Integrability and soliton solutions for a nonlinear model of spin transport in helical molecules

P. G. Estévez (joint work with P. Albares, E. Díaz, J. M. Cerveró, F. Domínguez-Adame, E. Diez)

Universidad de Salamanca, Universidad Complutense de Madrid

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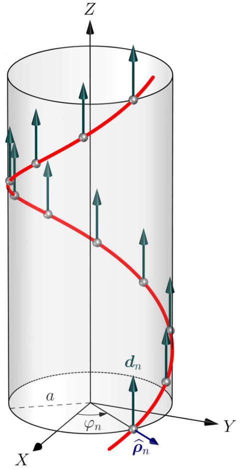
Electron spin dynamics in a deformable helical molecule

Albares *et al.*, 2018; Díaz *et al.*, 2018



Linear model for a rigid molecule

- **Spin-molecule interaction** $\rightarrow$ **Unconventional Rashba-like SOC**
- The Hamiltonian for the system is

$$\hat{\mathcal{H}} = \frac{\hat{p_z}^2}{2m} + \mu\boldsymbol{\sigma}\cdot(\hat{\boldsymbol{p}}\times\boldsymbol{E}), \quad \text{with } \mu = \frac{e\hbar}{(2mc)^2}$$

- The dimensionless Hamiltonian $\hat{H} = \frac{\hat{\mathcal{H}}}{E_b}$ reads

$$\hat{H} = -\partial_{\xi\xi} - 2\pi\gamma \begin{pmatrix} 0 & e^{-i2\pi\xi}(i\partial_\xi + \pi) \\ e^{i2\pi\xi}(i\partial_\xi - \pi) & \end{pmatrix}$$

with $E_b = \frac{\hbar^2}{2mb^2}$ and $\xi = \frac{z}{b}$

- γ is the spin-orbit parameter $\propto$ SOC
- **Time-dependent linear Schrödinger equation**

$$i\partial_t\chi(\xi,t) = \hat{H}\chi(\xi,t)$$

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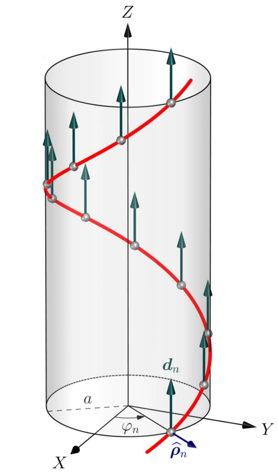

Rigid molecule → Linear Schrödinger equation

- Time-dependent Schrödinger eq. $i\partial_t \chi = \hat{H}\chi$

$$\hat{H} = -\partial_{\xi\xi} - 2\pi\gamma \begin{pmatrix} 0 & e^{-i2\pi\xi}(i\partial_\xi + \pi) \\ e^{i2\pi\xi}(i\partial_\xi - \pi) & \end{pmatrix}$$

Nonlinear model for a deformable molecule

- **Electron-lattice int.** → **Addional nonlinearity**

$$H_{\text{int}} = 2g\, \chi^\dagger(\xi, t) \cdot \chi(\xi, t), \quad g \text{ constant}$$

- **Modified NLS equation in 1+1 dimensions** for the spinor state $\chi = [\chi_1, \chi_2]^{\mathsf{T}}$

$$i\partial_t \chi(\xi, t) = \hat{H}\chi(\xi, t) + 2g \left[\chi^\dagger(\xi, t) \cdot \chi(\xi, t)\right] \chi(\xi, t)$$

where g is a free parameter

NLS eq. for a deformable helical molecule (GNLS)

Modified NLS equation in $1+1$ dimensions for a deformable molecule

$$i\partial_t \boldsymbol{\chi}(\xi,t) = \hat{H}\boldsymbol{\chi}(\xi,t) + 2g\left[\boldsymbol{\chi}^\dagger(\xi,t)\cdot\boldsymbol{\chi}(\xi,t)\right]\boldsymbol{\chi}(\xi,t)$$

$g>0 \rightarrow$ defocusing case, $g<0 \rightarrow$ focusing case

After the following change of variables, we get

$$\boldsymbol{\chi}(\xi,t) = N_g \begin{pmatrix} e^{-i\pi(\xi+\pi t)} & 0 \\ 0 & e^{i\pi(\xi-\pi t)} \end{pmatrix} \boldsymbol{\alpha}(\xi,t), \qquad N_g = \begin{cases} \sqrt{\dfrac{1}{g}} & \text{for } g>0 \\ i\sqrt{\dfrac{1}{|g|}} & \text{for } g<0 \end{cases}$$

Generalized NLS (GNLS) equation in $1+1$ dimensions

$$\begin{aligned} \left(i\partial_t + \partial_{\xi\xi} - 2i\pi\partial_\xi - 2\boldsymbol{\alpha}^\dagger\cdot\boldsymbol{\alpha}\right)\alpha_1 + 2i\pi\gamma\partial_\xi\alpha_2 &= 0 \\ 2i\pi\gamma\partial_\xi\alpha_1 + \left(i\partial_t + \partial_{\xi\xi} + 2i\pi\partial_\xi - 2\boldsymbol{\alpha}^\dagger\cdot\boldsymbol{\alpha}\right)\alpha_2 &= 0 \end{aligned}$$

where α_j with $j=1,2$ are the components of the spinor $\boldsymbol{\alpha}(\xi,t)$

Painlevé Test and SMM for GNLS

- The **Painlevé test** requires to consider the following **generalized Laurent expansion** for the components of the spinor $\boldsymbol{\alpha} = (\alpha_1, \alpha_2)^\intercal$

$$\alpha_1 = \sum_{j=0}^{\infty} a_j(\xi, t)[\phi(\xi, t)]^{j-\beta}, \qquad \alpha_2 = \sum_{j=0}^{\infty} b_j(\xi, t)[\phi(\xi, t)]^{j-\delta}, \qquad \beta, \delta \in \mathbb{N}$$

- If we apply the PT to GNLS: $\beta, \delta = 1$
  a_0, b_0 uniquely determined
  Resonances in $j = -1, 0$ (triple) $, 3$ (triple) $, 4$ ✓
  $\Bigg\} \rightarrow$ **Integrable**, with 1 P. branch

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- The **SMM** implies the **truncation of the series** (**auto-Bäcklund transformation**)

$$\alpha_1^{[1]} = \frac{A\phi_\xi}{\phi} + \alpha_1^{[0]}, \qquad \alpha_2^{[1]} = \frac{B\phi_\xi}{\phi} + \alpha_2^{[0]}$$

- ϕ obeys certain equations $\rightarrow$ **the singular manifold** (SM) **eqs.**

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- ϕ obeys certain equations $\rightarrow$ **the singular manifold** (SM) **eqs.**
- **Linearization** of the SM eqs. $\rightarrow$ **Lax pair**
  We need to introduce **three new functions** $\{\psi, \eta, \omega\}$

$$A = \omega/\psi, \quad B = \eta/\psi, \quad \omega\omega^\dagger + \eta\eta^\dagger - \psi\psi^\dagger = 0$$

Spectral problem for GNLS

Lax Pair for GNLS

$$\partial_\xi \boldsymbol{\Psi} = \begin{pmatrix} -i\lambda & -(\alpha_1^{[0]})^\dagger & -(\alpha_2^{[0]})^\dagger \\ -\alpha_1^{[0]} & i(\lambda+\pi) & -i\pi\gamma \\ -\alpha_2^{[0]} & -i\pi\gamma & i(\lambda-\pi) \end{pmatrix} \boldsymbol{\Psi},$$

$$\partial_t \boldsymbol{\Psi} = i \begin{pmatrix} \boldsymbol{\alpha}^{[0]}(\boldsymbol{\alpha}^{[0]})^\dagger + 2\lambda^2 & [(\alpha_1^{[0]})^\dagger]_\xi - 2i\lambda(\alpha_1^{[0]})^\dagger & [(\alpha_2^{[0]})^\dagger]_\xi - 2i\lambda(\alpha_2^{[0]})^\dagger \\ -[\alpha_1^{[0]}]_\xi - 2i\lambda\alpha_1^{[0]} & -\alpha_1^{[0]}(\alpha_1^{[0]})^\dagger - 2\lambda^2 & -\alpha_1^{[0]}(\alpha_2^{[0]})^\dagger \\ -[\alpha_2^{[0]}]_\xi - 2i\lambda\alpha_2^{[0]} & -\alpha_2^{[0]}(\alpha_1^{[0]})^\dagger & -\alpha_2^{[0]}(\alpha_2^{[0]})^\dagger - 2\lambda^2 \end{pmatrix} \boldsymbol{\Psi}$$

$$+\pi \begin{pmatrix} -i\pi(1+\gamma^2) & \gamma(\alpha_2^{[0]})^\dagger - (\alpha_1^{[0]})^\dagger & \gamma(\alpha_1^{[0]})^\dagger + (\alpha_2^{[0]})^\dagger \\ \gamma\alpha_2^{[0]} - \alpha_1^{[0]} & 0 & 0 \\ \gamma\alpha_1^{[0]} + \alpha_2^{[0]} & 0 & 0 \end{pmatrix} \boldsymbol{\Psi}$$

where $\boldsymbol{\Psi} = (\psi, \omega, \eta)^\intercal$ is the eigenvector and λ is the spectral parameter

- The SM reads $$d\phi = \psi\psi^\dagger d\xi - \left[2\lambda\psi\psi^\dagger + i\left(\psi_\xi\psi^\dagger - \psi\psi_\xi^\dagger\right)\right] dt$$

Binary Darboux transformations for GNLS

- Let $\boldsymbol{\alpha}^{[0]} = \left(\alpha_1^{[0]}, \alpha_2^{[0]}\right)^\mathsf{T}$ be a **seed solution** for GNLS and let $\boldsymbol{\Psi}_j = (\psi_j, \omega_j, \eta_j)^\mathsf{T}$ be **two seed eigenvectors**, with eigenvalues λ_j and ϕ_j as the SM, $j = 1, 2$.

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- The **first iterated solution** $\boldsymbol{\alpha}^{[1]} = \left(\alpha_1^{[1]}, \alpha_2^{[1]}\right)^{\intercal}$ can be constructed as

$$\alpha_1^{[1]} = \alpha_1^{[0]} + \frac{\omega_1 \psi_1^{\dagger}}{\phi_1}, \qquad \alpha_2^{[1]} = \alpha_2^{[0]} + \frac{\eta_1 \psi_1^{\dagger}}{\phi_1}$$

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- Lax pair for $\boldsymbol{\alpha}^{[1]}$ (with s.p. λ_2) $\rightarrow$ **coupled systems of nonlinear PDEs** for $\boldsymbol{\alpha}^{[1]}$ and $\boldsymbol{\Psi}_{1,2} \Rightarrow \boldsymbol{\Psi}_{1,2}$ and $\phi_{1,2}$ should follow the series expansions

$$\Psi_{1,2} = \Psi_2 - \Psi_1 \frac{\Delta_{1,2}}{\phi_1}, \qquad \phi_{1,2} = \phi_2 - \frac{\Delta_{1,2}\Delta_{1,2}^\dagger}{\phi_1}$$

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- The **second iteration** for the fields $\boldsymbol{\alpha}^{[2]}$ is computed as

$$\alpha_1^{[2]} = \alpha_1^{[1]} + \frac{\omega_{1,2} \psi_{1,2}^\dagger}{\phi_{1,2}}, \qquad \alpha_2^{[2]} = \alpha_2^{[1]} + \frac{\eta_{1,2} \psi_{1,2}^\dagger}{\phi_{1,2}}$$

which is given in terms of $\boldsymbol{\alpha}^{[0]}$ through the τ-function $\boldsymbol{\tau_{1,2} = \phi_1 \phi_2 - \Delta_{1,2}\Delta_{1,2}^\dagger}$

Soliton solutions

- **Exponential seed solution** $\alpha^{[0]} = j_0 e^{-2ij_0^2 t}(\beta_1, \beta_2)^\intercal$, with

$$\begin{pmatrix}\beta_1\\ \beta_2\end{pmatrix} = \frac{1}{2}\begin{pmatrix}(1+s)\cos\theta_0 + (1-s)\sin\theta_0\\ (1-s)\cos\theta_0 - (1+s)\sin\theta_0\end{pmatrix}, \; s=\pm 1,\ j_0,\ \theta_0 \text{ free}$$

- **Exponential eigenfunctions** for the Lax pair

$$\Psi_j = C_j e^{k_j\left(\xi + c_j t\right)} e^{\frac{im_0\pi(\xi - m_0\pi t)}{2}} e^{s_j i j_0^2 t}, \quad s=\pm 1,\ \gamma = \tan(2\theta_0)$$

where $m_0 = \frac{s}{\cos(2\theta_0)}$, $c_j = 2(m_0\pi - j_0\cos\theta_j)$, $k_j = j_0 \sin\theta_j$,for $j = 1, 2$.

- The **spectral parameter** is

$$\lambda_j = -\frac{m_0\pi}{2} + j_0\cos\theta_j, \qquad \theta_j \text{ free},\ j = 1, 2$$

- **Singular manifolds**

$$\phi_j = \frac{a_j + E_j^2}{2j_0\sin\theta_j}, \quad E_j = e^{j_0 \sin\theta_j\left[\xi + 2(m_0\pi - j_0\cos\theta_j)t\right]},\ j = 1, 2$$

Soliton solutions ($g > 0$, defocusing case)

- Δ-matrix $\to$ **τ-function**

$$\tau_{1,2} = \frac{1}{4k_1 k_2}\left(a_1 a_2 + a_2 E_1^2 + a_1 E_2^2 + A_{1,2} E_1^2 E_2^2\right)$$

with $A_{1,2} = 1 - \frac{2\sin\theta_1 \sin\theta_2 [1-\cos(\theta_1-\theta_2)]}{(\cos\theta_1 - \cos\theta_2)^2}$.

- First iteration

$$\left|\chi_1^{[1]}\right|^2 = j_0^2 \frac{1+s\cos(2\theta_0)}{2g}\left(1 - \frac{1}{j_0^2}\left[\frac{(\phi_1)_\xi}{\phi_1}\right]_\xi\right)$$

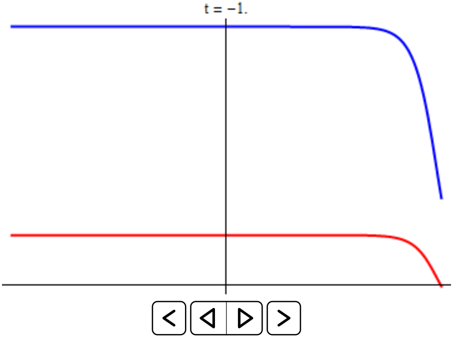
- Second iteration

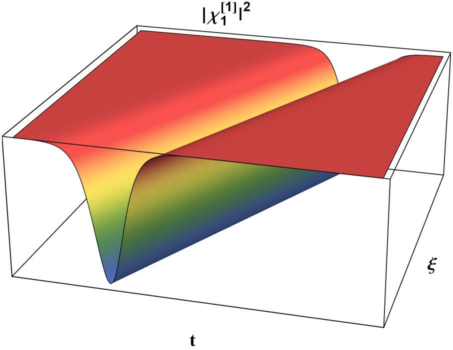
$$\left|\chi_1^{[2]}\right|^2 = j_0^2 \frac{1+s\cos(2\theta_0)}{2g}\left(1 - \frac{1}{j_0^2}\left[\frac{(\tau_{1,2})_\xi}{\tau_{1,2}}\right]_\xi\right)$$

- The lower component is related to the upper component through

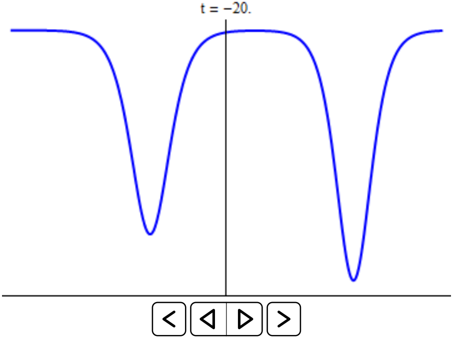
$$\left|\chi_2^{[j]}\right|^2 = \frac{1-s\cos(2\theta_0)}{1+s\cos(2\theta_0)}\left|\chi_1^{[j]}\right|^2, \qquad j = 1,2$$

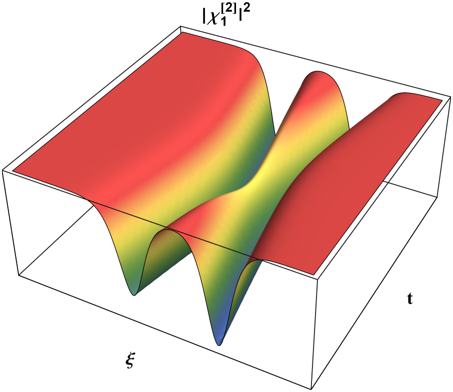
One-soliton solution $\left|\chi_1^{[1]}\right|^2$ → Travelling dark soliton





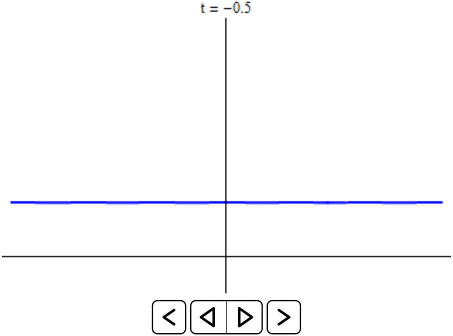
Two-soliton solution $\left|\chi_1^{[2]}\right|^2 \rightarrow$ **Interacting dark solitons**

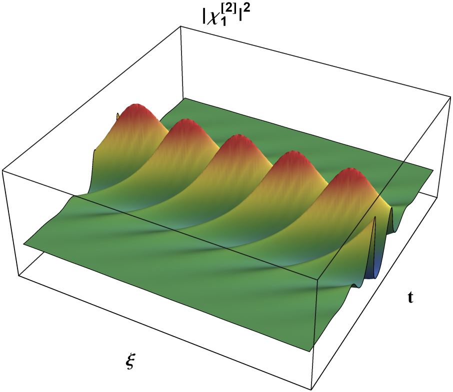




Akhmediev breather ($g < 0$, focusing case)

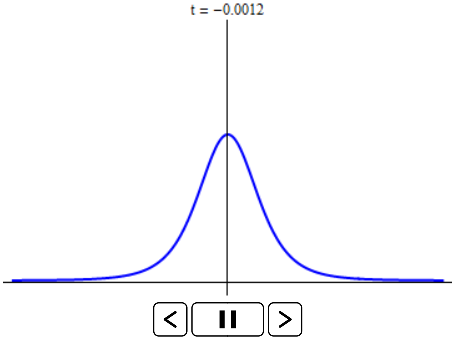
- $\boldsymbol{j_0 = i h_0}$, $h_0 \in \mathbb{R}$, $\boldsymbol{\theta_2 = \pi - \theta_1}$, $\boldsymbol{a_1 = a_2 = \cos\theta_1}$
- $\tau_{1,2} \sim \cosh\left[2h_0^2 \sin(2\theta_1) t\right] + \cos\theta_1 \cos\left[2h_0 \sin\theta_1 \left(\xi + \frac{2s\pi}{\cos(2\theta_0)} t\right)\right]$

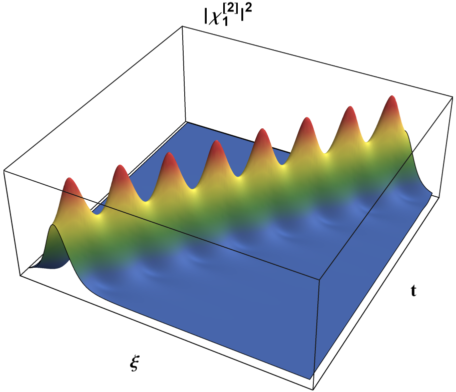




Kuznetsov–Ma breather ($g < 0$, focusing case)

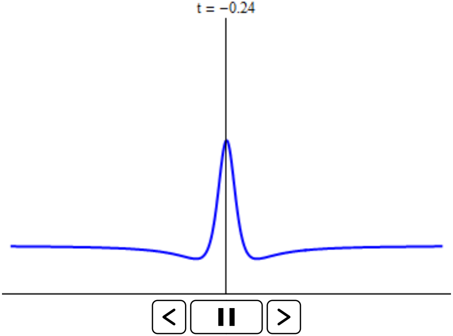
- $\boldsymbol{j_0 = i h_0}$, $h_0 \in \mathbb{R}$, $\boldsymbol{\theta_2 = \pi - \theta_1}$, $\boldsymbol{\theta_1 = i\hat{\theta}_1}$, $\hat{\theta}_1 \in \mathbb{R}$, $\boldsymbol{a_1 = a_2 = \cos\theta_1}$
- $\tau_{1,2} \sim \cos\left[2h_0^2 \sinh(2\hat{\theta}_1)\, t\right] + \cosh\hat{\theta}_1 \cosh\left[2h_0 \sinh\hat{\theta}_1 \left(\xi + \frac{2s\pi}{\cos(2\theta_0)}\, t\right)\right]$

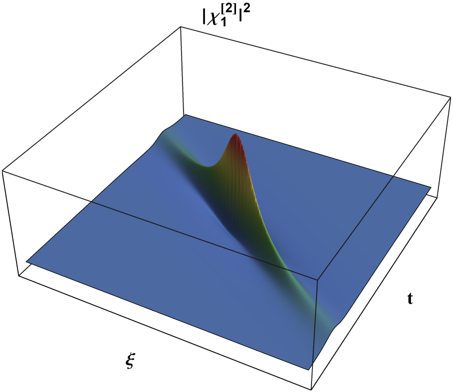




Rogue wave I ($g < 0$, focusing case)

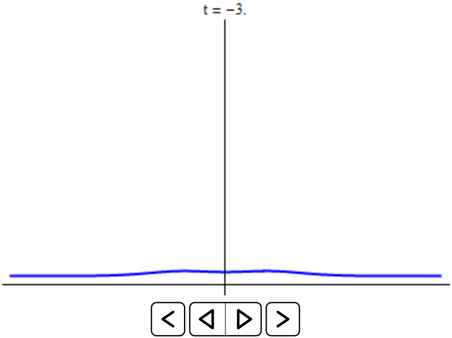
- Eigenfunct. 1: $\theta_1 = 0$, $\lambda_1 = -m_0\pi/2 + j_0$, $c_1 = 2\left(m_0\pi - j_0\right)$
- Eigenfunct. 2: $\theta_2 = \pi$, $\lambda_2 = -m_0\pi/2 - j_0$, $c_2 = 2\left(m_0\pi + j_0\right)$
- $\phi_1 = \xi + 2\pi m_0 t - 2ih_0 t$, $\phi_2 = \phi_1^{\dagger}$, $\tau_{1,2} = \left(\xi + 2\pi m_0 t\right)^2 + 4h_0^2 t^2 + \frac{1}{h_0^2}$

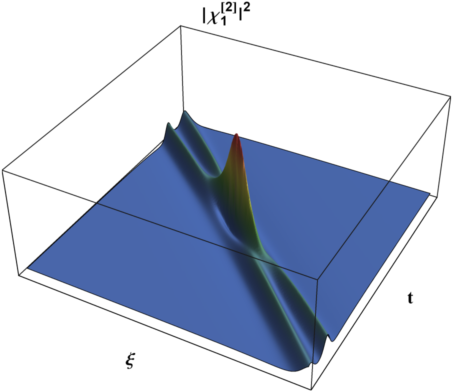




Rogue wave II ($g < 0$, focusing case)

- Eigenfunctions → product of a first degree polynomial & exponentials
- $\tau_{1,2}$ is a **polynomial** in (ξ, t) of **4th degree**





Cnoidal waves & bright solitons ($g < 0$, focusing case)

- Ansatz $\boldsymbol{\alpha} = e^{-i\varphi(\xi,t)}F(z)(\beta_1, \beta_2)^{\intercal}$ → **elliptic solution** of the form

$$\chi(\xi,t) = \frac{km\, e^{-i\varphi(\xi,t)}}{\sqrt{|g|(1-2m^2)}}\,\mathrm{cn}\left[\frac{kz}{\sqrt{2m^2-1}}, m\right]\begin{pmatrix} e^{-i\pi(\xi+\pi t)}\,\beta_1 \\ e^{i\pi(\xi-\pi t)}\,\beta_2\end{pmatrix}$$

where $\mathrm{cn}(\cdot)$ is the Jacobi elliptic cosine and $\varphi(\xi,t) = \frac{c}{2}\left(\xi + \frac{c}{2}t\right) - k^2 t - \pi m_0(\xi + \pi m_0 t)$.

- The hyperbolic limit $m = 1$ yields the normalized solution

$$\chi(\xi,t) = \frac{\sqrt{|g|}}{2}\,\frac{e^{-i(\varphi(\xi,t)+\pi^2 t)}}{\cosh\left[\frac{|g|}{2}\left(\xi + ct\right)\right]}\begin{pmatrix} e^{-i\pi\xi}\,\beta_1 \\ e^{i\pi\xi}\,\beta_2\end{pmatrix}$$

→ generalization of the **Davydov soliton**

- This solution presents a **well defined spin polarization**

$$|\mathrm{SP}_{\mathrm{sol}}| = \frac{1}{\sqrt{1+\gamma^2}}$$

Generalization of the Davydov soliton