# Domain Walls in Continuous Spin Chains with application to Protein Folding

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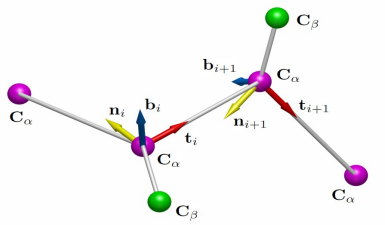
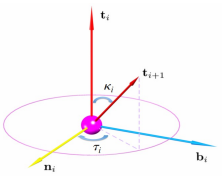
## Proteins as Spin Chains




The (simplified) geometry of a protein can be characterized by the bond and torsion angles of the backbone $\kappa_i$ and $\tau_i$.

Then the values for $\kappa_i$ and $\tau_i$ are determined by minimizing the energy function, where b,c,d,e,q and m are global parameters, that are specific to a given secondary superstructure and determine size, twist and chirality of a loop.




$$E=-\sum_{i=1}^{N} 2\kappa_{i+1}\kappa_i+\sum_{i=1}^{N}(2\kappa_i^2+c\cdot(\kappa_i^2-m^2)^2)+\sum_{i=1}^{N}(b\kappa_i^2\tau_i^2+d\tau_i+e\tau_i^2+q\kappa_i^2\tau_i)$$

## Generalized Discrete Nonlinear Schrödinger Equation

The GDNLS-equation emerges, when the energy is extremized. The auxilary variable $\tau_i$ is eliminated first by:

$$\frac{\partial E}{\partial \tau_i}=2b\kappa_i^2\tau_i+2e\tau_i+d+q\kappa_i^2=0 \quad \Rightarrow \quad \tau_i[\kappa_i]=-\frac{d+q\kappa_i^2}{2(b\kappa_i^2+e)}$$

This is substituted into the variation of E with respect to $\kappa_i$ and gives:

$$\kappa_{i+1}-2\kappa_i+\kappa_{i-1}=\frac{\partial U[\kappa_i^2]}{\partial \kappa_i^2}\kappa_i=U'[\kappa_i]\kappa_i$$

Where

$$U'[\kappa_i]=2c(\kappa_i^2-m^2)+b\frac{d+q\kappa_i^2}{2(b\kappa_i^2+e)}^2-q\frac{d+q\kappa_i^2}{2(b\kappa_i^2+e)}$$

## Iterative Solution and Dark Solitons

The GDNLS-equation in general exhibits chaotic behaviour, but some special solutions can be found[2]. There is an energy maximum at constant bond angle κ=0 and a minimum at $\kappa_\infty=\pm m$, that corresponds to a helix.

Furthermore it was shown that for energy functions that are bounded from below with $U'[\kappa_\infty]>0$ there exist dark soliton solutions, that interpolate between the asymptotic solutions $\kappa_{-\infty}=m$ and $\kappa_\infty=-m$.

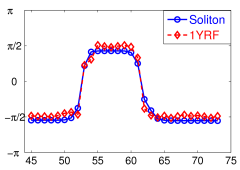
Those can be found iteratively, starting from a step function, that changes sign in the center of the soliton with the following iteration:

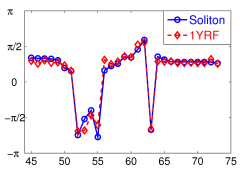
$$\kappa_i^{(n+1)}=\kappa_i^n-\epsilon(\kappa_i^n U'[\kappa_i^n]-(\kappa_{i+1}^n-2\kappa_i^n+\kappa_{i-1}^n))$$

In order to model loops in real life proteins we have to explicitly break the κ↔-κ reflection symmetry and choose different values for m at both sides of the soliton $m_i$ and $m_f$.

Using a monte carlo simulations we find the best parameter values b,c,d,e,q,$m_i$ ,$m_f$ to describe a given helix-loop-helix configuration.

## Application to HP35

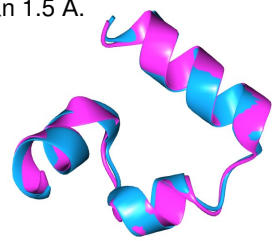



***Top**: Bond angles of 1YRF(red) sites 45-78 and the best fit with our model.*

***Bottom**: Torsion angles of 1YRF(red) sites 45-78 and the best fit with our model.*

Here we have used this method to model the chicken villin headpiece subdomain HP35 (1YRF) [3].
The best parameters gave an overall RMSD of 0.74 Å.
The same parameters for the first and second soliton each describe several thousands of solitons in the PDB with an accuracy better than 1.5 Å.



*Comparison between 1YRF backbone (pink), soliton solution (blue)*

[1] U.H. Danielsson, M. Lundgren and A.J. Niemi, Phys.Rev. E82, 021910 (2010)
[2] M. Herrmann, e-print arXiv:1002.1591v1 [math-ph]
[3] N.Molkenthin, S.Hu and A.J.Niemi, e-print arXiv:1009.1078v1 [physics.bio-ph]