Inhomogeneous Alpha Helical Proteins

8.1 Introduction

Inhomogeneity in alpha helical protein molecules may occur due to different reasons. It may arise due to defects caused by the presence of additional molecules such as drugs, carcinogens, mutants and dyes in specific sites of the alpha helical protein sequence. Also the reasons for inhomogeneity or site dependence in exchange interactions may be one of the following reasons: (i) The distance between neighbouring atoms may vary along the protein lattices, (ii) the atomic wave function may vary from site to site, (iii) there may be imperfections in the vicinity of a bond, (iv) deviations in aminoacid sequence or (v) geometric effects. In inhomogeneous system, it may have impact on the parameters of the soliton, namely, the amplitude, the velocity, the position and the phase. The in-
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Homogeneities due to the presence of drug molecules weakens or even breaks the hydrogen bonding in the helix and hence changes the localized structure within the alpha helix. These changes cause the soliton to slow down or stop disrupting the energy and information transfer in the protein matrix leading to a disruption in normal consciousness. Thus it has become important and necessary to investigate the internal dynamics of solitons in inhomogeneous alpha helical proteins with intra and interspine coupling. Motivated by this, we propose a model for inhomogeneous alpha helical proteins by including internal molecular excitations, dipole-dipole interactions between nearest neighbours and next nearest neighbours with intra and interspine coupling. The effect of inhomogeneity is investigated by solving the governing equations of motion.

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To study the effect of inhomogeneity in a single spine (intra spine) of alpha helical proteins, we consider a higher order model described in Chapter 3 and include the site dependent inhomogeneity $F_n$ and $G_n$. The Hamiltonian associated with the model can be written as

$$H = \sum_n \{ B_n^\dagger [E_0 B_n + E_1 B_n B_n^\dagger B_n - J_0 F_n (B_{n+1}^\dagger B_{n+1} + B_{n+1}^\dagger B_{n+1})]$$

$$- J_1 G_n (B_{n+1}^\dagger B_{n+1} B_n^\dagger + B_{n+1}^\dagger B_{n+1} B_{n+1}^\dagger B_n) + \frac{1}{2} \left( \frac{p_n^2}{m} + K_1 (u_n^2) \right) \}.$$
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\[-u_{n-1})^2 + K_2(u_n - u_{n-2})^2 \] 

\[+ \chi_1(u_{n+1} - u_{n-1})B_n^1B_n^2 \]

\[+ \chi_2(u_{n+2} - u_n)B_n^1B_{n+1}^1 + \chi_3(u_n - u_{n-2})B_n^1B_{n-1}^1 \]

\[-u_{n-1})B_n^1B_{n+1}^1\}

\[(8.1)\]

The functions \(F_n\) and \(G_n\) characterize the variation of the dipole and quadrupole interactions along the hydrogen bonding spine due to inhomogeneities. Having constructed the Hamiltonian for the inhomogeneous alpha helical protein molecules, the corresponding dynamical equation can be obtained by deriving the associated Heisenberg’s equations of motions using Eqs. (2.12)-(2.14). The equations of motion for the dynamical variable \(a_n\) is found to be

\[i\hbar \frac{da_n}{dt} = (E_0 + W - 3E_1)a_n + 2E_1a_n^2a_n - J_0F_n\sigma_{n+1} - J_0F_{n-1}\sigma_{n-1} \]

\[-2J_1G_n^2a_{n+1}^2 - 2J_1G_{n-1}^2a_{n-1}^2 + (\chi_1 - 3\chi_4)(b_{n+1} - b_{n-1})a_n \]

\[+ \chi_2(b_{n+2} - b_n)a_n + \chi_3(b_n - b_{n-2})a_n \]

\[+ 2\chi_4(b_{n+1} - b_{n-1})a_n a_n^* \]

\[(8.2)\]

The equation for \(b_n\) is same as given in Eq. (3.7).

When the functions \(a_n, b_n, F_n\) and \(G_n\) change smoothly over one link of the chain, it is appropriate to make a continuum approximation for \(a_{n\pm 1}, b_{n\pm 1}, F_{n\pm 1}\) and \(G_{n\pm 1}\) using the Taylor expansions given in Eqs. (2.17) and

\[F_{n\pm 1} = F + \tau F_x \pm \frac{\tau^2}{2}F_{xx} \pm \frac{\tau^3}{6}F_{xxx} \pm \frac{\tau^4}{24}F_{xxxx} \cdots \]

\[(8.3)\]

\[G_{n\pm 1} = G + \tau G_x \pm \frac{\tau^2}{2}G_{xx} \pm \frac{\tau^3}{6}G_{xxx} \pm \frac{\tau^4}{24}G_{xxxx} \cdots \]

\[(8.4)\]
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Here \( \epsilon \) and \( \tau \) are the lattice parameters and suffix \( x \) represents partial derivative with respect to \( x \). Eq. (8.2) then becomes

\[
i \hbar \frac{\partial a}{\partial t} = (E_0 + W - 3E_1 - 2J_0F + 2E_1a^a)a + 2eb_x[\Omega_1 - 3\chi_1 + 2\chi_1|a|^2]a
\]

\[
+ \epsilon^2[-J_0a_x - 4GJ_1(a_x^2 + aa_x)a^* + 2\Omega_0(a_x b_x + ab_x)]
\]

\[
+ \frac{\epsilon^3}{3}[6\Omega_5(a_x b_x + a_x b_x) + (\Omega_1 - 3\chi_1 + \Omega_5 + \Omega_6 + \chi_2 + 2\chi_1|a|^2)ab_{xxx}]
\]

\[
- \frac{\epsilon^4}{12}[J_0F_{xxxx} + 4GJ_1(3a_x^2 + 4a_x a_{xxx} + a_{xxxx})a^* - 4\Omega_6(a_{xxxx} b_x
\]

\[
+ 3a_x b_x + 4a_x b_{xxx} + 2ab_{xxxx})] + \rho[J_0F_x + 2G_x J_1|a|^2]a
\]

\[
- \rho^2[\frac{1}{2}F_x J_0 + G_{xx} J_1|a|^2]a + \rho^3[\frac{1}{6}[J_0F_{xxxx} + 2G_{xxx} J_1|a|^2]
\]

\[
- \frac{\rho^4}{24}[J_0F_{xxxx} + 2G_x J_1 G_{xxx}|a|^2]a - \epsilon \rho a_x[F_x J_0 + 4G_x J_1|a|^2]
\]

\[
+ \epsilon^2 \rho[-\frac{1}{2}F_x J_0 a_x + 2G_x J_1(a_x^2 + aa_x)a^* - \frac{\epsilon^3}{6}\rho a_{xxxx} F_x J_0
\]

\[
+ 4J_1G_x(3a_x a_{xx} + aa_{xxx})a^*) + \epsilon^4 \rho\frac{1}{24}a_{xxxx}F_x J_0 + G_x J_1(\frac{1}{2}a_x^2
\]

\[
+ \frac{2}{3}a_x a_{xxx} + \frac{1}{6}aa_{xxx})a^*) + \epsilon^2 \rho a_x[\frac{1}{6}F_x J_0 + 2aG_x J_1 a^*
\]

\[
+ \epsilon^3\rho[-\frac{1}{6}a_x F_{xxxx} J_0 - \frac{2}{3}aa_x G_{xxx} J_1 a^*] + \epsilon^4 \rho \frac{1}{24}F_{xxxx} J_0
\]

\[
+ \frac{1}{6}|a|^2G_{xxxx} J_1]a_x + \epsilon^2 \rho^2[-\frac{1}{4}a_{xx} F_{xx} J_0 - G_{xx} J_1(a_x^2
\]

\[
+ aa_{xx})a^*]
\]

\[
(8.5)
\]

where \( \Omega_1 = \chi_1 + \chi_2 + \chi_3; \Omega_2 = \chi_1 - \chi_2 + \chi_3; \Omega_3 = \chi_1 - \chi_2 - \chi_3; \Omega_4 = \chi_1 - 4\chi_2 - 4\chi_3; \Omega_5 = \chi_2 + \chi_3, \Omega_6 = \chi_2 - \chi_3.

Assuming the lattice constants \( \epsilon \) and \( \tau \) to be equal and substituting Eq. (3.10)
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in Eq. (8.5), we obtain

\[ i \hbar \frac{\partial a}{\partial t} = \beta_1 a + \beta_2 a_x + \beta_3 a_{xx} + \beta_4 a_{xxx} + \beta_5 a_{xxxx} + \beta_6 |a|^2 a + \beta_7 |a|^2 a_x \\
+ \beta_8 |a|^2 a_{xx} + \beta_9 a_x^2 a^* + \beta_{10} |a|^4 a + \beta_{11} a^2 a_{xx}^* + \beta_{12} |a_x|^2 a \\
+ \beta_{13} a^2 a_x^*, \]  

where \( \beta_1 = (E_0 + W) - 2J_0 F + \epsilon J_0 F_x - \frac{J_0 \epsilon^2 F_{xx}}{2} + \frac{4J_0 \epsilon^3 F_{xxx}}{6} - \frac{J_0 \epsilon^4 F_{xxxx}}{24} \), \( \beta_2 = -\epsilon^2 J_0 F_x + \frac{J_0 \epsilon^3 F_{xx}}{2} - \frac{4J_0 \epsilon^4 F_{xxx}}{6} \), \( \beta_3 = -\epsilon^2 J_0 F + \frac{J_0 \epsilon^3 F_x}{2} - \frac{4J_0 \epsilon^4 F_{xx}}{4} \), \( \beta_4 = \frac{J_0 \epsilon^4 F_x}{6} \), \( \beta_5 = -\frac{J_0 \epsilon^3 F}{12} \), \( \beta_6 = 2(E_1 - 2\Omega_1^2 \beta) \epsilon^2 + \frac{2}{3} \Omega_1 \Omega_3 \beta \epsilon^4 - \frac{J_1}{2} (G_{xx} \epsilon^4 + 4G_x \epsilon^3) \), \( \beta_7 = -4J_1 G_x \epsilon^4 - 8\beta \Omega_6 \Omega_2 \epsilon^3 \), \( \beta_8 = \epsilon^4 (-2J_1 + \frac{2}{3} \Omega_1 \Omega_3 \beta - 4\beta \Omega_5 \Omega_2) \), \( \beta_9 = -4GJ_1 \epsilon^4 \), \( \beta_{10} = 4\chi_4 \Omega_1 \beta \epsilon^4 \), \( \beta_{11} = \beta \epsilon^4 (\frac{2}{3} \Omega_1 \Omega_4 - 4\Omega_5 \Omega_6) \), \( \beta_{12} = -8\beta \Omega_5 \Omega_6 \epsilon^4 \), \( \beta_{13} = -4\beta \Omega_2 \Omega_6 \epsilon^3 \).

Eq. (8.6) describes the dynamics of inhomogeneous alpha helical proteins, which is a perturbed higher order NLS equation.

8.2.1 Effect of Inhomogeneity

Since Eq. (8.6) is a perturbed equation, to study the effect of inhomogeneity on soliton excitations, we solve it using perturbation techniques. Here we use the sine-cosine method which is explained in Section 1.3.6.1. To use this method we make the transformation \( a = u e^{i(kx - \omega t)} \) in Eq. (8.6) and it becomes

\[ \hbar \omega u = \beta_1 u + \beta_2 u_x + \beta_3 (u_{xx} - k^2 u) + \beta_4 (u_{xxx} - 3k^2 u_x) \\
+ \beta_5 (u_{xxxx} - 6k^2 u_{xx} + k^4 u) + \beta_6 u^3 + \beta_7 u^2 u_x \\
+ \beta_8 u^2 (u_{xx} - k^2 u) + \beta_9 (u_x^2 - k^2 u_x^2) u + \beta_{10} u^5 \]
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\[ +\beta_{11}u^2(u_{xx} - k^2u) + \beta_{12}(u_x^2 + k^2u^2)u + \beta_{13}u^2u_x, \quad (8.7) \]

\[ \hbar u_t = \beta_2ku - 2\beta_3k u_x + \beta_4(3ku_{xx} - k^3u) + 4\beta_5(ku_{xxx} - k^3u_x) + \beta_7\delta u_x^2u - k\beta_{13}u^3. \quad (8.8) \]

Using the wave variable \( \xi = t - \delta x \), Eqs. (8.7) and (8.8) can be written as

\[ \hbar \omega u = \beta_1u - \delta \beta_2u_\xi + \beta_3(\delta^2u_{\xi\xi} - k^2u) + \beta_4(-\delta^3u_{\xi\xi\xi} + 3k^2\delta u_\xi) + \beta_5(\delta^4u_{\xi\xi\xi\xi} - 6k^2\delta^2u_{\xi\xi} + k^4u) + \beta_6u^3 \]

\[ -\beta_7\delta u_x^2u_\xi + \beta_8u^2(\delta^2u_{\xi\xi} - k^2u) + \beta_9(\delta^2u_\xi^2 - k^2u) \]

\[ -k^2u^2)u + \beta_{10}u^5 + \beta_{11}u^2(\delta^2u_{\xi\xi} - k^2u) \]

\[ +\beta_{12}(\delta^2u_\xi^2 + k^2u^2)u - \beta_{13}\delta u_x^2u_\xi, \quad (8.9) \]

\[ \hbar u_\xi = \beta_2ku + 2\beta_3k\delta u_\xi + \beta_4(3k\delta^2u_{\xi\xi} - k^3u) \]

\[ +4\beta_5(-k\delta^3u_{\xi\xi\xi} + k^3\delta u_\xi) + \beta_7ku^3 - 2\beta_8k\delta u_x^2u_\xi \]

\[ -2\beta_9k\delta u_x^2u_\xi + 2\beta_{11}k\delta u_x^2u_\xi - k\beta_{13}u^3. \quad (8.10) \]

Now we assume that Eqs. (8.9) and (8.10) admit the solution

\[ u(\xi) = \kappa \sin^3(\mu \xi), \quad (8.11) \]

where \( \kappa, \beta \) and \( \mu \) are constant parameters to be determined. In order to find the parameter \( \beta \), we balance the linear higher order derivative term with the
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nonlinear term of equations (8.9) and (8.10) and finally we obtain, \( \beta = -1 \).

Using Eq. (8.11) with \( \beta = -1 \) in Eqs. (8.9) and (8.10) we get the system of algebraic equations

\[
\sin^{-1}(\mu \xi) : h\omega \lambda = \beta_1 \lambda + \beta_3(\delta^2 \mu^2 \lambda - k^2 \lambda) + \beta_5(-3\delta^4 \mu^4 - 6k^2 \delta^2 \mu^2 + k^4)\lambda \\
- k^2 \lambda \beta_8 - 2\beta_3 \delta^2 \mu^2 \lambda - 6\beta_5(3\delta^4 \mu^4 + 2k^2 \delta^2 \mu^2)\lambda
\]  

(8.12)

\[
\sin^{-2}(\mu \xi) : 6\beta_4 \delta^3 \mu^3 \lambda = 0,
\]  

(8.13)

\[
\sin^{-3}(\mu \xi) : \beta_6 \lambda^3 + \beta_8 \lambda^3 \mu \delta^2 - \beta_9 k^2 \lambda^3 - \beta_{11} k^2 \lambda^3 + \beta_{11} \delta^2 \lambda^3 \mu^2 + \beta_{12} k^2 \lambda^3 = 0
\]  

(8.15)

\[
\sin^{-4}(\mu \xi) : 6\beta_4 \delta^3 \mu^3 \lambda = 0,
\]  

(8.16)

\[
\sin^{-5}(\mu \xi) : 2\beta_8 \lambda^3 \mu^2 \delta^2 - k^2 \lambda^3 \beta_9 + \beta_{10} \lambda^2 + 2\beta_{11} \lambda^3 \delta^2 \mu^2 + \beta_{12} \delta^2 \mu^2 \lambda^3 = 0,
\]  

(8.17)

\[
\sin^{-2}(\mu \xi) \cos(\mu \xi) : \beta_2 \delta \mu \lambda + \beta_4(5\delta^3 \mu^3 \lambda + 3k^2 \lambda \mu) = 0,
\]  

(8.18)

\[
\sin^{-3}(\mu \xi) \cos(\mu \xi) : 24\beta_5 \delta^4 \mu^4 \lambda = 0,
\]  

(8.19)

\[
\sin^{-4}(\mu \xi) \cos(\mu \xi) : \beta_7 \delta \mu \lambda^3 + \beta_{13} \delta \mu \lambda^3 = 0,
\]  

(8.20)

\[
\sin^{-5}(\mu \xi) \cos(\mu \xi) : 24\beta_5 \delta^4 \mu^4 \lambda = 0,
\]  

(8.21)

\[
\sin^{-1}(\mu \xi) : \beta_2 k + \beta_4(3k \delta^2 \mu^2 - k^2)\lambda + \beta_7 k \lambda^3 + 6\beta_4 k \lambda \delta^2 \mu^2,
\]  

(8.22)

\[
\sin^{-2}(\mu \xi) : 24\beta_5 k \lambda \delta^3 \mu^3 = 0,
\]  

(8.23)

\[
\sin^{-3}(\mu \xi) : 6\beta_4 k \delta^2 \mu^2 \lambda - k \lambda^3 \beta_{13} = 0, \beta_{13} = 0
\]  

(8.24)
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\[
\sin^{-4}(\mu \xi) : 24\beta_5 k \lambda \delta^3 \mu^3 = 0, \tag{8.25}
\]

\[
\sin^{-2}(\mu \xi) \cos(\mu \xi) : h \lambda \mu - 2\lambda \mu \delta k \beta_3 + 20k \lambda \delta^3 \mu^3 - 4k^3 \delta \lambda \mu \beta_5 = 0, \tag{8.26}
\]

\[
\sin^{-4}(\mu \xi) \cos(\mu \xi) : 2\beta_8 k \delta \mu \lambda^3 + 2\beta_9 k \delta \lambda^3 \mu - 2\beta_{11} k \delta \mu \lambda^3 = 0. \tag{8.27}
\]

Solving the above system of algebraic equations using symbolic computation, we obtain

\[
\beta_2 = \beta_3 = \beta_4 = \beta_5 = \beta_7 = \beta_{10} = \beta_{13} = 0, \tag{8.28}
\]

\[
\mu = \pm \sqrt{2k \hbar \delta \left(\beta_1 - \hbar \omega - \frac{h k}{2\delta} - \beta_8 k^2\right)}, \tag{8.29}
\]

and

\[
\kappa = \left(\frac{-B \pm \sqrt{B^2 - 4AC}}{2A}\right)^{1/2}, \tag{8.30}
\]

where \(A = \beta_{10}, B = \beta_6 - \beta_9 \delta^2 \mu^2 + (\beta_8 + \beta_{12})k^2\) and \(C = \frac{\hbar \delta \mu^2}{k^3}\).

Hence the solution of Eq. (8.6) becomes

\[
a(x, t) = \kappa \csc[\pm \sqrt{2k h \delta \left(\beta_1 - \hbar \omega - \frac{h k}{2\delta} - \beta_8 k^2\right)(t - \delta x + \rho)}] \\
\times e^{ikx - \omega t} \tag{8.31}
\]

or

\[
a(x, t) = \kappa \sec[\pm \sqrt{2k h \delta \left(\beta_1 - \hbar \omega - \frac{h k}{2\delta} - \beta_8 k^2\right)(t - \delta x + \rho)}] \\
\times e^{ikx - \omega t}. \tag{8.32}
\]

This gives the soliton solution for the inhomogeneous alpha helical proteins with higher order molecular excitations.
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Figure 8.1: (a) Unperturbed soliton, (b) Perturbed soliton with the inhomogeneity $F = G = \sin(x)$.

When the perturbation due to inhomogeneity is switched on, it may have impact on the parameters of the soliton namely the amplitude, the velocity, the position and the phase. To understand the nature of evolution of the amplitude and velocity of the soliton, we assume the inhomogeneity as periodic. Periodic inhomogeneity may represent periodic repetition of defects or molecules along the helical chain which can be expressed as $F(x) = G(x) = \sin(x)$. On substituting this form we obtain the solitary wave solution for the perturbed NLS equation as shown in Figure 8.1. It shows that when there is periodic inhomogeneity present in the lattice, the amplitude and velocity of the soliton decrease with time (however when there is no inhomogeneity the amplitude and velocity of the soliton remains the same during propagation). When the soliton moves along the spines of alpha helical proteins with periodic inhomogeneity, starting from rest with a finite amplitude, the soliton amplitude decreases and when the velocity reaches a particular value, it suddenly splits and slows down.
8.3 Inhomogeneous Alpha Helical Proteins with Interspine Coupling

We consider the model with interspine coupling explained in Chapter 4 and include the inhomogeneity by introducing the site dependent function $F_n$. The Hamiltonian in this case becomes

$$H = \sum_{n, \alpha, \rho} \left\{ E_0 B_{n, \alpha}^\dagger B_{n, \alpha} - J F_n (B_{n, \alpha}^\dagger B_{n+1, \alpha} + B_{n+1, \alpha}^\dagger B_{n, \alpha}) - \frac{1}{2} \frac{F_n^2}{m} \right\} + \frac{s_n^2}{m} + K (u_{n, \alpha} - u_{n-1, \alpha})^2 + I (v_{n, \alpha} - v_{n, \alpha-1})^2 \right\} + (\chi_1 B_{n, \alpha}^\dagger B_{n, \alpha}$$

$$+ \chi_2 B_{n+1, \alpha}^\dagger B_{n+1, \alpha} + \chi_3 B_{n, \alpha-1}^\dagger B_{n, \alpha-1} (u_{n+1, \alpha} - u_{n-1, \alpha}) + (\chi_4 B_{n, \alpha}^\dagger B_{n+1, \alpha}$$

$$+ \chi_5 B_{n+1, \alpha+1} B_{n, \alpha+1} + \chi_6 B_{n, \alpha-1}^\dagger B_{n, \alpha-1} (u_{n+2, \alpha} - u_{n, \alpha}) + (\chi_7 B_{n, \alpha}^\dagger B_{n-1, \alpha}$$

$$+ \chi_8 B_{n+1, \alpha+1} B_{n-1, \alpha+1} + \chi_9 B_{n, \alpha-1}^\dagger B_{n, \alpha-1} (u_{n, \alpha} - u_{n-2, \alpha}) + [\eta_n B_{n, \alpha}$$

$$+ \eta_2 (B_{n+1, \alpha} - B_{n-1, \alpha})] [\{v_{n, \alpha+\rho} - 2v_{n, \alpha}\}] \right\}. \quad (8.33)$$

The function $F_n$ characterize the variation of the dipole - dipole interactions along the hydrogen bonding spine due to inhomogeneities. The corresponding dynamical equations are found to be

$$i \hbar \frac{d a_{n, \alpha}}{d t} = \sum_{\rho} \left\{ (E_0 + W) a_{n, \alpha} - J (F_n a_{n+1, \alpha} + F_{n-1} a_{n-1, \alpha}) - L a_{n, \alpha+\rho}$$

$$+ a_{n, \alpha} [\chi_1 (b_{n+1, \alpha} - b_{n-1, \alpha}) + \chi_2 (b_{n+1, \alpha-1} - b_{n-1, \alpha-1})$$

$$+ \chi_3 (b_{n+1, \alpha+1} - b_{n-1, \alpha+1})] + a_{n+1, \alpha} [\chi_4 (b_{n+2, \alpha} - b_{n, \alpha})$$

$$+ \chi_5 (b_{n+2, \alpha-1} - b_{n, \alpha-1}) + \chi_6 (b_{n+2, \alpha+1} - b_{n, \alpha+1})]$$

$$+ \chi_7 (b_{n, \alpha} - b_{n, \alpha-1}) + \chi_8 (b_{n, \alpha+1} - b_{n, \alpha})$$

$$+ \chi_9 (b_{n+1, \alpha} - b_{n-1, \alpha}) + \chi_10 (b_{n+2, \alpha} - b_{n, \alpha})$$

$$+ \eta_{n+1, \alpha} a_{n, \alpha+1} + \eta_{n-1, \alpha} a_{n, \alpha-1} + \eta_{n, \alpha+2} a_{n, \alpha+2} a_{n, \alpha-2} + \eta_{n, \alpha+1} a_{n, \alpha+1} a_{n, \alpha-1} + \eta_{n, \alpha} a_{n, \alpha} a_{n, \alpha}$$

$$+ \eta_{n+1, \alpha} a_{n+1, \alpha} a_{n+1, \alpha} + \eta_{n+2, \alpha} a_{n+2, \alpha} a_{n+2, \alpha} + \eta_{n+1, \alpha} a_{n+1, \alpha} a_{n+1, \alpha} + \eta_{n+2, \alpha} a_{n+2, \alpha} a_{n+2, \alpha}.$$
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\[ +a_{n-1,\alpha}[\chi_1(b_{n,\alpha} - b_{n-2,\alpha}) + \chi_8(b_{n,\alpha-1} - b_{n-2,\alpha-1})] \]
\[ +\chi_0(b_{n,\alpha+1} - b_{n-2,\alpha+1})] + A[\eta_1a_{n,\alpha} + \eta_2(a_{n+1,\alpha} - a_{n-1,\alpha})] \]
\[ \times \left[ \eta_1|a_{n,\alpha+\rho}|^2 - 2|a_{n,\alpha}|^2 + \eta_2(a_{n,\alpha+\rho}(a_{n+1,\alpha+\rho} - a_{n-1,\alpha+\rho}) \right. \]
\[ -2a_{n,\alpha}^*(a_{n+1,\alpha} - a_{n-1,\alpha}) \} \] \tag{8.34}

and equations of motion for the variables \( \phi_{n,\alpha} \) and \( \tau_{n,\alpha} \) are the same as given in Eqs. (4.10) and (4.11). Making continuum approximation using Taylor series expansions (2.17) and (8.4) we get the equation of motion for the inhomogeneous alpha helical proteins in the continuum limit as

\[ i\hbar a_{\alpha,t} = (E_0 + W - 2JF)a_{\alpha} - La_{\alpha+\rho} - 2[\delta_1\gamma_\alpha + \delta_2\gamma_{\alpha-1} + \delta_3\gamma_{\alpha+1}] \]
\[ +2\epsilon[\eta_1\eta_2(|a_{\alpha+\rho}|^2 - 2|a_{\alpha}|^2)a_{\alpha,x} + \frac{\eta_1\eta_2}{2}a_{\alpha+\rho}^*a_{\alpha+\rho,x}a_{\alpha} - \eta_1\eta_2|a_{\alpha}|^2a_{\alpha,x}] \]
\[ +2\epsilon^2[-\frac{JF^2}{2} - \frac{J}{2}a_{\alpha,xx} + \eta_2^2a_{\alpha+\rho}^*a_{\alpha+\rho,x}a_{\alpha,x} - 2\eta_2^2a_{\alpha}^*a_{\alpha,x} + J\tau(F_x) \]
\[ -\frac{\tau F_{xx}}{2})a_{\alpha} - \epsilon\tau(JF_x - \frac{\tau JF_{xx}}{2})a_{\alpha,x} + \epsilon^2\tau(\frac{JF_x}{2} - \frac{\tau F_{xx}}{4})a_{\alpha,xx}. \] \tag{8.35}

Substituting Eq. (4.17) in Eq. (8.35) and choosing the lattice parameter \( \epsilon = \tau \) we get the following equation:

\[ i\hbar \frac{\partial a_{\alpha}}{\partial t} = \sigma a_{\alpha} - J\epsilon^2F_xa_{\alpha,x} - JF\epsilon^2a_{\alpha,xx} - La_{\alpha+\rho} + (\beta_1|a_{\alpha}|^2 \]
\[ +\beta_2|a_{\alpha+1}|^2 + \beta_3|a_{\alpha-1}|^2)a_{\alpha} + (\beta_4a_{\alpha+1}a_{\alpha+1,x} \]
\[ +\beta_5a_{\alpha-1}a_{\alpha-1,x} + \beta_6a_{\alpha+1}^*a_{\alpha+1,x} + \beta_7a_{\alpha}^*a_{\alpha-1,x})a_{\alpha} \]
\[ +(|\beta_8|a_{\alpha}|^2 + \beta_9|a_{\alpha+1}|^2 + \beta_{10}|a_{\alpha-1}|^2)a_{\alpha,x}. \] \tag{8.36}
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with \( \sigma = E_0 + W - 2JF + J\epsilon F_x - \frac{J^2}{2} F_{xx} \). For \( \alpha = 1, 2, 3 \), Eq. (8.36) can be written as

\[
i\hbar \frac{\partial a_1}{\partial t} = \sigma a_1 - J\epsilon F_x a_{1,x} - J\epsilon F_x^2 a_{1,xx} - L(a_2 + a_3) + \left( \beta_1 |a_1|^2 + \beta_2 |a_2|^2 \right) + \beta_4 |a_3|^2 a_1 + \left( \beta_5 a_2^* a_{2,x} + \beta_6 a_3^* a_{3,x} \right) a_1 + \left( \beta_7 a_3^* a_{3,x} \right) a_1 \\
+ \left( \beta_8 |a_1|^2 + \beta_9 |a_2|^2 + \beta_{10} |a_3|^2 \right) a_{1,x},
\]

(8.37)

\[
i\hbar \frac{\partial a_2}{\partial t} = \sigma a_2 - J\epsilon F_x a_{2,x} - J\epsilon F_x^2 a_{2,xx} - L(a_3 + a_1) + \left( \beta_1 |a_1|^2 + \beta_3 |a_2|^2 \right) + \beta_2 |a_3|^2 a_2 + \left( \beta_3 a_1^* a_{1,x} + \beta_4 a_3^* a_{3,x} \right) a_2 + \left( \beta_5 a_1^* a_{1,x} + \beta_6 a_3^* a_{3,x} \right) a_2 \\
+ \left( \beta_{10} |a_1|^2 + \beta_8 |a_2|^2 + \beta_9 |a_3|^2 \right) a_{2,x},
\]

(8.38)

\[
i\hbar \frac{\partial a_3}{\partial t} = \sigma a_3 - J\epsilon F_x a_{3,x} - J\epsilon F_x^2 a_{3,xx} - L(a_1 + a_2) + \left( \beta_1 |a_1|^2 + \beta_3 |a_2|^2 \right) + \beta_1 |a_3|^2 a_3 + \left( \beta_4 a_1^* a_{1,x} + \beta_5 a_2^* a_{2,x} \right) a_3 + \left( \beta_6 a_1^* a_{1,x} + \beta_7 a_2^* a_{2,x} \right) a_3 \\
+ \left( \beta_8 |a_1|^2 + \beta_{10} |a_2|^2 + \beta_9 |a_3|^2 \right) a_{3,x}.
\]

(8.39)

Eqs. (8.37)-(8.39) are a set of three coupled perturbed NLS equations representing the dynamics of inhomogeneous alpha helical proteins with interspine coupling. We derive the exact solutions for Eqs. (8.37)-(8.39) using the extended tanh method and study the effect of inhomogeneity in energy transfer in alpha helical proteins and the details are presented in the next section.

8.3.1 Effect of Inhomogeneity

To study the effect of inhomogeneity in alpha helical proteins with interspine coupling, we solve Eqs. (8.37)-(8.39) using the extended tanh method explained
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in Section 1.3.6.4 which is again a perturbation technique. To apply this method, we make the transformations

\[ a_1 = e^{i(kx + \omega t)}U_1(\mu \xi), \quad a_2 = e^{i(kx + \omega t)}U_2(\mu \xi), \quad a_3 = e^{i(kx + \omega t)}U_3(\mu \xi) \quad (8.40) \]

to Eqs. (8.37)-(8.39) which give

\[
- \omega \hbar U_1 = (E_0 + W - 2JF + J\partial_x F)U_1 - J\epsilon^2 \partial_x FU_1' \mu c_1 - JF \epsilon^2 (U_1'' \mu^2 c_1^2
-k^2 U_1) - L(U_2 + U_3) + (\beta_1 |U_1|^2 + \beta_2 |U_2|^2 + \beta_3 |U_3|^2) U_1 + (\beta_4 U_2 U_2')^2
+ \beta_5 U_3 U_3') mc_1 U_1 + (\beta_6 U_2 U_2' + \beta_7 U_3 U_3') mc_1 U_1 + (\beta_8 U_1^2
+ \beta_9 U_2^2 + \beta_{10} U_3^2) mc_1 U_1',
\]

\[
h \mu c_2 U_1' = [k(-\beta_4 + \beta_9) u_1^2 + k(-\beta_5 + \beta_7 + \beta_{10}) u_2^2 + k(-\beta_6 + \beta_8
+ \beta_{11}) u_3^2 u_1] - 2J\epsilon^2 k \mu c_1 U_1',
\]

\[
- \omega \hbar U_2 = (E_0 + W - 2JF + J\partial_x F)U_2 - J\epsilon^2 \partial_x FU_2' \mu c_1 - JF \epsilon^2 (U_2'' \mu^2 c_1^2
-k^2 U_2) - L(U_3 + U_1) + (\beta_3 |U_2|^2 + \beta_1 |U_2|^2 + \beta_2 |U_3|^2) U_2 + (\beta_5 U_1 U_1')
+ \beta_1 U_3 U_3') mc_1 U_2 + (\beta_6 U_3 U_3' + \beta_{10} U_3 U_3') mc_1 U_2 + (\beta_{10} U_1^2
+ \beta_8 U_2^2 + \beta_9 U_3^2) mc_1 U_2',
\]

\[
h \mu c_2 U_2' = [k(-\beta_4 + \beta_9) u_1^2 + k(-\beta_5 + \beta_7 + \beta_{10}) u_2^2 + k(-\beta_6 + \beta_8
+ \beta_{11}) u_3^2 u_3] - 2J\epsilon^2 k \mu c_1 U_2',
\]

\[
- \omega \hbar U_3 = (E_0 + W - 2JF + J\partial_x F)U_3 - J\epsilon^2 \partial_x FU_3' \mu c_1 - JF \epsilon^2 (U_3'' \mu^2 c_1^2
\]
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\[-k^2 U_3) - L(U_1 + U_2) + (\beta_2|U_1|^2 + \beta_3|U_2|^2 + \beta_1|U_3|^2)U_3 + (\beta_4 U_1U')_1 \\
+ \beta_5 U_2 U'_2 \mu c_1 U_3 + (\beta_6 U_1U'_1 + \beta_7 U_2 U'_2) \mu c_1 U_3 + (\beta_9 U_1^2) \\
+ \beta_{10} U_2^2 + \beta_8 U_3^2) \mu c_1 U_3', \quad (8.45)\]

\[h\mu c_2 u'_3 = [k(-\beta_4 + \beta_5)u_3^2 + k(-\beta_5 + \beta_7 + \beta_9)u_1^2 + k(-\beta_6 + \beta_8) \\
+ \beta_{11} u_2^2 u_3] - 2Je^2k\mu c_1 u'_1, \quad (8.46)\]

Balancing the higher order linear terms and nonlinear terms in Eqs. (8.41)-(8.46) we get \( N = 1 \), so that the solution takes the form

\[U_1(\xi) = a_{10} + a_{11}\phi + a_{12}\phi^{-1}, \quad (8.47)\]

\[U_2(\xi) = a_{20} + a_{21}\phi + a_{22}\phi^{-1}, \quad (8.48)\]

\[U_3(\xi) = a_{30} + a_{31}\phi + a_{32}\phi^{-1}. \quad (8.49)\]

Substituting Eqs. (8.47)-(8.49) in Eqs. (8.41)-(8.46) 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) \( a_{10} = a_{20} = a_{30} = 0; \)**

The solutions of Eqs. (8.37)-(8.39) are

\[a_1(x,t) = \sqrt{-2\zeta_3^2\Omega'} \sqrt{b(\zeta_1 + \zeta_2 + \zeta_3)} e^{(kx+\omega t)} \]

\[\times \sqrt{b} \left( \frac{-\Omega'}{4bc^2_Je^2} \xi \right) + b \coth(\sqrt{b} \left( \frac{-\Omega'}{4bc^2_Je^2} \xi \right) \right), \quad (8.50)\]
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\[ a_2(x, t) = \sqrt{-2(\zeta_1^2 - \zeta_3^2)^2/\Omega'} e^{i(kx + \omega t)} \]
\[ \times \sqrt{b} \left( \tanh(\sqrt{b} \sqrt{-\Omega'/4bc_1^2Je^2\xi}) + b \coth(\sqrt{b} \sqrt{-\Omega'/4bc_1^2Je^2\xi}) \right), \quad (8.51) \]

\[ a_3(x, t) = \sqrt{-2(\zeta_1^2 - \zeta_3^2 - \zeta_2^2 + \zeta_1\zeta_2 + \zeta_1\zeta_3 + \zeta_2\zeta_3)^2/\Omega'} e^{i(kx + \omega t)} \]
\[ \times \sqrt{b} \left( \tanh(\sqrt{b} \sqrt{-\Omega'/4bc_1^2Je^2\xi}) + b \coth(\sqrt{b} \sqrt{-\Omega'/4bc_1^2Je^2\xi}) \right), \quad (8.52) \]

where

\[ \Omega' = E_0 + W - 2JF + J\epsilon\partial_x F - \frac{J\epsilon^2}{2} F_{xx} - JF\epsilon^2k^2 - 2L + \hbar\omega \quad (8.53) \]

and

\[ \zeta_1 = \beta_1 + \beta_8 + \beta_9, \quad \zeta_2 = \beta_2 + 2\beta_6 + 2\beta_9, \quad \zeta_3 = \beta_3 + 2\beta_7 + 2\beta_{10}. \quad (8.54) \]

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

The solutions of Eqs. (8.37)-(8.39) in this case are

\[ a_1(x, t) = \sqrt{-2(\zeta_1^2 - \zeta_3^2)^2/\Omega'} e^{i(kx + \omega t)} \sqrt{b} \left( \tanh(\sqrt{b} \sqrt{-\Omega'/4bc_1^2Je^2\xi}) + b \coth(\sqrt{b} \sqrt{-\Omega'/4bc_1^2Je^2\xi}) \right), \quad (8.55) \]

\[ a_2(x, t) = \sqrt{-2(\zeta_1^2 - \zeta_3^2 - \zeta_2^2 + \zeta_1\zeta_2 + \zeta_1\zeta_3 + \zeta_2\zeta_3)^2/\Omega'} e^{i(kx + \omega t)} \sqrt{b} \left( \tanh(\sqrt{b} \sqrt{-\Omega'/4bc_1^2Je^2\xi}) + b \coth(\sqrt{b} \sqrt{-\Omega'/4bc_1^2Je^2\xi}) \right), \quad (8.56) \]

\[ a_3(x, t) = \sqrt{-2(\zeta_1^2 - \zeta_2^2 - \zeta_2^2 + \zeta_1\zeta_2 + \zeta_1\zeta_3 + \zeta_2\zeta_3)^2/\Omega'} e^{i(kx + \omega t)} \sqrt{b} \left( \tanh(\sqrt{b} \sqrt{-\Omega'/4bc_1^2Je^2\xi}) + b \coth(\sqrt{b} \sqrt{-\Omega'/4bc_1^2Je^2\xi}) \right). \quad (8.57) \]
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Figure 8.2: Soliton in homogeneous alpha helical proteins with interspine coupling.

Figure 8.3: Plot of soliton splitting in an inhomogeneous alpha helical proteins with cubic inhomogeneity for $P = 0.00005$ and $Q = 1 \times 10^{-5}$.

Figure 8.4: Plot of soliton splitting in an inhomogeneous alpha helical proteins with biquadratic inhomogeneity for $R = 0.00009$ and $S = 1 \times 10^{-5}$.

Figure 8.5: Plot of soliton splitting in an inhomogeneous alpha helical proteins with periodic inhomogeneity for $K = 0.009$. 

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Figure 8.6: Plot of soliton splitting in an inhomogeneous alpha helical proteins with localized inhomogeneity for \( L = 0.3 \).

We analyse the solution for various types of nonlinear inhomogeneities arising due to the defects caused by the presence of additional molecules in alpha-helical proteins. As we are concerned with whether nonlinear type of inhomogeneities in the lattice modifies the soliton propagation qualitatively or not, we choose cubic and biquadratic interactions which are nonlinear first neighbour interactions. In addition, we study the effect of periodic type inhomogeneities caused by the periodic repetition of defects or molecules along the helical chain. To start with, we consider the alpha-helical protein lattice with cubic inhomogeneity of the form \( F(x) = P x^3 + Q x^2 \) where the strength of inhomogeneity is determined by the parameters \( P \) and \( Q \). In the absence of such inhomogeneity the system supports stable propagation of soliton which is depicted in Figure 8.2. It is further noticed, that for small values of inhomogeneities \( P < 0.0005 \) and \( Q < 1 \times 10^{-12} \), the soliton nature is preserved. When the strength of inhomogeneity exceeds this limit, splitting in the soliton as shown in Figure 8.3 occurs which predicts the instability of soliton. If the inhomogeneity increases further, the splitting is too
larger to cause disorder in the system. The process of energy transfer is suddenly interrupted and the protein can no longer assure its biological tasks. The larger the inhomogeneities, the higher the soliton instability which in turn affects the normal functioning of the proteins. Similar behaviour is observed in the case of biquadratic type inhomogeneity of the form $F(x) = Rx^4 + Sx^2$. The optimum values of $R$ and $S$ are found to be $0.00005$ and $1 \times 10^{-12}$ respectively for the normal functioning of proteins. A plot of the evolution of the soliton for the parametric values $R = 0.00005$ and $S = 1 \times 10^{-12}$ is given in Figure 8.4 which shows again a split in the soliton and hence its instability. A periodic type inhomogeneity arising due to periodic repetition of different sites or simple defects along the strands is incorporated in the form $F(x) = 1 + K \sin(x)$. For $K > 0.009$, fluctuation in the localized region of the soliton appears which is indicated in Figure 8.5. The fluctuation that appears in the localized region is periodic in nature which also leads to a disorder in the smooth functioning of the protein molecular systems. The localized form of inhomogeneity $F(x) = L \sech(x)$ may correspond to the intercalation of a compound between neighbouring atoms similar to the insertion of a drug molecule and the alpha helical protein has to unwind, which leads to distortion of the helix at intercalated sites. For $L > 0.3$, fluctuations appear in the tail of the soliton.
8.4 Conclusion

In this Chapter we have introduced the Hamiltonian model for the dynamics of inhomogeneous alpha helical proteins with intraspine and interspine coupling. To study the effect of inhomogeneity in an alpha helical protein chain with intraspine coupling, we have solved the resulting perturbed fourth order NLS equation. The effect of inhomogeneity is understood by carrying out a perturbation analysis. As an example we have considered periodic inhomogeneity in hydrogen bonding spines of alpha helical proteins which is found to introduce small fluctuations in the tail of the soliton. In the case of interspine coupling, the resulting three coupled inhomogeneous equations have been solved by the extended tanh function analysis and from the results we have studied the effect of inhomogeneity. We have investigated the behaviour of the propagation of soliton in the inhomogeneous protein chain for various types of nonlinear inhomogeneities such as cubic, biquadratic, periodic and localized types and our results indicate fluctuations in the soliton when the amount of inhomogeneity exceeds a limiting value. Above this limit the energy is not transferred with good efficiency. Splitting of soliton indicates the instability in soliton propagation and a sudden interruption in the energy transfer which in turn affects the normal biological functioning of proteins.