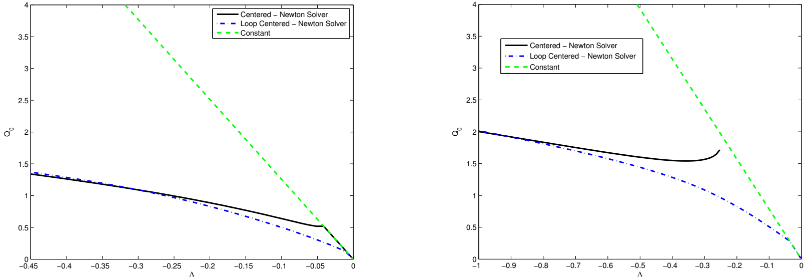

Figure: The bifurcation diagram for $L = 2\pi$ (left) and $L = \pi/2$ (right).

Symmetric state has larger mass than the asymmetric state.
The asymmetric state is the ground state of NLS on the dumbbell graph.
(Marzuola–P, 2016) (Goodman, 2018)

Bifurcation diagram: large mass $Q(\Psi) = \mu$

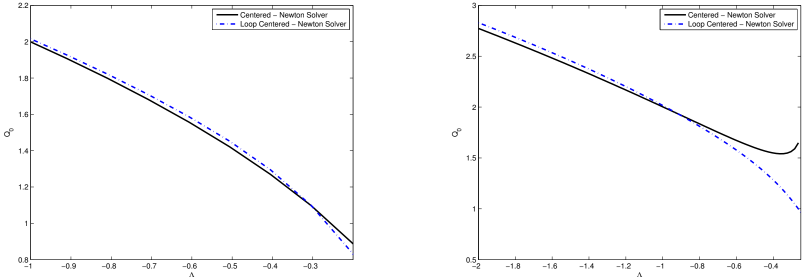

Figure: The bifurcation diagram for $L = 2\pi$ (left) and $L = \pi/2$ (right).

Symmetric state has smaller mass than the asymmetric state.
Which state is the ground state of NLS on the dumbbell graph?

Stationary states: large mass $Q(\Psi) = \mu$

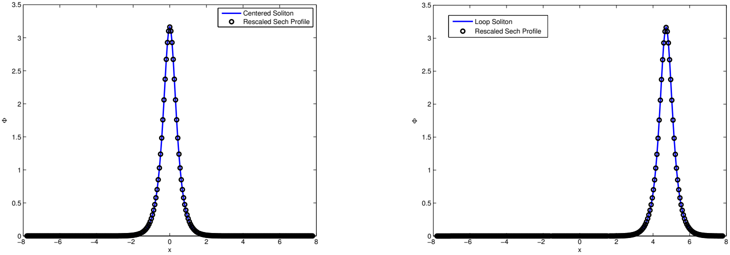

Figure: Comparison of the two stationary states (solid line) with the solitary wave (dots) for $L = \pi/2$ and $\Lambda = -10.0$.

Both stationary states are close to the NLS solitary wave:

$$\phi_\infty(x) = \sqrt{|\Lambda|}\mathrm{sech}(\sqrt{|\Lambda|}x), \quad x \in \mathbb{R},$$

with mass $Q(\phi_\infty) = 2\sqrt{|\Lambda|}$.

Main result in the limit of large mass

Question: If there exist two monotone branches $\Lambda \mapsto Q$ which satisfy

$$\left| Q_{1,2}(\Lambda) - 2|\Lambda|^{\frac{1}{2}} \right| \leq \frac{C}{|\Lambda|^{1+\varepsilon}}, \qquad \Lambda \in (-\infty, \Lambda_0), \qquad \varepsilon > 0,$$

which branch gives minimum of energy $E(\Psi)$ for fixed mass $Q(\Psi) = \mu$?

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which branch gives minimum of energy $E(\Psi)$ for fixed mass $Q(\Psi) = \mu$?

Theorem (Berkolaiko–Marzuola–P, 2018)

If $Q_1(\Lambda) < Q_2(\Lambda)$ for every $\Lambda \in (-\infty, \Lambda_0)$, then

$$Q_1(\Lambda_1) = Q_2(\Lambda_2) = \mu \;\Rightarrow\; E_1(\Lambda_1) > E_2(\Lambda_2),$$

for every $\mu \in (\mu_0, \infty)$ with sufficiently large positive μ_0.

Asymmetric state is the ground state on the dumbbell graph.
(Adami–Serra, 2018)

Analytical technique in the limit of large mass

After rescaling

$$\Phi(x) = |\Lambda|^{1/2}\Psi(z), \quad z = |\Lambda|^{1/2}x,$$

the existence problem becomes

$$-\Delta_z\Psi + \Psi - 2|\Psi|^2\Psi = 0, \qquad z \in J_- \cup J_0 \cup J_+,$$

where

$$\begin{aligned} J_- &:= \left[-(L+2\pi)|\Lambda|^{1/2}, -L|\Lambda|^{1/2}\right], \\ J_0 &:= \left[-L|\Lambda|^{1/2}, L|\Lambda|^{1/2}\right], \\ J_+ &:= \left[L|\Lambda|^{1/2}, (L+2\pi)|\Lambda|^{1/2}\right]. \end{aligned}$$

Question: How to justify the approximation $\psi_\infty(z) = \text{sech}(z)$. as $|\Lambda| \to \infty$?

One stationary state with "surgery" technique

Break the dumbbell graph into two parts:

- Central edge

$$-\psi_0''(z) + \psi_0 - \psi_0^3 = 0, \quad z \in J_0 = \left[-L|\Lambda|^{1/2}, L|\Lambda|^{1/2}\right].$$

- Two loops

$$-\psi_\pm''(z) + \psi_\pm - \psi_\pm^3 = 0, \quad z \in J_\pm.$$

with symmetry condition $\psi_-(-z) = \psi_+(z)$.

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  with symmetry condition $\psi_-(-z) = \psi_+(z)$.

Two exact solutions exist for the central edge:

$$\psi_0(z) = \frac{k}{\sqrt{2k^2-1}} \mathrm{cn}\left(\frac{z}{\sqrt{2k^2-1}}; k\right),$$

and

$$\psi_0(z) = \frac{1}{\sqrt{2-k^2}} \mathrm{dn}\left(\frac{z}{\sqrt{2-k^2}}; k\right),$$

where $k \in (0,1)$ is elliptic modulus. As $k \to 1$, $\psi_0(z) \to \psi_\infty(z) = \mathrm{sech}(z)$.

Define

$$p(k,\Lambda) := \psi_0(L|\Lambda|^{1/2}) \qquad \text{and} \qquad q(k,\Lambda) := |\psi_0'(L|\Lambda|^{1/2})|$$

and consider solution in the right loop (use symmetry for the left loop):

$$-\psi_+''(z) + \psi_+ - \psi_+^3 = 0, \quad z \in \left[L|\Lambda|^{1/2}, (L+2\pi)|\Lambda|^{1/2}\right],$$

subject to the Dirichlet conditions:

$$\psi_+(L|\Lambda|^{1/2}) = \psi_+((L+2\pi)|\Lambda|^{1/2}) = p(k,\Lambda)$$

with $p(k,\Lambda)$ assumed to be small as $\Lambda \to -\infty$.

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with $p(k,\Lambda)$ assumed to be small as $\Lambda \to -\infty$.

Lemma

There exists a unique solution of the boundary value problem satisfying

$$\|\psi_+\|_{H^2(J_+)} \leq C|p(k,\Lambda)|.$$

Moreover, the Dirichlet-to-Neumann map satisfies

$$\psi_+'(L|\Lambda|^{1/2}) = -p(k,\Lambda) + \text{smaller terms}.$$

The remaining Kirchhoff condition

$$\psi'_+((L+2\pi)|\Lambda|^{1/2}) - \psi'_+(L|\Lambda|^{1/2}) = q(k,\Lambda)$$

leads to the root finding problem for k

$$q(k,\Lambda) = 2p(k,\Lambda) + \text{smaller terms.}$$

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Lemma

There exists a unique solution as $|\Lambda| \to \infty$:

$$k = 1 - \frac{8}{3} e^{-2L|\Lambda|^{1/2}} + \text{smaller terms},$$

in the case if ψ_0 is the cn-function:

$$\psi_0(z) = \frac{k}{\sqrt{2k^2-1}} \mathrm{cn}\left(\frac{z}{\sqrt{2k^2-1}}; k\right).$$

The branch $\Lambda \mapsto Q$ for the mass of Ψ can be computed:

$$Q(\Lambda) = 2|\Lambda|^{1/2} - \frac{16}{3} L|\Lambda| e^{-2L|\Lambda|^{1/2}} + \mathcal{O}(e^{-2L|\Lambda|^{1/2}}) \;\; < 2|\Lambda|^{1/2}.$$

The other stationary state with "surgery" technique

Break the dumbbell graph into two parts:

- The right loop

$$-\psi_+''(z) + \psi_+ - \psi_+^3 = 0, \quad z \in \left[L|\Lambda|^{1/2}, (L+2\pi)|\Lambda|^{1/2}\right]$$

- The rest of the dumbbell graph

$$\begin{aligned} -\psi_0''(z) + \psi_0 - \psi_0^3 &= 0, \quad z \in J_0, \\ -\psi_-''(z) + \psi_- - \psi_-^3 &= 0, \quad z \in J_-. \end{aligned}$$

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Again, two exact solutions exist for the right loop

$$\psi_+(z) = \frac{k}{\sqrt{2k^2-1}} \mathrm{cn}\left(\frac{z-(L+\pi)|\Lambda|^{1/2}}{\sqrt{2k^2-1}}; k\right),$$

and

$$\psi_+(z) = \frac{1}{\sqrt{2-k^2}} \mathrm{dn}\left(\frac{z-(L+\pi)|\Lambda|^{1/2}}{\sqrt{2-k^2}}; k\right).$$

Solve the system for the rest of the graph under the Dirichlet condition at $z = L|\Lambda|^{1/2}$ and use Dirichlet-to-Neumann map to satisfies the Kirchhoff boundary condition at $z = L|\Lambda|^{1/2}$:

$$2q(k,\Lambda) = p(k,\Lambda) + \text{smaller terms}.$$

Lemma

There exists a unique solution as $|\Lambda| \to \infty$:

$$k = 1 - \frac{8}{3} e^{-2\pi|\Lambda|^{1/2}} + \text{smaller terms}.$$

in the case if ψ_+ is the dn-function.

The branch $\Lambda \mapsto Q$ for the mass of Ψ can be computed:

$$Q(\Lambda) = 2|\Lambda|^{1/2} + \frac{16}{3}|\Lambda|\pi e^{-2\pi|\Lambda|^{1/2}} + \mathcal{O}(e^{-2\pi|\Lambda|^{1/2}}) \;\; > 2|\Lambda|^{1/2}.$$

By the main result, this stationary state localized in the loop is the ground state of NLS on the dumbbell graph in the limit of large mass.

Ground state for bounded graphs

Main question: Let $\Gamma = \{E, V\}$ be bounded.
What is the ground state as $Q \to \infty$ (or $\Lambda \to -\infty$)?

1. If E includes terminal edges (pendants), the ground state is the half-soliton in the longest pendant.

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2. If E does not have pendants but includes loops connected to a single edge, the ground state is the soliton in the shortest loop.

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3. If E has none of the above, the ground state is the soliton in the longest edge or the longest loop.

Ground state for unbounded graphs

Main question: Let $\Gamma = \{E, V\}$ be unbounded.
Does there exist a ground state?

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2. If E does not have pendants but includes loops connected to a single edge, the ground state exists at the soliton in the shortest loop.

3. If E has none of the above and includes unbounded edges, the ground state does not exist.

Numerical example: ground state in the loop

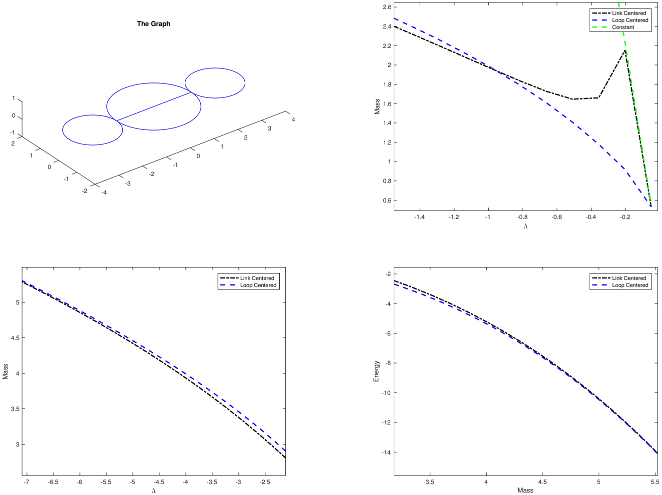

Figure: The generalized dumbbell graph (top left), the Q vs Λ plot bifurcating from linear theory (top right), the Q vs Λ plot in the strongly nonlinear limit (bottom left), and the Q vs. E plot for large E (bottom right).

Numerical example: ground state on the central edge

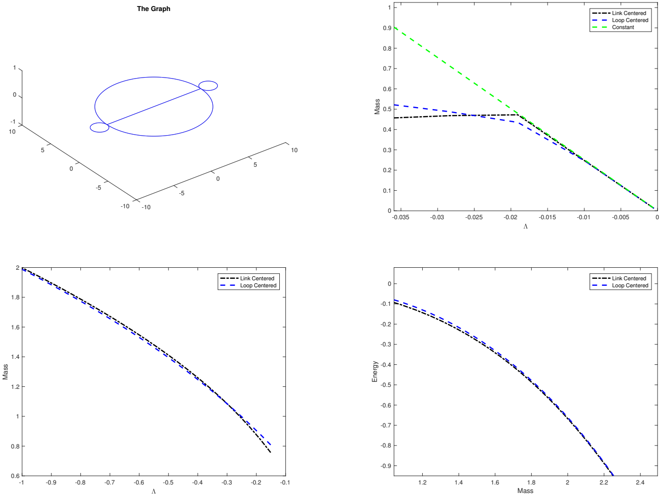

Figure: The generalized dumbbell graph (top left), the Q vs Λ plot bifurcating from linear theory (top right), the Q vs Λ plot in the strongly nonlinear limit (bottom left), and the Q vs. E plot for large E (bottom right).