4

Soliton Excitations in Continuum
Alpha Helical Proteins with
Interspine Coupling

4.1 Introduction

In most of the works on Davydov soliton, mainly a single channel or hydrogen bonding spine of the alpha helical protein molecule has been considered as it is assumed that the study of the dynamics of a single molecular chain will reproduce the dynamics of the full alpha helical molecular chain. Based on that in the previous chapter, we presented the results of the multisoliton propagation along a single hydrogen bonding spine. However in reality a sequence of amide units (-CONH-) forms a helical structure, which is stabilized by three quasilinear strands of hydrogen bonds [149]. In such a situation there exists a possible interaction
(interspine coupling) between the nearest neighbouring peptide units of the adjacent molecular spines. Thus it has become important and necessary to investigate the internal dynamics of alpha helical protein with interspine coupling. Only a few number of related works have been reported in the literature in the recent past [267-273]. Motivated by this we propose a model for alpha helical proteins by including excitations, dipole-dipole interactions between nearest neighbours and next nearest neighbours and interspine coupling. The underlying dynamics is studied for specific choice of parameters which leads to integrable models both in the continuum and discrete levels.

4.2 The Model

The Hamiltonian with interspine coupling for a system of three coupled infinite molecular chains with unit cells H-N-C=O characterizing the three hydrogen bonding spines of peptide groups running parallel to the helical axis in an alpha helical protein can be written as

\[ H = H_{11} + H_{12} + H_{13} + H_{14} + H_{15}. \]  

(4.1)

In Eq. (4.1), \( H_{11} \) stands for the exciton Hamiltonian representing internal molecular excitations. If \( E_0 \) is the amide - I excitation energy and \( B_{n,\alpha}^{\dagger} \) is an operator for creation of this excitation on the n-th peptide group in the \( \alpha \)-th spine, then
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\[ H_{11} \text{ is given by} \]

\[ H_{11} = \sum_{n,\alpha} B^\dagger_{n,\alpha} [E_0 B_{n,\alpha} - J_0 (B_{n+1,\alpha} + B_{n-1,\alpha}) - L (B_{n,\alpha+1} + B_{n,\alpha-1})]. \]  

(4.2)

The summation with respect to \( n \) runs over the unit cells \((H - N - C = O)\) along the infinite hydrogen bonding spines and the summation over \( \alpha \) runs over the three hydrogen bonding spines \((\alpha = 1, 2, 3)\). \( B^\dagger_{n,\alpha} \) and \( B_{n,\alpha} \) represent the creation and annihilation operators for the internal molecular excitation of the peptide group labeled by \( n \) in the \( \alpha \)-th spine. The first term \( E_0 B^\dagger_{n,\alpha} B_{n,\alpha} \) defines the amide-I excitation energy and the second term the resonance dipole-dipole interaction between nearest neighbours. The operator \( B^\dagger_{n,\alpha} B_{n+1,\alpha} \) and \( B^\dagger_{n,\alpha} B_{n-1,\alpha} \) represent the transfer of amide-I energy from peptide group \( n \) to \( n \pm 1 \) due to the dipole-dipole interaction. \( L \) is the interspine transfer matrix element accomplishing the transport between covalently linked peptide groups of different spines. The energy \( H_{12} \) associated with displacing the peptide groups away from their equilibrium positions is given in the harmonic approximation by

\[ H_{12} = \sum_{n,\alpha} \frac{1}{2} \left( \frac{p^2_{n,\alpha}}{m} + \frac{s^2_{n,\alpha}}{m} + K (u_{n,\alpha} - u_{n-1,\alpha})^2 + I (v_{n,\alpha} - v_{n,\alpha-1})^2 \right), \]  

(4.3)

where \( u_{n,\alpha} \) is the operator for the longitudinal displacement of peptide group parallel to the helical axis from its equilibrium position in each hydrogen bonding spine and \( v_{n,\alpha} \) that for the displacement along the helical radius. \( p_{n,\alpha} \) and \( s_{n,\alpha} \) are the momentum operators conjugate to \( u_{n,\alpha} \) and \( v_{n,\alpha} \) respectively. \( m \) is the
mass of the peptide group. \( K \) and \( I \) are the elasticity coefficients relative to change in helix pitch and helix radius respectively. \( H_{13} \) is the Hamiltonian for the interaction between amide - I excitation and the displacement of the peptide groups and is given by

\[
H_{13} = \sum_{n,\alpha} (\chi_1 B_{n,\alpha}^\dagger B_{n,\alpha} + \chi_2 B_{n,\alpha+1}^\dagger B_{n,\alpha+1} + \chi_3 B_{n,\alpha-1}^\dagger B_{n,\alpha-1})(u_{n+1,\alpha} - u_{n-1,\alpha}),
\]

where \( \chi_1, \chi_2 \) and \( \chi_3 \) represent the nonlinear couplings which give rise to change in energy of the amide-I bond at different levels caused by the stretching of the helix between two nearest neighbouring unit cells of the same spine. The energy \( H_{14} \) for the interaction between amide-I excitation and the displacement of the next nearest peptide groups for same spines is written as

\[
H_{14} = \sum_{n,\alpha} (\chi_4 B_{n,\alpha}^\dagger B_{n+1,\alpha} + \chi_5 B_{n,\alpha+1}^\dagger B_{n+1,\alpha+1} + \chi_6 B_{n,\alpha-1}^\dagger B_{n+1,\alpha-1})(u_{n+2,\alpha} - u_{n,\alpha}) + (\chi_7 B_{n,\alpha}^\dagger B_{n-1,\alpha} + \chi_8 B_{n,\alpha+1}^\dagger B_{n-1,\alpha+1} + \chi_9 B_{n,\alpha-1}^\dagger B_{n-1,\alpha-1})
\times (u_{n,\alpha} - u_{n-2,\alpha}),
\]

where \( \chi_4, \chi_5, \ldots, \chi_9 \) represent the nonlinear couplings which give rise to change in energy of the amide-I bond at different levels caused by the stretching of the helix between two next nearest neighbouring unit cells of the same spine. The Hamiltonian \( H_{15} \) for the interaction between the amide - I excitation and the displacement of the peptide groups in the nearest neighbouring spines can be
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written as

\[ H_{15} = \sum_{n,\alpha} [\eta_1 B_{n,\alpha} + \eta_2 (B_{n+1,\alpha} - B_{n-1,\alpha})] (v_{n,\alpha+1} + v_{n,\alpha-1} - 2v_{n,\alpha}), \quad (4.6) \]

where \( \eta_1 \) and \( \eta_2 \) describe the change in amide-I energy caused by the stretching of the helix between two neighbouring unit cells of the two nearest neighbour spines along the radial direction of the helix.

Using the wave function (2.7), the Hamiltonian corresponding to the large amplitude collective modes of the coherent states can be expressed as

\[ \langle H \rangle = \sum_{n,\alpha,\rho} \{ a^*_{n,\alpha} [(E_0 + W)a_{n,\alpha} - Ja_{n+\rho,\alpha} - L(a_{n,\alpha+1} + a_{n,\alpha-1})] + (\chi_1 a^*_{n,\alpha}a_{n,\alpha} \\
+ \chi_2 a^*_{n+1,\alpha}a_{n,\alpha+1} + \chi_3 a^*_{n,\alpha+1}a_{n-1,\alpha} (b_{n+1,\alpha} - b_{n-1,\alpha})] + (\chi_4 a^*_{n,\alpha}a_{n+1,\alpha} \\
+ \chi_5 a^*_{n+1,\alpha}a_{n+1,\alpha+1} + \chi_6 a^*_{n,\alpha+1}a_{n-1,\alpha+1} (b_{n+2,\alpha} - b_{n,\alpha})] + (\chi_7 a^*_{n,\alpha}a_{n-1,\alpha} \\
+ \chi_8 a^*_{n,\alpha+1}a_{n-1,\alpha+1} + \chi_9 a^*_{n,\alpha+1}a_{n-1,\alpha-1} (b_{n,\alpha} - b_{n+2,\alpha})] + a^*_{n,\alpha}\eta_1 a_{n,\alpha} \\
+ \eta_2 (a_{n+1,\alpha} - a_{n-1,\alpha}) [c_{n,\alpha+\rho} - 2c_{n,\alpha}] \}, \quad (4.7) \]

where \( \rho = \pm 1 \) and

\[ W = \frac{1}{2} \left( \frac{\phi_{n,\alpha}^2}{m} + \frac{\pi_{n,\alpha}^2}{m} + K(b_{n,\alpha} - b_{n-1,\alpha})^2 + I(c_{n,\alpha} - c_{n-1,\alpha})^2 \right) \quad (4.8) \]

is the deformation energy of the spines.

Using the Hamiltonian (4.7) in the equation of motion (2.6) and after using the commutation relations (2.13) and (2.14), the equations of motion for the variables \( a_{n,\alpha}, b_{n,\alpha} \) and \( c_{n,\alpha} \) can be written as

\[ i\hbar \frac{da_{n,\alpha}}{dt} = \sum_{\rho} [(E_0 + W)a_{n,\alpha} - Ja_{n+\rho,\alpha} - La_{n+\rho+\alpha}] + a_{n,\alpha} \chi_1 (b_{n+1,\alpha} \]

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\[-b_{n-1,\alpha} + \chi_2(b_{n+1,\alpha-1} - b_{n-1,\alpha-1}) + \chi_3(b_{n+1,\alpha+1} - b_{n-1,\alpha+1})\]

\[+ a_{n+1,\alpha}[\chi_4(b_{n+2,\alpha} - b_{n,\alpha}) + \chi_5(b_{n+2,\alpha-1} - b_{n,\alpha-1}) + \chi_6(b_{n+2,\alpha+1} - b_{n,\alpha+1}) - b_{n,\alpha+1})] + a_{n-1,\alpha}[-\chi_7(b_{n,\alpha} - b_{n-2,\alpha}) + \chi_8(b_{n,\alpha-1} - b_{n-2,\alpha-1}) + \chi_9(b_{n,\alpha+1} - b_{n-2,\alpha+1})]\]

\[+ \eta_1a_{n,\alpha} + \eta_2(a_{n+1,\alpha} - a_{n-1,\alpha})]\]

\[= (c_{n,\alpha+\rho} - 2c_{n,\alpha})\]

\[\frac{\partial}{\partial t} = \sum_\rho \{K(b_{n+\rho,\alpha} - 2b_{n,\alpha}) + \chi_1(|a_{n+1,\alpha}|^2 - |a_{n-1,\alpha}|^2)\]

\[+ \chi_2(|a_{n+1,\alpha+1}|^2 - |a_{n-1,\alpha+1}|^2) + \chi_3(|a_{n+1,\alpha-1}|^2 - |a_{n-1,\alpha-1}|^2)\]

\[+ \chi_4(a_{n+1,\alpha}^*a_{n+1,\alpha} - a_{n-2,\alpha}^*a_{n-2,\alpha}) + \chi_5(a_{n+1,\alpha+1}^*a_{n+1,\alpha+1} - a_{n-2,\alpha+1}^*a_{n-2,\alpha+1})\]

\[+ \chi_7(a_{n+2,\alpha}^*a_{n+2,\alpha} - a_{n,\alpha}^*a_{n,\alpha}) + \chi_8(a_{n+2,\alpha+1}^*a_{n+2,\alpha+1} a_{n+1,\alpha+1}\]

\[+ \chi_9(a_{n+2,\alpha-1}^*a_{n+2,\alpha-1}) - a_{n,\alpha-1}^*a_{n-1,\alpha-1})\}\] (4.9)

\[\frac{m}{d^2c_{n,\alpha}} dt^2 = \sum_\rho \{I(c_{n,\alpha+\rho} - 2c_{n,\alpha}) - \eta_1(|a_{n,\alpha+\rho}|^2 - 2|a_{n,\alpha}|^2)\]

\[\frac{\partial}{\partial t} = \sum_\rho \{I(c_{n,\alpha+\rho} - 2c_{n,\alpha}) - \eta_1(|a_{n,\alpha+\rho}|^2 - 2|a_{n,\alpha}|^2)\] \[\frac{\partial}{\partial t} = \sum_\rho \{I(c_{n,\alpha+\rho} - 2c_{n,\alpha}) - \eta_1(|a_{n,\alpha+\rho}|^2 - 2|a_{n,\alpha}|^2)\]

The set of coupled equations (4.9), (4.10) and (4.11) describes the dynamics of the homogeneous protein lattice with interspine coupling. Assuming that the time rate of change in amplitude of the lateral displacement, i.e., \(\frac{d^2c_{n,\alpha}}{dt^2}\) is

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slow and proportional to the change in amplitude of the lateral displacement with respect to $\alpha$, we replace the left-hand side of Eq. (4.11) by the discrete form

$$\frac{d^2 c_{n,\alpha}}{dt^2} \rightarrow \sum_{\rho=1,-1} \left\{ \frac{1}{\sigma^2} (c_{n,\alpha+\rho} - 2c_{n,\alpha}) \right\},$$

(4.12)

where $\sigma$ is a parameter which represents a small change in $t$. Using Eq. (4.12), Eq. (4.11) can be written as

$$\sum_{\rho} (c_{n,\alpha+\rho} - 2c_{n,\alpha}) = A_1 \sum_{\rho} \left\{ \eta_1 (|a_{n,\alpha+\rho}|^2 - 2|a_{n,\alpha}|^2) + \eta_2 [(a^*_{n,\alpha+\rho} a_{n+1,\alpha+\rho} - 2a^*_{n,\alpha} a_{n+1,\alpha})$$

$$- (a^*_{n,\alpha+\rho} a_{n-1,\alpha+\rho} - 2a^*_{n,\alpha} a_{n-1,\alpha})] \right\},$$

(4.13)

where $A_1 = \frac{n \sigma^2}{I \sigma^2 - m}$. Substituting Eq. (4.13) in Eq. (4.9) we get

$$i \hbar \frac{da_{n,\alpha}}{dt} = \sum_{\rho} \left\{ (E_0 + W)a_{n,\alpha} - Ja_{n+\rho,\alpha} - L a_{n,\alpha+\rho} + a_{n,\alpha} [\chi_1 (b_{n+1,\alpha} - b_{n-1,\alpha})$$

$$+ \chi_2 (b_{n+1,\alpha-1} - b_{n-1,\alpha-1}) + \chi_3 (b_{n+1,\alpha+1} - b_{n-1,\alpha+1})]$$

$$+ a_{n+1,\alpha} [\chi_4 (b_{n+2,\alpha} - b_{n,\alpha}) + \chi_5 (b_{n+2,\alpha-1} - b_{n,\alpha-1})$$

$$+ \chi_6 (b_{n+2,\alpha+1} - b_{n,\alpha+1})] + a_{n-1,\alpha} [\chi_7 (b_{n,\alpha} - b_{n-2,\alpha})$$

$$+ \chi_8 (b_{n,\alpha-1} - b_{n-2,\alpha-1}) + \chi_9 (b_{n,\alpha+1} - b_{n-2,\alpha+1})]$$

$$+ A_1 [\eta_1 a_{n,\alpha} + \eta_2 (a_{n+1,\alpha} - a_{n-1,\alpha})] \left[ \eta_1 (|a_{n,\alpha+\rho}|^2 - 2|a_{n,\alpha}|^2)$$

$$+ \eta_2 [(a^*_{n,\alpha+\rho} a_{n+1,\alpha+\rho} - 2a^*_{n,\alpha} a_{n+1,\alpha}) - (a^*_{n,\alpha+\rho} a_{n-1,\alpha+\rho}$$

$$- 2a^*_{n,\alpha} a_{n-1,\alpha})] \right\}.$$  (4.14)

When the function $a_{n,\alpha}$ and $b_{n,\alpha}$ change smoothly over one link of the chain, it is appropriate to make a continuum approximation for $a_{n+1,\alpha}$ and $b_{n+1,\alpha}$ using the
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Taylor series expansion (2.17) in Eqs. (4.10) and (4.14). The resulting equations are:

\[
\begin{align*}
i \hbar a_{\alpha,t} &= \left[ \delta_0 + \eta^2 \bar{A}_1 \left( |a_{\alpha+\rho}|^2 - 2|a_\alpha|^2 \right) \right] a_\alpha - L a_{\alpha+\rho} + 2\epsilon [\delta_1 b_{\alpha,x} \\
&+ \delta_2 b_{\alpha-1,x} + \delta_3 b_{\alpha+1,x} + A_1 \eta \eta_2 \left( |a_{\alpha+\rho}|^2 - 2|a_\alpha|^2 \right) a_{\alpha,x} + \frac{1}{2} a^*_{\alpha+\rho} a_{\alpha+\rho,x} a_\alpha - |a_\alpha|^2 a_{\alpha,x} \right] \\\n&+ 2\epsilon \left[ \frac{-J}{2} a_{\alpha,xx} + A_1 \eta^2 a^*_{\alpha+\rho} a_{\alpha+\rho,x} a_{\alpha,x} - 2A_1 \eta_2 a^*_{\alpha} a_{\alpha,x} \right],
\end{align*}
\]

(4.15)

\[
\begin{align*}
mb_{\alpha,tt} &= -\frac{d}{dx} \left\{ 2\epsilon [\delta_1 |a_\alpha|^2 + \delta_2 |a_{\alpha+1}|^2 + \delta_3 |a_{\alpha-1}|^2] + 2\epsilon \left[ -\delta_4 a_\alpha a^*_x \right. \\
&\left. -\delta_5 a_{\alpha+1} a^*_{\alpha+1,x} - \delta_6 a_{\alpha-1} a^*_{\alpha-1,x} \right] \right\},
\end{align*}
\]

(4.16)

where \( \delta_0 = E_0 + W - 2J, \delta_1 = \chi_1 + \chi_4 + \chi_7, \delta_2 = \chi_2 + \chi_5 + \chi_8, \delta_3 = \chi_3 + \chi_6 + \chi_9, \delta_4 = \chi_4 - \chi_7, \delta_5 = \chi_5 - \chi_8 \) and \( \delta_6 = \chi_6 - \chi_9. \)

Defining \( \gamma_{1,\alpha} = -\epsilon b_{\alpha,x} \) and \( \xi = x - v_1 t, \) Eq. (4.16) can be solved for \( \gamma_{1,\alpha} \)

\[
\gamma_{1,\alpha} = \beta \left\{ 2\epsilon [\delta_1 |a_\alpha|^2 + \delta_2 |a_{\alpha+1}|^2 + \delta_3 |a_{\alpha-1}|^2] + 2\epsilon \left[ -\delta_4 a_\alpha a^*_x \right. \\
&\left. -\delta_5 a_{\alpha+1} a^*_{\alpha+1,x} - \delta_6 a_{\alpha-1} a^*_{\alpha-1,x} \right] \right\}.
\]

(4.17)

where \( \beta = \frac{1}{K(1-s^2)}, s^2 = \frac{v^2}{v_0^2} \) and \( v_0 = \epsilon^3 \left( \frac{K}{m} \right)^{\frac{1}{2}}. \)

Substituting Eq. (4.17) in Eq. (4.15) and rescaling \( a_\alpha \to \epsilon a_\alpha \) we get the equation of motion as

\[
\begin{align*}
i \hbar a_{\alpha,t} &= \delta_0 a_\alpha - \epsilon J^2 a_{\alpha,xx} - L a_{\alpha+\rho} + \beta_1 |a_\alpha|^2 a_\alpha + \beta_2 |a_{\alpha+1}|^2 a_\alpha \\
&+ \beta_3 |a_{\alpha-1}|^2 a_\alpha + \beta_4 a_\alpha a_{\alpha+1} a^*_{\alpha+1,x} + \beta_5 a_\alpha a_{\alpha-1} a^*_{\alpha-1,x}
\end{align*}
\]

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\[ + \beta_6 a_\alpha \alpha^{*+1} a_{\alpha+1,x} + \beta_7 a_\alpha \alpha^{*-1} a_{\alpha-1,x} + \beta_8 |a_{\alpha+1}|^2 a_{\alpha,x} \]
\[ + \beta_9 |a_{\alpha-1}|^2 a_{\alpha,x} + \beta_{10} |a_{\alpha}|^2 a_{\alpha,x}, \quad \text{(4.18)} \]

where \( \beta_1 = -4 \beta (\delta_1^2 + \delta_2^2 + \delta_3^2) - 2 A_1 \eta_1^2, \beta_2 = \beta_3 = -4 \beta \Omega_1 + \eta_2^2, \beta_4 = \beta_5 = -4 \beta \epsilon (\Omega_3 + \Omega_4), \beta_6 = \epsilon (A_1 \eta_1 \eta_2 - 4 \beta \Omega_4), \beta_7 = \epsilon (A_1 \eta_1 \eta_2 - 4 \beta \Omega_3), \beta_8 = \epsilon (2 A_1 \eta_1 \eta_2 - 4 \beta \Omega_4), \beta_9 = \epsilon (A_1 \eta_1 \eta_2 - 4 \beta \Omega_3), \beta_{10} = -4 \epsilon (A_1 \eta_1 \eta_2 + \beta \Omega_4), \Omega_1 = \delta_1 \delta_2 + \delta_2 \delta_3 + \delta_1 \delta_3, \Omega_2 = \delta_4 \delta_1 + \delta_5 \delta_2 + \delta_6 \delta_3, \Omega_3 = \delta_5 \delta_1 + \delta_6 \delta_2 + \delta_4 \delta_3, \Omega_4 = \delta_6 \delta_1 + \delta_4 \delta_2 + \delta_5 \delta_3. \]

Using \( \alpha = 1, 2, 3 \), Eq. (4.18) can be explicitly written in the form

\[ i a_{1,x} = \delta_0 a_1 - J \epsilon^2 a_{1,xx} - L (a_2 + a_3) + (\beta_1 |a_1|^2 + \beta_2 |a_2|^2 + \beta_3 |a_3|^2) a_1 + (\beta_4 a_2 a_{2,x}^*) a_1 \]
\[ + \beta_5 a_3 a_{3,x}^* a_1 + (\delta_4 a_{2,x} a_{3,x}^*) a_1 \]
\[ + (\beta_6 |a_1|^2 + \beta_7 |a_2|^2 + \beta_8 |a_3|^2) a_{1,x}, \quad \text{(4.19)} \]

\[ i a_{2,x} = \delta_0 a_2 - J \epsilon^2 a_{2,xx} - L (a_3 + a_1) + (\beta_1 |a_1|^2 + \beta_2 |a_2|^2 + \beta_3 |a_3|^2) a_2 + (\beta_4 a_1 a_{1,x}^*) a_2 \]
\[ + \beta_5 a_3 a_{3,x}^* a_2 + (\beta_7 a_{1,x}^* a_{1,x} + \delta_6 a_{2,x} a_{3,x}) a_2 \]
\[ + (\beta_8 |a_1|^2 + \beta_9 |a_2|^2 + \beta_10 |a_3|^2) a_{2,x}, \quad \text{(4.20)} \]

\[ i a_{3,x} = \delta_0 a_3 - J \epsilon^2 a_{3,xx} - L (a_1 + a_2) + (\beta_1 |a_1|^2 + \beta_2 |a_2|^2 + \beta_3 |a_3|^2) a_3 + (\beta_4 a_1 a_{1,x}^*) a_3 \]
\[ + \beta_5 a_2 a_{2,x}^* a_3 + (\beta_7 a_{1,x} a_{1,x} + \delta_6 a_{2,x} a_{2,x}) a_3 \]
\[ + (\beta_9 |a_1|^2 + \beta_{10} |a_2|^2 + \beta_8 |a_3|^2) a_{3,x}. \quad \text{(4.21)} \]

Eqs. (4.19)-(4.21) are a set of three coupled perturbed NLS equations which represent the dynamics of alpha helical proteins with nearest and next nearest
neighbour interactions and interspine coupling. In order to solve Eqs. (4.19)-(4.21) we employ the extended tanh method and study the soliton dynamics. The details are given in the next section.

### 4.3 Soliton Solutions

The extended tanh method is one of most direct and effective algebraic method for finding exact solutions to nonlinear equations. To use the method as given in section 1.3.6.4, we make the transformations

\[ a_1 = e^{i(kx + \omega t)}U_1(\mu \xi), \quad a_2 = e^{i(kx + \omega t)}U_2(\mu \xi), \quad a_3 = e^{i(kx + \omega t)}U_3(\mu \xi) \]  

(4.22)

in Eqs. (4.19)-(4.21). The resulting equations are

\[ -\omega \hbar U_1 = \delta_0 U_1 - J e^2(U'_1 \mu^2 c_1^2 - k^2 U_1) - L(U_2 + U_3) + (\beta_1 |U_1|^2 + \beta_2 |U_2|^2) \]
\[ + \beta_3 |U_3|^2 U_1 + (\beta_4 U_2 U'_2 + \beta_5 U_3 U'_3) \mu c_1 U_1 + (\beta_6 U_2 U'_2) \]
\[ + \beta_7 U_3 U'_3) \mu c_1 U_1 + (\beta_8 U_1^2 + \beta_9 U_2^2 + \beta_{10} U_3^2) \mu c_1 U'_1, \]  

(4.23)

\[ \hbar \mu c_2 U'_1 = [k(-\beta_4 + \beta_5) U_2^2 + k(-\beta_5 + \beta_7 + \beta_{10}) U_2^2 + k(-\beta_6 + \beta_8) \]
\[ + \beta_{11} |U_3|^2 U_1 - 2 Je^2 k \mu c_1 U'_1, \]  

(4.24)

\[ -\omega \hbar U_2 = \delta_0 U_2 - J e^2(U'_2 \mu^2 c_1^2 - k^2 U_2) - L(U_3 + U_1) + (\beta_3 |U_1|^2 + \beta_1 |U_2|^2) \]
\[ + \beta_2 |U_3|^2 U_2 + (\beta_4 U_1 U'_1 + \beta_6 U_3 U'_3) \mu c_1 U_2 + (\beta_7 U_1 U'_1) \]
\[ + \beta_8 U_3 U'_3) \mu c_1 U_2 + (\beta_{10} U_1^2 + \beta_8 U_2^2 + \beta_9 U_3^2) \mu c_1 U'_2, \]  

(4.25)
We propose the following series expansion as a solution of Eqs. (4.23)-(4.28)

\[ U_j(\xi) = a_{j0} + \sum_{i=1}^{N} a_{ji}\phi^i + b_{ji}\phi^{-i}, \quad j = 1, 2, 3 \]  

(4.29)

with a new variable \( \phi = \phi(\xi) \) which is a solution of the Ricatti equation

\[ \phi' = b + \phi^2, \]  

(4.30)

where \( b \) is a parameter to be determined. Balancing the higher order linear terms and nonlinear terms in Eqs. (4.23)-(4.28) we get \( N = 1 \), so that the solution takes the form

\[ U_1(\xi) = a_{10} + a_{11}\phi + a_{12}\phi^{-1}, \]  

(4.31)

\[ U_2(\xi) = a_{20} + a_{21}\phi + a_{22}\phi^{-1}, \]  

(4.32)

\[ U_3(\xi) = a_{30} + a_{31}\phi + a_{32}\phi^{-1}. \]  

(4.33)
Substituting Eqs. (4.31)-(4.33) in Eqs. (4.23)-(4.28) we obtain a system of algebraic equations. Solving the resulting algebraic equations by hand is cumbersome and laborious. We solve these algebraic equations using mathematica and get two different sets of solutions.

**case(i) $a_{10} = a_{20} = a_{30} = 0;$**

\[
\begin{align*}
a_{11} &= \sqrt{-\frac{2\zeta_2^2\Omega}{b(\zeta_1 + \zeta_2 + \zeta_3)}}, & a_{12} &= b\sqrt{-\frac{2\zeta_2^2\Omega}{b(\zeta_1 + \zeta_2 + \zeta_3)}}, \\
a_{21} &= \sqrt{-\frac{2(\zeta_3^2 - \zeta_2^2)\Omega}{b(\zeta_1 + \zeta_2 + \zeta_3)}}, & a_{22} &= b\sqrt{-\frac{2(\zeta_3^2 - \zeta_2^2)\Omega}{b(\zeta_1 + \zeta_2 + \zeta_3)}}, \\
a_{31} &= \sqrt{\frac{2(-\zeta_1^2 - \zeta_2^2 - \zeta_3^2 + \zeta_1\zeta_2 + \zeta_1\zeta_3 + \zeta_2\zeta_3)\Omega}{b(\zeta_1 + \zeta_2 + \zeta_3)}}, & a_{32} &= b\sqrt{\frac{2(-\zeta_1^2 - \zeta_2^2 - \zeta_3^2 + \zeta_1\zeta_2 + \zeta_1\zeta_3 + \zeta_2\zeta_3)\Omega}{b(\zeta_1 + \zeta_2 + \zeta_3)}},
\end{align*}
\]

\[
\mu = \sqrt{-\frac{\Omega}{4bc_1^2J^2}},
\]

where $\Omega = E_0 + W - 2J + Je^2k^2 - 2L + \hbar\omega$, $\zeta_1 = \beta_1 + \beta_8$, $\zeta_2 = \beta_2 + 2\beta_6 + 2\beta_9$, and $\zeta_3 = \beta_3 + 2\beta_7 + 2\beta_{10}$.

The solutions of Eqs. (4.19)-(4.21) are then written as

\[
\begin{align*}
a_1(x, t) &= \sqrt{-\frac{2\zeta_2^2\Omega}{b(\zeta_1 + \zeta_2 + \zeta_3)}} e^{i(kx + \omega t)} \\
&\times \sqrt{b}\left( \tanh\left(\sqrt{b}\sqrt{-\frac{\Omega}{4bc_1^2J^2}}\xi\right) + b\coth\left(\sqrt{b}\sqrt{-\frac{\Omega}{4bc_1^2J^2}}\xi\right) \right), \\
a_2(x, t) &= \sqrt{-\frac{2(\zeta_3^2 - \zeta_2^2)\Omega}{b(\zeta_1 + \zeta_2 + \zeta_3)}} e^{i(kx + \omega t)} \\
&\times \sqrt{b}\left( \tanh\left(\sqrt{b}\sqrt{-\frac{\Omega}{4bc_1^2J^2}}\xi\right) + b\coth\left(\sqrt{b}\sqrt{-\frac{\Omega}{4bc_1^2J^2}}\xi\right) \right),
\end{align*}
\]
4.3 Soliton Solutions

\[ a_3(x, t) = \sqrt{\frac{2(-\zeta_1^2 - \zeta_2^2 - \zeta_3^2 + \zeta_1 \zeta_2 + \zeta_1 \zeta_3 + \zeta_2 \zeta_3) \Omega}{b(\zeta_1^2 + \zeta_2^2 + \zeta_3^2 - 3\zeta_1 \zeta_2 \zeta_3)}} e^{i(kx + \omega t)} \]

\[ \times \sqrt{b} \left( \tanh(\sqrt{b} \sqrt{-\frac{\Omega}{4bc J_2^2 \xi^2}}) + b \coth(\sqrt{b} \sqrt{-\frac{\Omega}{4bc J_2^2 \xi^2}}) \right). \] (4.41)

case(ii) \( a_{10} = a_{20} = a_{30} = a_{12} = a_{22} = a_{32} = 0; \)

\[ a_{11} = \sqrt{\frac{-2\zeta_2^2 \Omega}{b(\zeta_1 + \zeta_2 + \zeta_3)}}, \quad a_{21} = \sqrt{\frac{-2(\zeta_1^3 - \zeta_3^3)^2 \Omega}{b(\zeta_1 + \zeta_2 + \zeta_3)}}, \] (4.42)

\[ a_{31} = \sqrt{\frac{2(-\zeta_1^2 - \zeta_2^2 - \zeta_3^2 + \zeta_1 \zeta_2 + \zeta_1 \zeta_3 + \zeta_2 \zeta_3) \Omega}{b(\zeta_1^2 + \zeta_2^2 + \zeta_3^2 - 3\zeta_1 \zeta_2 \zeta_3)}}, \] (4.43)

\[ \mu = \sqrt{\frac{-\Omega}{4bc J_2^2 \xi^2}}. \] (4.44)

The solutions of Eqs. (4.19)-(4.21) in this case become

\[ a_1(x, t) = \sqrt{\frac{-2\zeta_2^2 \Omega}{b(\zeta_1 + \zeta_2 + \zeta_3)}} e^{i(kx + \omega t)} \sqrt{b} \left( \tanh(\sqrt{b} \sqrt{-\frac{\Omega}{4bc J_2^2 \xi^2}}) \right), \] (4.45)

\[ a_2(x, t) = \sqrt{\frac{-2(\zeta_1^3 - \zeta_3^3)^2 \Omega}{b(\zeta_1 + \zeta_2 + \zeta_3)}} e^{i(kx + \omega t)} \sqrt{b} \left( \tanh(\sqrt{b} \sqrt{-\frac{\Omega}{4bc J_2^2 \xi^2}}) \right), \] (4.46)

\[ a_3(x, t) = \sqrt{\frac{2(-\zeta_1^2 - \zeta_2^2 - \zeta_3^2 + \zeta_1 \zeta_2 + \zeta_1 \zeta_3 + \zeta_2 \zeta_3) \Omega}{b(\zeta_1^2 + \zeta_2^2 + \zeta_3^2 - 3\zeta_1 \zeta_2 \zeta_3)}} e^{i(kx + \omega t)} \]

\[ \times \sqrt{b} \left( \tanh(\sqrt{b} \sqrt{-\frac{\Omega}{4bc J_2^2 \xi^2}}) \right). \] (4.47)

The above set of solutions represent solitons which are plotted in Figure 4.1.

Thus the molecular excitations in the alpha helical proteins represented by the model (4.1) in the low temperature limit under continuum approximation is governed by solitons and it is expected that each soliton along the three different
spines transports an amount of energy approximately equal to $E_0$ with different amplitudes.

It is found that equation (4.18) is completely integrable for the parametric choices $L = 0$, $\chi_4 = -\chi_7$, $\chi_5 = -\chi_8$, $\chi_6 = -\chi_9$, $\eta_1 = \frac{i}{3\epsilon \eta_2}$, $\chi_2 = \chi_3$, $\chi_1 = -2\chi_2$, $\chi_2^2 = \frac{-5\eta_1^2}{12}$, $\chi_4 = \frac{-5}{16}\chi_1$ and $\chi_5 = \frac{1}{32\chi_2}$. By making the transformation

$$a_\alpha = e^{q_\alpha \exp \left( \frac{-i\epsilon(E_0 + W - 2J)}{2\hbar} \right)}$$  \hspace{1cm} (4.48)

Eq. (4.18) can be transformed into the completely integrable Chen - Lee - Liu equation [112]

$$iq_{\alpha,t} + q_{\alpha,xx} + i(|q_\alpha|^2 + |q_{\alpha+p}|^2)q_{\alpha,x} = 0.$$  \hspace{1cm} (4.49)

For $\alpha = 1, 2, 3$, Eq. (4.49) can be explicitly written in the form

$$iq_{1,t} + q_{1,xx} + i(|q_1|^2 + |q_2|^2 + |q_3|^2)q_{1,x} = 0,$$  \hspace{1cm} (4.50)

$$iq_{2,t} + q_{2,xx} + i(|q_1|^2 + |q_2|^2 + |q_3|^2)q_{2,x} = 0,$$  \hspace{1cm} (4.51)

$$iq_{3,t} + q_{3,xx} + i(|q_1|^2 + |q_2|^2 + |q_3|^2)q_{3,x} = 0.$$  \hspace{1cm} (4.52)

Equations (4.50)-(4.52) are a set of completely integrable three coupled derivative NLS equations (Chen - Lee - Liu equations). A matrix generalization of the Lax pair for the three coupled Chen - Lee - Liu equations and its soliton solutions are given by Takayuki and Wadati [112-114].
4.4 Integrable Discretization

A suitable discretization can reproduce most of the important properties of the differential equation in the small-value range of the difference interval and can be considered a 'generalization' of the original continuous equation. Such a discretization facilitates a better and more intuitive understanding of the differential equation without using a limiting procedure, which is needed to define differentiation, and is ideal for performing numerical experiments. Ablowitz and Ladik [100] have formulated a technique to find a Lax pair for an integrable discrete NLS equation. In this section we extend the same technique to arrive at the three coupled discrete derivative NLS equations and study the nature of energy transfer in discrete alpha helical protein lattice. The Lax pair formulation in a discrete lattice comprises a pair of linear equations

\[ V_{n+1} = L_n V_n, \]  
\[ V_{nt} = M_n V_n. \]  

Here, \( V_n = (V_{n1}, V_{n2})^T \) is a column-vector function. The square matrices \( L_n \) and \( M_n \) depend on the spectral parameter \( \xi \), which is an arbitrary constant independent of \( n \) and \( t \). The compatibility condition is given by

\[ L_{n,t} = M_{n+1} L_n - L_n M_n \]  

is a discrete version of the zero-curvature condition with

\[ L = \begin{pmatrix} i\xi^2 & q_n \\ r_n & i\xi^{-2} + q_n / r_n \end{pmatrix} \]  

and
It yields the difference - difference equation

\[ M = [M_{l,m}], \quad l, m = 1, 2, \tag{4.57} \]

where

\[
M_{n,1,1} = -\frac{i}{\sigma^2} \xi^4 - \frac{i}{\sigma^2} \xi^2 - \frac{i}{\sigma^2} q_n r_{n-1} - \frac{i}{\sigma^2} + \frac{1}{\sigma^2} (q_n r_{n-1} - q_n r_{n+1} - q_n r_{n-1} q_n r_{n-2}) \xi^{-2}, \tag{4.58}
\]

\[
M_{n,1,2} = \frac{1}{\sigma^2} q_n \xi^3 + \left( -\frac{1}{\sigma^2} q_n r_n - \frac{2}{\sigma^2} q_n \right) \xi + \frac{1}{\sigma^2} q_n - 1 \xi^{-1}, \tag{4.59}
\]

\[
M_{n,2,1} = \frac{1}{\sigma^2} r_{n-1} \xi + \left( -\frac{1}{\sigma^2} q_{n-1} r_{n-1} - \frac{2}{\sigma^2} r_{n-1} \right) \xi^{-1} + \xi^{-1}, \tag{4.60}
\]

\[
M_{n,2,2} = -\frac{i}{\sigma^2} \xi^{-4} - \frac{i}{\sigma^2} \xi^{-2} - \frac{i}{\sigma^2} q_n - 1 \xi^{-2} - \frac{i}{\sigma^2} \xi^2. \tag{4.61}
\]

It yields the difference - difference equation

\[
i q_{n,t} + \frac{1}{\epsilon^2} (q_{n+1} + q_{n-1} - 2q_n + iq_{n,1} (q_{n+1} - q_{n+1} r_{n+1} q_{n+2}) = 0. \tag{4.62}
\]

By choosing \( q_n \) and \( r_n \) as the column and row vector solutions as \( q_n = (q_{n,1}, q_{n,2}, q_{n,3}) \)

and \( r_n = (q_{n,1}^*, q_{n,2}^*, q_{n,3}^*)^T \), we get a set of three coupled discrete derivative NLS equations

\[
i q_{n,1,t} + \frac{1}{\epsilon^2} (q_{n+1,1} + q_{n-1,1} - 2q_{n,1} + \sum_{k=1}^{3} |q_{n,k}|^2 (q_{n+1,1} - q_{n-1,1} - q_{n+1,1} q_{n+2,1})) = 0, \tag{4.63}
\]

\[
i q_{n,2,t} + \frac{1}{\epsilon^2} (q_{n+1,2} + q_{n-1,2} - 2q_{n,2} + \sum_{k=1}^{3} |q_{n,k}|^2 (q_{n+1,2} - q_{n-1,2} - q_{n+1,2} q_{n+2,2})) = 0, \tag{4.64}
\]

\[
i q_{n,3,t} + \frac{1}{\epsilon^2} (q_{n+1,3} + q_{n-1,3} - 2q_{n,3} + \sum_{n=1}^{3} |q_{n,k}|^2 (q_{n+1,3} - q_{n-1,3} - q_{n+1,3} q_{n+2,3})) = 0. \tag{4.65}
\]
4.5 Conclusion

One can verify that in the continuum limit equations (4.63)-(4.65) become the set of completely integrable three coupled derivative NLS equations (Chen-Lee-Liu equations) (4.50)-(4.52) with appropriate scalings. By means of numerical analysis, we study the dynamics of a set of three coupled equations (4.63)-(4.65). The space - time plot of the energy density profile corresponding to Eqs. (4.63)-(4.65) is shown in Figure 4.2 which shows two co propagating solitons interacting between each other during its propagation through the alpha helical protein chain. The total energy of each soliton is found to be conserved and it is expected that when the solitons propagate along the three hydrogen bonding spine and during collision there will be no change in the distribution of energy among them in the neighbouring spines keeping the total energy conserved.

4.5 Conclusion

In this Chapter we have studied the nonlinear dynamics of alpha helical proteins with interspine coupling. For this, we propose a Hamiltonian model which includes internal molecular excitations, dipole - dipole interactions and nonlinear coupling between the internal molecular excitations with the displacements. We also incorporate the nonlinear couplings which give rise to change in amide -I bond at different levels caused by stretching of the helix between two nearest neighbour unit cells. Under coherent representation in the continuum limit, the collective molecular excitations are found to be governed by a set of perturbed three cou-
4.5 Conclusion

pled NLS equation. In the unperturbed limit which is also the homogeneous limit, the dynamics is governed by the completely integrable three coupled derivative NLS equations (Chen - Lee - Liu equations) which exhibit soliton solution. We have identified the equivalent integrable three coupled discrete derivative NLS equation through an appropriate generalization of the Lax pair of the original Ablowitz - Ladik lattice. One can verify in the continuum limit the three coupled discrete derivative NLS model is reduced to the completely integrable Chen - Lee - Liu model. By means of numerical analysis we have studied the propagation of solitons and the energy transfer in discrete alpha helical protein lattices. It is observed that when the solitons propagate along the hydrogen bonding spines of alpha helical proteins, they collide among themselves and during collision there is no change in the distribution of energy among them in the neighbouring spines keeping the total energy conserved.
Figure 4.1: Density profiles of solitons in continuum alpha helical proteins with interspine coupling.
Figure 4.2: Two soliton interaction and the energy transfer in alpha helical proteins at the discrete level.