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Temperature effects on Two Exciton Energy Transfer in Continuum Alpha-helical Proteins

5.1 Introduction

After studying the dynamics of two exciton energy transfer in alpha-helical protein molecular chains, we investigate the effect of temperature on two exciton states in the continuum level. Since the alpha-helical protein molecules in the living systems work always at biological temperature 300K, the influence of the temperature on solitons at 300K should be considered and studied in a realistic model of the bio-energy transport in the alpha-helical protein molecules.

To introduce the temperature in the system, Davydov [134] calculated the Hamiltonian function by averaging over all possible phonon occupation numbers,
and applying the random-phase approximation. Kapor et al [139] formulated Dayvdov’s soliton theory for finite temperature by generating the simple product trial function in order to estimate the temperature stability of the soliton. They evaluated the relative displacement of the molecule at a certain temperature $T$ and arrived at the conclusion that the displacement due to the thermal fluctuation is not sufficient to destroy the soliton localization. Cruzeiro et al. [157] examined temperature effects on the Davydov’s soliton assuming an anisotropic model with different values of the left- and right-sides exciton-phonon coupling constant. They derived quantum mechanically without approximation, the basic equations of the system from Davydov’s original theory. Their calculations showed that the Davydov soliton is stable at 310$^\circ$K. Other simulations also showed that the Davydov soliton is stable at 300$^\circ$K. Förner [161,162] also did some works on the quantum and temperature effects on alpha-helical proteins. In all the above models, the temperature effect on a single exciton energy is studied. Hence we now turn to study the influence of temperature of the heat bath on two exciton in the alpha-helical protein analytically. We adopt Förner’s way and investigate in this chapter the temperature effect on two exciton states in alpha-helical proteins. A multiple scale perturbation analysis is carried out to find the solution of the dynamical equation in the continuum level.
5.2 Model and Equations of Motion for $|\psi_1\rangle$

We consider the Davydov model in which the protein chain is idealised as a discrete chain with peptide groups at each site of the chain. These peptide groups are in turn linked together by amino-acids. The model then couples the quantum compressional motion of the amino acids to the peptide groups by the exchange of phonons which can excite transitions in the peptides and vice-versa. In this model we also include higher order excitations and interactions to represent two exciton and write the Hamiltonian in the dimensionless form as

$$H = \sum_n \left\{ E_0 B_n^\dagger B_n - J (B_{n+1}^\dagger B_n + B_n^\dagger B_{n+1}) + E_1 B_n^\dagger B_n B_n^\dagger B_n \right. \\
+ J_1 (B_{n+1}^\dagger B_n B_n^\dagger B_{n+1} + B_n^\dagger B_{n+1} B_{n+1}^\dagger B_n) \right\} \\
+ \sum_q \hbar \omega_q \left\{ b_q^\dagger b_q + 1/2 + \sum_n [K_{n,q}(b_q + b_q^\dagger)B_n^\dagger B_n] \right. \\
+ \sum_n [B_{n,q}(b_q + b_q^\dagger)B_n^\dagger B_n B_n^\dagger B_n] \right\}, \quad (5.1)$$

where

$$K_{n,q} = \left( \frac{\chi_n}{\omega_q} \right) \left( \frac{1}{\sqrt{2\hbar \omega_q}} \right) \left( \frac{U_{n+1,q}}{\sqrt{M_{n+1}}} - \frac{U_{n,q}}{\sqrt{M_n}} \right). \quad (5.2)$$

In Hamiltonian (5.1), $K_{n,q}$ is a matrix and is real. The other parameters have the usual meanings. Note that we use the asymmetric interaction model where only the coupling of the oscillator $n$ to the hydrogen bond between $n$ and $n+1$ in which the oscillator takes part is considered. $\omega_q$ is the eigenfrequency of
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The normal mode $q$ and $U$ contains the normal mode coefficients. $\omega$ and $U$ are obtained by numerical diagonalization of the matrix $V$ which is given by [194]

$$V_{n,m} = \{(W_{n,m}(1 - \delta_{nN}) + W_n - 1(1 - \delta_{n1})|\delta_{nm} - W_n(1 - \delta_{nN})\delta_{m,n+1}
-W_n - 1(1 - \delta_{n})\delta_{m,n-1}\}(M_nM_m)^{-1/2}. \tag{5.3}$$

The form of $V$ implies that we use free chain ends and $N$ units.

5.2.1 $|\psi_1\rangle$ Ansatz

In our modified ansatz, we use a lattice already prepared with a thermal phonon distribution $|T\rangle$ instead of starting from a thermally averaged Lagrangian. The wave function we use is

$$|\psi_1, T\rangle = \left[\sum_n A_n B_n^\dagger\right]\sum_n A_n B_n^\dagger|0\rangle_e \hat{W}_n(t)|T\rangle, \tag{5.4}$$

where $|0\rangle_e$ is the exciton vacuum, $|A_n|^2$ is the probability of finding an amide-I vibrational quantum at site $n$, $|T\rangle$ is a coherent state with $|K_q|^2$ thermal phonons in each normal mode $q$ and $\hat{W}_n$ is a unitary displacement operator which is given by

$$\hat{W}_n = exp(\hat{S}_n), \quad \hat{S}_n = \sum_q [\beta_{n,q}(t)b_q^\dagger - \beta_{n,q}^*(t)b_q]. \tag{5.5}$$

In Eq. (5.5), $|\beta_{n,q}(t)|^2$ is the number of phonons excited by exciton-phonon coupling in the lattice at site n and wavenumber q, and $|T\rangle$ is a coherent state with $|K_q|^2$ thermal phonons in each normal mode q.
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\[
|T\rangle = exp(\hat{T})|0\rangle,
\quad \hat{T} = \sum_q (K_q b_q^\dagger - K_q^* b_q).
\tag{5.6}
\]

$|K_q|^2$ is computed according to Bose-Einstein statistics:

\[
|K_q|^2 = 1/exp[\hbar \omega / K_q T - 1] = v_q^2.
\tag{5.7}
\]

$|T_q\rangle$ is an exact solution of the time-dependent schrödinger equation

\[
\frac{i\hbar}{\partial t} |T_q\rangle = \hbar \omega_q (b_q^\dagger b_q + 1/2) |T_q\rangle.
\tag{5.8}
\]

If

\[
K_q(t) = |K_q| exp(-i\omega_q t),
\tag{5.9}
\]

we obtain the final ansatz state as

\[
|\psi_1\rangle = \left[ \sum_n A_n K_n^\dagger \right] \sum_n A_n K_n^\dagger |0\rangle e^{\sum_n \beta_{q,n} K_q^* - \beta_{q,n}^* K_q} 
\times \exp(\sum_q (C_{n,q} b_q^\dagger - C_{n,q} b_q)) |\bar{p}\rangle,
\tag{5.10}
\]

where

\[
C_{n,q}(t) = b_{n,q}(t) + v_q exp(-i\omega_q t).
\]

Thus the phonon part consists of coherent states with amplitudes $C_{n,q}(t)$ modulated by a phase factor. The Lagrangian of the system is written as

\[
L = \frac{i\hbar}{2} \sum_n \{ A_n^* \dot{A}_n - \dot{A}_n^* A_n - E_0 |A_n|^2 + J (A_{n+1}^* A_n D_{n+1,n}
\]

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\[ + A_n^* A_{n+1} D_{n,n+1} - \sum_q \hbar \omega_q B_{n,q} (\beta_{n,q} + \beta_{n,q}^*) + 2v_q \cos(\omega_q t) \]

\[ + \beta_{n,q}^2 + v_q^2 + 1/2 + v_q(\beta_{n,q} \exp(i \omega_q t)) - E_1 |A_n|^4 \]

\[ - J_1 (A_{n+1}^* A_n^2 D_{n+1,n} + A_n^2 A_{n+1}^* D_{n,n+1}) \]

\[ - \sum_q \hbar \omega_q [K_{n,q}(\beta_{n,q} + \beta_{n,q}^*) + 2v_q \cos(\omega_q t)] |A_n|^4 \}, \quad (5.11) \]

where

\[ D_{n,m} = \exp[\sum_q (\beta_{n,q}^* \beta_{m,q} - 1/2(|\beta_{n,q}|^2 + |\beta_{m,q}|^2) \]

\[ + (\beta_{n,q}^* - \beta_{m,q}^*) v_q \exp(-i \omega_q t) - (\beta_{n,q} - \beta_{m,q}) v_q \exp(i \omega_q t)]]. \quad (5.12) \]

Note, that in contrast with Davydov’s model the exponent in $D_{n,m}$ contains no temperature-dependent real part (besides the implicit temperature dependence in the $\beta_{n,q}$) and thus there is nothing like a Debye-Waller factor present. From this, the equations of motion are obtained with the help of the Euler-Lagrange equations

\[ \frac{d}{dt} \left( \frac{\partial L}{\partial A_n^*} \right) - \frac{\partial L}{\partial A_n} = 0, \quad (5.13) \]

\[ \frac{d}{dt} \left( \frac{\partial L}{\partial \beta_{n,q}^*} \right) - \frac{\partial L}{\partial \beta_{n,q}} = 0. \quad (5.14) \]

From the Euler-Lagrange equations we obtain

\[ i \hbar A_n = E_0 A_n - J(A_{n-1} D_{n,n-1} + A_{n+1} D_{n,n+1}) + \sum_q \hbar \omega_q [K_{n,q}[\beta_{n,q} \]

\[ + \beta_{n,q}^* ] + 2v_q \cos(\omega_q t) + |\beta_{n,q}|^2 + v_q[\beta_{n,q} \exp(i \omega_q t) \]

\[ + \beta_{n,q}^* \exp(-i \omega_q t) A_n] + 2E_1 |A_n|^2 A + J_1 (2A_n^* A_{n-1}^* D_{n,n-1}) \]
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\[ +2A_n^* A_{n+1}^2 D_{n,n+1} + \sum_q \hbar \omega_q \{ K_{n,q} [\beta_{n,q} + \beta_{n,q}^*] \} + 2v_q \cos(\omega_q t)2|A_n|^2 A_n \}, \quad (5.15) \]

\[ i\hbar \beta_{n,q} = \sum_q J(q) \left( \frac{1}{2} A_{n+1}^* A_n \beta_{n,q} D_{n+1,n} + (\beta_{n-1,q} - \frac{1}{2} \beta_{n,q}) A_n^* A_{n-1}^* D_{n,n-1} \right) \]

\[ + \left( \beta_{n+1,q} - \frac{1}{2} \beta_{n,q} \right) A_n^* A_{n+1}^* D_{n,n+1} + \frac{1}{2} A_n^* A_{n-1}^* D_{n-1,n} \right) \]

\[ + J_1 (A_{n+1}^* 2A_n^2 D_{n,n+1} (\beta_{n+1,q} - \frac{1}{2} \beta_{n,q}) + A_n^2 A_{n-1}^* \frac{1}{2} \beta_{n,q} D_{n,n-1} \right) \]

\[ + A_n^2 A_{n+1}^2 (\beta_{n+1,q} - \frac{1}{2} \beta_{n,q}) - \frac{1}{2} A_n^2 A_{n-1}^2 A_n^2 + A_n \}

\[ + \hbar \omega_q \{ [K_{n,q} + \exp(-i\omega q t)] A_n^2 + |A_n|^4 \}. \quad (5.16) \]

For analytical treatment, we turn to the analysis in the continuum limit. For single phonon mode, we transform Eqs. (5.15) and (5.16) to the following system of equations using the continuum approximations Eqs. (3.14) and (3.15):

\[ i\hbar \dot{A} = \kappa_0 + \epsilon \kappa_1 + \epsilon^2 \kappa_2 + \epsilon^3 \kappa_3 + \epsilon^4 \kappa_4, \quad (5.17) \]

and

\[ i\hbar \dot{\beta} = \Gamma_0 + \epsilon \Gamma_1 + \epsilon^2 \Gamma_2 + \epsilon^3 \Gamma_3 + \epsilon^4 [\Gamma_4 + \Gamma_5]. \quad (5.18) \]

where

\[ \kappa_0 = (E_0 - 2J)A + (2E_1 + 4J_1 + 2J_1 c(\beta^* - \beta))|A|^2 A \]

\[ + (4J_1 A_2 |A|^2 - J c A)(\beta^* - \beta) + \hbar \omega \{ K[A(\beta + \beta^* \right) \]

\[ + 2v_q \cos(\omega t)] + A_1 |\beta|^2 + Av_q [d(\beta + \beta^*)] \]

\[ + 2B ||A|^2 A(\beta + \beta^* + 2v_q \cos(\omega t))] \}, \quad (5.19) \]
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\[ \kappa_1 = J(c A_z (\beta^* - \beta) + A (\beta_z - \beta_z^*)) + J_1(c A_z (4A (\beta^* - \beta)) - 2A (\beta_z - \beta_z^*)), \]  
\[ (5.20) \]

\[ \kappa_2 = J(A_{zz}(\frac{c}{2} - 1) + A_z(c - 2d)(\beta_z + \beta_z^*) + A(\beta_{zz}(\frac{c}{2} - d) + \frac{1}{2}\beta_z^*)) + J_1(|A|^2(4A_{zz} + A_z(\beta_z(c - 4\beta^*)) + 4\beta_z^*)) + A(\beta_{zz}(2d - c) - \beta_z^*)), \]  
\[ (5.21) \]

\[ \kappa_3 = J\{c(\frac{1}{6}A_{zzz} + \frac{1}{2}A_{zz} + \frac{1}{2}A_z)\} + J_1(c|A|^2(\frac{2}{3}A_{zzz}) - 2A_{zz} - A_z(\beta_z^* - \beta_{zz})) + \frac{1}{3}A(\beta_{zzz} - \beta_{zzz}) - 2A^*A_z(\beta - \beta^*), \]  
\[ (5.22) \]

\[ \kappa_4 = J\{A_{zzzz}(\frac{1}{24}c(\beta - \beta^*) - 1) + A_{zzzz}(\beta_z^*(\frac{1}{6}\beta + c) + \beta_z(c - \beta^* + \frac{1}{3}d)) + A_{zz}(\frac{1}{2}|\beta_z|^2 + \frac{1}{2}(\beta_z^* \beta_z^*) - \beta_{zz}(\beta + 1))) + A_z(\frac{1}{2}(\beta_z\beta_z^* + \beta_z^* \beta_z) + \frac{1}{6}(\beta_z^* \beta_z)) + (\beta + c) + \beta_{zzz}(c - \beta^* - \frac{1}{3}d) + A(\frac{1}{4}|\beta_{zz}|^2 + \beta_{zzz}^* \times (\beta + c) + \beta_{zzz}(c - \beta^* + 2d))\} + J_1\{A_{zzzz}(|A|^2(\frac{1}{3}(1 + 2c(\beta^* - \beta))))) + A_{zz}(A^*(A_{zz} \times \beta_z^*(\frac{2}{3}A_z\beta^* - 1 + 4d + 2\beta^*)) - \frac{2}{3}A_z\beta_{zz}^* + \beta_{zzz} \times \frac{2}{3}A_z|A|^2(\beta^* - c + \frac{4}{3}dA_z + \frac{1}{3}|A|^2A\beta_z^*)) - \beta_{zzz}^*|A|^2(\frac{2}{3}A_z\beta + \frac{1}{3}A^*A_z) - \frac{1}{2}|\beta_{zz}|^2 + \frac{1}{12}|A|^2A \times (\beta_{zzzz}(\beta^* - c + 2d) - \frac{1}{12}\beta_{zzzz}^*(\beta + c)))\}, \]  
\[ (5.23) \]
with \( c = 1/d = \exp(-i\omega t) \).

As the co-efficients \( \Gamma_0, \Gamma_1, \Gamma_2, \Gamma_3... \) are very lengthy in form, in which it contains a large number of terms, they are separately presented in Appendix.

After rescaling \( A \rightarrow \epsilon A \) and \( \beta \rightarrow \epsilon \beta \) and making a transformation \( \beta = \beta_0 \exp(ivt) \), where \( v \) is the velocity of the wave, we obtain from Eq. (5.18)

\[
\beta = \gamma |A|^2, \quad (5.24)
\]

where \( \gamma = h\omega B \). Substituting Eq. (5.24) in Eq. (5.17), we get

\[
i\hbar \dot{A} = a_0 A + a_1 A_{zz} + a_2 |A|^2 A + a_3 A_{zzzz} + a_4 |A|^4 A + a_5 (A^* A_z^2 \\
+ A|A_z|^2) + a_6 (A^* A_{zz} + 2|A_z|^2 + AA_{zz}^*), \quad (5.25)
\]

where \( a_0 = \epsilon(E_0 - 2J + 2h\omega \cos(\omega t)), \quad a_1 = -\epsilon^3 J, \quad a_2 = [\epsilon^2(2h\omega K + 2v_\eta \cos(\omega t)) + \epsilon^3(2E_1 + 4J_1)], \quad a_3 = \epsilon^4 J, \quad a_4 = \epsilon^4 h\omega 2K, \quad a_5 = \epsilon^4 4Ji\nu_\eta \sin(\omega t), \quad a_6 = \epsilon^4 2Ji\nu_\eta \sin(\omega t).

Making the transformation \( A \rightarrow q\sqrt{2\hbar/a_2} \) and a rescaling \( t \rightarrow -(\frac{\hbar}{\epsilon})t \), Eq. (5.25) reduces to

\[
iq_t + q_{zz} + 2|q|^2 q + \alpha_1 q_{zzzz} + \alpha_2 |q|^4 q + \alpha_3 (q^* q_z^2 \\
+ q|q_z|^2) + \alpha_4 (|q|^2 q_{zz} + 2q|q_z|^2 + q^2 q_{zz}^*) = 0, \quad (5.26)
\]

where \( \alpha_1 = -Je^5, \quad \alpha_2 = 2\epsilon^4 h^3 \omega K/p, \quad \alpha_3 = \alpha_4 = 2i\epsilon^4 hJi\nu_\eta \sin(\omega t)/p \), and \( p = \epsilon^2(2h\omega B + 2v_\eta \cos(\omega t)) + \epsilon^3(2E_1 + 4J_1) \).

Eq. (5.26) describes the dynamics of alpha-helical proteins in the continuum.
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limit. It is a perturbed NLS equation which may be rewritten as

\[ iq_t + q_{zz} + 2|q|^2q + \gamma\{q_{zzzz} + \delta_1|q|^4q \]
\[ + \delta_2(q^*q_z^2 + 3q|q_z|^2) + \delta_3(|q|^2q_{zz} + q^2q_{zz}^*) \} = 0, \tag{5.27} \]

where \( \gamma = \alpha_1, \quad \delta_1 = \alpha_2/\alpha_1, \quad \delta_2 = \delta_3 = \alpha_3/\alpha_1 \). When \( \gamma = 0 \), Eq. (5.26) reduces to the completely integrable cubic NLS equation which admits soliton solutions.

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To study the effect of temperature on the two exciton energy transfer in alpha-helical protein, we solve Eq. (5.27) using a suitable perturbation technique. The perturbed equation that is going to be studied here is

\[ iq_t + q_{zz} + |q|^2q + \gamma R = 0, \tag{5.28} \]

where \( R = q_{zzzz} + \delta_1|q|^4q + \delta_2(q^*q_z^2 + 3q|q_z|^2 + |q|^2q_{zz} + q^2q_{zz}^*) \) and \( \gamma \) is a perturbation parameter. In the presence of these perturbation terms, the soliton parameters namely the soliton amplitude, width and velocity may vary because of temperature dependence. The one soliton solution of the cubic NLS equation is as given in Eq. (3.33).

Introducing Eq. (3.33) into Eq. (5.28), one gets

\[ - \eta^2 \dot{q} + \dot{q}_{\theta\theta} + 2|\dot{q}|^2\dot{q} = \alpha_0 F(\dot{q}), \tag{5.29} \]
Using Eqs. (3.41) and (3.42), the real and imaginary parts are written as

where

\[ F(\dot{q}) = -i[\dot{q}_r + 4\xi \dot{q}_{\theta\theta} + 4\xi^3 \dot{q}_\theta + \delta_2 \dot{q}^2 \dot{q}_{\theta\theta} + 4\delta_2 (1 + \xi^2) \dot{q} |\dot{q}|^2 \]

\[ + \delta_2 |\dot{q}|^2 |q_{\theta\theta}|^2 - \delta_2 \xi^2 |q|^2 q - \delta_2 \xi^2 |\dot{q}|^2 \dot{q} \]

\[ + \delta_2 \xi^2 \dot{q}^2 + \delta_2 \xi^3 q^2 + \dot{q} [\xi \dot{q} - (\xi \theta_{\theta\theta} + \sigma_{\theta\theta})] \]

\[ - \xi^4 - \delta_1 |\dot{q}|^4 + 2\delta_2 \xi \dot{q} \dot{q}_\theta + 4\delta_2 \xi \dot{q}^* \dot{q}_{\theta\theta} + 3\delta_2 \xi^2 \dot{q}^* \dot{q}_\theta \]

\[ - \dot{q}_{\theta\theta\theta} - 6\xi^2 \dot{q}_{\theta\theta}. \quad (5.30) \]

Using Eq. (3.37) in Eq. (5.28), we get

\[- \eta^2 \dot{q}_1 + \dot{q}_{1\theta \theta} + 4\xi_0 \dot{q}_1 + q_0 \dot{q}_1 = F(\dot{q}_0). \quad (5.31)\]

where

\[ F(\dot{q}_0) = -i[\dot{q}_{0r} + 4\xi \dot{q}_{0\theta \theta} + 4\xi^3 \dot{q}_{0\theta} + \delta_2 \dot{q}^2 \dot{q}_{0\theta \theta} + \delta_2 \xi^2 \dot{q}_0 \dot{q}_{0\theta} \]

\[ + 4\delta_2 (1 + \xi^2) \dot{q}_0 |\dot{q}_0|^2 + \delta_2 |\dot{q}_0|^2 \dot{q}_{0\theta \theta} - \delta_2 \xi^2 |\dot{q}_0|^2 \dot{q}_0 \]

\[ + \delta_2 \xi^2 \dot{q}_0 \dot{q}_{0\theta} - \delta_2 \xi^2 |\dot{q}_0|^2 q_0 + \delta_3 \xi^3 q_0^2 \dot{q}_{0\theta} \]

\[ + \delta_3 \xi^3 q_0^3 + \dot{q}_0 [\xi \dot{q}_0 - (\xi \theta_{\theta\theta} + \sigma_{\theta\theta})] \]

\[ - \delta_1 |\dot{q}_0|^4 + 2\delta_2 \xi \dot{q}_0 \dot{q}_{0\theta} + 4\delta_2 \xi \dot{q}_0^* \dot{q}_{0\theta} \]

\[ + 3\delta_2 \xi^2 \dot{q}_0^* \dot{q}_{0\theta} - \dot{q}_{0\theta\theta \theta} - 6\xi^2 \dot{q}_{0\theta \theta}. \quad (5.32)\]

Using Eqs. (3.41) and (3.42), the real and imaginary parts are written as

\[ \text{Re}(\hat{F}_1) = \dot{q}_0 [\xi \dot{q}_r (\theta - \theta_0) - (\xi \theta_{\theta\theta} + \sigma_{\theta\theta})] - \xi^4 - \delta_1 |\dot{q}_0|^4 \]

\[- 2\delta_2 \xi \dot{q}_0 \dot{q}_{0\theta} - 4\delta_2 \xi \dot{q}_0 \dot{q}_{0\theta} + \delta_2 \xi^2 \dot{q}_0 \dot{q}_{0\theta} \]

\[ + 2\delta_3 \xi^2 \dot{q}_0^* \dot{q}_{0\theta} - \dot{q}_{0\theta\theta \theta} + 6\xi^2 \dot{q}_{0\theta \theta}. \quad (5.33)\]
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Figure 5.1: velocity of the soliton.

and

\[ Im(\hat{F}_1) = -\left[ \ddot{q}_0 + 4\xi \dot{q}_0 q_{0\theta\theta} - 4\xi^3 \dot{q}_0 q_{0\theta} + \delta_2 \dot{q}_0^2 q_{0\theta\theta} + \delta_2 \xi^2 \dot{q}_0^2 \dot{q}^2 \right. \]

\[ \left. -4\delta_2 (1 + \xi^2) |\dot{q}_0|^2 \dot{q} + \delta_2 |q_0|^2 q_{0\theta\theta} \right] \]

\[ -\delta_2 \xi^2 |\dot{q}_0|^2 \dot{q} + \delta_2 |q_0|^2 q_{0\theta\theta} - \delta_2 \xi q_0^2 \dot{q}_0^2 \right]. \]  \hspace{1cm} (5.34)

Using the leading order solution \( \dot{q}_0 \) given in Eqs. (3.45) and (3.46) and on evaluating the integrals, we get \( \xi_r = 2/3\delta_2 \xi \eta^4 \), and \( \eta_r = (28/15+16/15\xi - 8/3\xi^2 - 26/5\eta^2) \delta_2 \eta^2 \), which imply that the velocity and amplitude of the soliton may vary with temperature. We have plotted the velocity of soliton in Fig. (5.1) and the amplitude in Fig. (5.2). From the figures we observe that as time passes on, the velocity and amplitude of the soliton increase and when reaching a maximum value a phase change occurs and the soliton moves in the opposite direction.

The perturbed solution of Eq. (5.28) can be determined by solving Eqs.
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Figure 5.2: Amplitude of the soliton.

Figure 5.3: Evolution of $|q|^2$ at temperature 30K.

(3.42) and (3.43) for $\hat{\phi}_1$ and $\hat{\psi}_1$ and using the conditions $\xi_r = 2/3\delta_2\xi^4$, and $\eta_r = (28/15 + 16/15\xi - 8/3\xi^2 - 26/5\eta^2)\delta_2\eta^2$, and appropriate initial conditions.

Evaluating the integrals using the particular solutions as in Eqs. (3.47), (3.48) and the general solution as in (3.49), we obtain $\hat{\phi}_1$ after removing the secular terms (terms proportional to $\sinh\eta(\theta - \theta_0)$) and applying the boundary conditions $\hat{\phi}_1(0) = \hat{\phi}_{1\theta}(0) = 0|_{\theta_0=0}$ as
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Figure 5.4: Evolution of $|q|^2$ at temperature 100K.

Figure 5.5: Evolution of $|q|^2$ at temperature 250K.

Figure 5.6: Evolution of $|q|^2$ at temperature 300K.
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\[
\hat{\phi}_1 = -\text{sech}(\theta - \theta_0)\tanh(\theta - \theta_0)\{P_1\text{sech}^2 \eta(\theta - \theta_0)
+ P_2\text{sech}^4 \eta(\theta - \theta_0) + P_3\tanh(\theta - \theta_0) + P_4 \times
\tanh^3 \eta(\theta - \theta_0) + P_5\tanh^4 \eta(\theta - \theta_0) + P_6
\tanh^5 \eta(\theta - \theta_0) + P_7\tanh^{10} \eta(\theta - \theta_0) + p_8 \theta + p_9 \theta^2
+ p_{10}\log[\text{sech}(\theta - \theta_0)]\} + \left[\frac{3}{2}(\theta - \theta_0)\text{sech}(\theta - \theta_0)\right]
- \frac{1}{2\eta}\tanh(\theta - \theta_0)\sinh(\theta - \theta_0)
- \frac{1}{\eta}\text{sech}(\theta - \theta_0)) \times \{P_{11}\text{sech}^2 \eta(\theta - \theta_0)
+ P_{12}\text{sech}^4 \eta(\theta - \theta_0) + P_{13}\text{sech}^6 \eta(\theta - \theta_0)
+ p_{14}\tanh \eta(\theta - \theta_0) + p_{15}\tanh^3 \eta(\theta - \theta_0)\},
\]

(5.35)

where

\[
p_1 = (\theta - \theta_0)^2 \left[\frac{3}{4}\xi_\tau + (\theta - \theta_0)(\frac{3}{2}(\xi_\theta + \sigma_\theta) + \xi^4) - \frac{27}{2} \eta^4\right]
- \frac{4}{5}\left[\frac{3}{2}(\delta_2 + \delta_3)\xi_\eta^2 + \frac{1}{4}\eta^3\right],
\]

(5.36)

\[
p_2 = (\theta - \theta_0)^2 \left[\frac{9}{4}\eta^2 - \frac{5}{8}\eta^3 + \frac{1}{4}(3\delta_2 + 2\delta_3)\xi_\eta^2\right],
\]

(5.37)

\[
p_3 = (\theta - \theta_0)^2 \left[\frac{9}{8}\xi_\tau + (\frac{3}{4}\eta^2 + \frac{1}{2})(\xi_\theta + \sigma_\theta) + \xi^4\right]
+ \frac{1}{4}\eta^3(\delta_1 + 21) + \frac{27}{4}\eta^2\xi,
\]

(5.38)

\[
p_4 = (\theta - \theta_0)^2 \left[\frac{15}{4}(-\frac{9}{2}\delta_2 + 3\delta_3)\xi_\eta^3 - \frac{1}{6}\eta^2(4\delta_1 + 25) + \frac{23}{4}\eta^2 + \frac{3}{4}(5.39)\right],
\]

\[
p_5 = (\theta - \theta_0)^2 \left[\frac{27}{48}\eta^4 - \frac{9}{4}\xi^2 \eta^2\right] + \frac{1}{20}(\frac{9}{2}\delta_2 + 3\delta_3)\xi - \frac{11}{4}\eta^3
\]

(5.39)
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\[ p_6 = (\theta - \theta_0)(\frac{1}{5}(\frac{9}{2}\delta_2 + 3\delta_3)\xi\eta^3) + (-\frac{3}{20} + \frac{1}{4})\eta^2 + \frac{1}{5}(\delta_1 + 5)\eta^2, \]  
\[ p_7 = \frac{1}{2}\eta^4(\theta - \theta_0), \quad p_8 = 11\eta^4 - \frac{3}{4}\xi^2\eta^2, \quad p_9 = -\frac{1}{4}\xi_r, \]  
\[ p_{10} = \frac{2\xi_r}{\eta} + (\frac{12}{5}\delta_2 - \frac{8}{5}\delta_3)\xi\eta^3, \]  
\[ p_{11} = \xi_r(\theta - \theta_0) + \frac{1}{2}(\xi\theta_0 + \sigma_0r + \xi^4) - 5\eta^4 + 3\xi^2\eta^2, \]  
\[ p_{12} = \delta_2\xi\eta^3 - \frac{9}{2}\eta^4 + \frac{1}{2}\eta^4 - \frac{3}{4}\xi^2\eta^2, \]  
\[ p_{13} = \frac{\eta^4}{3}(\frac{\delta_1}{2} - 7), \quad p_{14} = \frac{\xi_r}{2\eta} + (\delta_2 - 2\delta_3)\xi\eta^3, \]  
\[ p_{15} = \frac{2}{3}\xi\eta^3(\delta_2 + \delta_3). \]  

After evaluating the integrals, using the particular solution, on applying the boundary conditions and after removing the secular terms, we obtain

\[ \hat{\psi}_1 = -\text{sech}\eta(\theta - \theta_0)\{S_1\text{sech}^2\eta(\theta - \theta_0) + S_2\text{sech}^4\eta(\theta - \theta_0) \]
\[ + s_3\text{sech}^6\eta(\theta - \theta_0) + S_4\tanh\eta(\theta - \theta_0) + S_5\tanh^3\eta(\theta - \theta_0) \]
\[ + S_6\tanh^4\eta(\theta - \theta_0) + s_7\tanh^5\eta(\theta - \theta_0) + s_8\log[\text{sech}\eta(\theta - \theta_0)] \]
\[ + S_9\theta + (\frac{1}{2}(\theta - \theta_0)\text{sech}\eta(\theta - \theta_0) + \frac{1}{2\eta}\sinh(\theta - \theta_0)) \times \]
\[ \{S_{10}\text{sech}^2\eta(\theta - \theta_0) + S_{11}\text{sech}^4\eta(\theta - \theta_0) + s_{12}\text{sech}^6\eta(\theta - \theta_0) \]
\[ + s_{13}\tanh\eta(\theta - \theta_0) + s_{14}\tanh^3\eta(\theta - \theta_0) + s_{15}\tanh^5\eta(\theta - \theta_0)\}, \]  

where
### 5.3 Effect of Temperature on Soliton

\[s_1 = \frac{(\theta - \theta_0)^2}{2} \eta_r + (\theta - \theta_0)(2\xi^2 \eta^2 - \frac{1}{6}(\delta_2(\frac{5}{2} + 2\xi) + \frac{1}{2}\delta_3)\eta^3)\]

\[+ \delta_2(-\frac{13}{30} \eta^5 - \frac{1}{4}\xi \eta^2 + \frac{1}{12}\xi^2 \eta + \frac{1}{4}\xi \eta^2) + \frac{1}{4}\delta_3 \xi \eta^2, \quad (5.49)\]

\[s_2 = \frac{5}{2}\xi \eta^3(\theta - \theta_0) + \frac{1}{4}\delta_2 \eta^3, \quad s_3 = -\frac{1}{12}\delta_2 \eta^4(\theta - \theta_0), \quad (5.50)\]

\[s_4 = \frac{(\theta - \theta_0)(\frac{7}{12}\delta_2 \eta^3 + \delta_2 \eta^2 \xi^2) + 2\eta^2(\xi - \xi^2)}{s}, \quad (5.51)\]

\[s_5 = (\theta - \theta_0)(-\frac{1}{3}\xi \eta^2 + \frac{1}{3}(\delta_2(\frac{5}{2} + 2\xi) + \frac{1}{2}\delta_3)\eta^4\]

\[-\frac{1}{6}\delta_2 \xi^2 \eta^2) + \frac{5}{6}\xi \eta^5 + \eta^3(\frac{2}{3}\xi - \frac{2}{9}\delta_2 - \frac{10}{3}\xi) + \frac{2}{3}\xi \eta^2, \quad (5.52)\]

\[s_6 = 2\xi \eta^3(\theta - \theta_0) + \eta^3(2\xi - \frac{99}{40}\delta_2 + \frac{1}{2}\delta_3), \quad (5.53)\]

\[s_7 = (\theta - \theta_0)(-2\delta_2 - 2\xi + \frac{1}{2}\delta_3)\eta^5 - \frac{1}{2}\delta_2 \eta^4 + \frac{1}{5}\delta_2 \eta^6, \quad (5.54)\]

\[s_8 = \eta^4(\delta_2 + 2\xi + \frac{1}{2}\delta_3) + \frac{\eta r}{\eta}, \quad s_9 = \frac{1}{2}\eta_r (\theta - \theta_0) + \frac{1}{2}\eta + 2\xi \eta^3, \quad (5.55)\]

\[s_{10} = (\theta - \theta_0)(\eta_r + \eta), \quad s_{11} = -4\xi \eta^3, \quad s_{12} = \frac{1}{6}\delta_2 \eta^5, \quad (5.56)\]

\[s_{13} = \frac{\eta r}{2\eta} + \delta_2 \eta^5 - (2\delta_2 + \delta_3)\xi \eta^2, \quad (5.57)\]

\[s_{14} = -\frac{2}{3}\delta_2 \eta^5 + \frac{1}{3}(2\delta_2 + \delta_3)\xi \eta^2 + \eta^4(\frac{2}{3}\delta_2(5 + 4\xi) + \delta_3), \quad (5.58)\]

\[s_{15} = \frac{-29}{60}\delta_2 \eta^3 - \frac{1}{10}\delta_2 \eta^3 - (\delta_2(\frac{5}{2} + 2\xi) + \frac{1}{2}\delta_3)\frac{1}{5}(\theta - \theta_0). \quad (5.59)\]

Using Eqs. (5.35) and (5.48), the first-order perturbed solution \(\hat{q}_1\) is written as

\[\hat{q}_1 = -\text{sech}\eta(\theta - \theta_0)\text{tanh}(\theta - \theta_0)[P_1\text{sech}^2\eta(\theta - \theta_0)\]

\[+P_2\text{sech}^4\eta(\theta - \theta_0) + P_3\text{tanh}(\theta - \theta_0)\]
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\[ +P_4 \tanh^3 \eta (\theta - \theta_0) + P_5 \tanh^4 \eta (\theta - \theta_0) \]
\[ +P_6 \tanh^5 \eta (\theta - \theta_0) + P_7 \tanh^6 \eta (\theta - \theta_0) + p_8 \theta - p_9 \theta^2 \]
\[ +\left( \frac{3}{2} (\theta - \theta_0) \text{sech}(\theta - \theta_0) \tanh(\theta - \theta_0) \right) \]
\[ -\frac{1}{2\eta} \tanh(\theta - \theta_0) \sinh(\theta - \theta_0) \]
\[ -1/\eta \text{sech}(\theta - \theta_0) [P_{10}\text{sech}^2 \eta (\theta - \theta_0) \]
\[ +P_{11}\text{sech}^4 \eta (\theta - \theta_0) + P_{12}\text{sech}^6 \eta (\theta - \theta_0) \]
\[ +p_{13}\tanh(\theta - \theta_0) + p_{14}\tanh^3 \eta (\theta - \theta_0) \]
\[ +i\{-\text{sech}(\theta - \theta_0) [S_1\text{sech}^2 \eta (\theta - \theta_0) \]
\[ +S_2\text{sech}^4 \eta (\theta - \theta_0) + s_3\text{sech}^6 \eta (\theta - \theta_0) \]
\[ +S_4\tanh(\theta - \theta_0) + S_5\tanh^3 \eta (\theta - \theta_0) \]
\[ +S_6\tanh^4 \eta (\theta - \theta_0) + s_7\tanh^5 \eta (\theta - \theta_0) \]
\[ +s_8 \log[\text{sech}(\theta - \theta_0) + S_9 \theta] + \left( \frac{1}{2} (\theta - \theta_0) \right) \]
\[ +\frac{1}{2\eta} \sinh(\theta - \theta_0) [S_{10}\text{sech}^2 \eta (\theta - \theta_0) \text{sech}(\theta - \theta_0) \]
\[ +S_{11}\text{sech}^4 \eta (\theta - \theta_0) + s_{12}\text{sech}^6 \eta (\theta - \theta_0) \]
\[ +s_{13}\tanh(\theta - \theta_0) + s_{14}\tanh^3 \eta (\theta - \theta_0) \]
\[ +s_{15}\tanh^5 \eta (\theta - \theta_0) \} \]. \quad (5.60) \]

To discuss some of the cases in more detail we show in Figs. (5.3-5.5) the time evolution of \(|q(t)|^2\) for some parameter values. We see that the formation of the solitary wave is a clear temperature effect, since at temperature \(T < 200K\).
5.4 Site Independent Dynamics, $|\psi_2\rangle$ Ansatz

The most simple form of the ansatz for $|\psi\rangle$ is the so called $|\psi_2\rangle$ state, which is a product state of exact solutions for the isolated oscillators and the isolated amide-I subsystems with unknown time-dependent parameters given by

$$|\psi_2\rangle = \left[ \sum_n A_n B_n^\dagger \right] \sum_n A_n B_n^\dagger |0\rangle e^{i\omega t} \exp\left( \frac{1}{2} \sum_q (\beta_q B_q^\dagger - \beta_q^* B_q) \right) \times \exp\left( \sum_q (C_q b_q^\dagger - C_q b_q) \right) |0\rangle_p,$$

where

$$C_q(t) = b_q(t) + v_q e^{i\omega_q t}.$$  

Thus the phonon part consists of coherent states with amplitudes $C_q$ modulated by a phase factor. Then the Lagrangian is given by

$$L = \frac{i\hbar}{2} \sum_n \{ A_n^* \dot{A}_n - A_n^* A_n - E_0 |A_n|^2 + J (A_{n+1}^* A_n + A_n^* A_{n+1}) \}$$

$$- \sum_q \hbar \omega_q [K_q (\beta_q + \beta_q^*) + 2v_q \cos(\omega_q t) + |\beta_q|^2 + v_q^2 + 1/2]$$

$$+ v_q (\beta_q e^{i\omega_q t}) |A_n|^2 - E_1 |A_n|^4 - J_1 (2A_n^2 A_{n-1}^2 + \beta_q^* e^{i\omega_q t} |A|^2$$
\[ +2A^*A_{n+1}^2 - \sum_q \hbar \omega_q |K_q(\beta_q + \beta_q^*) + 2v_q \cos(\omega_q t)|A_n|^4 \}. \] (5.62)

The equations of motion are obtained as

\[
\nonumber
ih \dot{A}_n = E_0 A_n - J(A_{n-1} + A_{n+1}) \\
+ \sum_q \hbar \omega_q \{ [K_q(\beta_q + \beta_q^*) + 2v_q \cos(\omega_q t)] \\
+ |\beta_q|^2 + v_q[\beta_q \exp(i\omega_q t) + \beta_q^* \exp(-i\omega_q t)]A_n \} \\
+ 2E_1 |A_n|^2 A + J1(2A_n^2A_{n-1})^2 \\
+ 2A_n^2A_{n+1}^2 + \sum_q \hbar \omega_q \{ K_q[\beta_q + \beta_q^*] \\
+ 2v_q \cos(\omega_q t)]2|A_n|^2A_n \}, \] (5.63)

\[
ih \dot{\beta}_{n,q} = \hbar \omega q K_q(|A_n|^2 + |A_n|^4). \] (5.64)

Using continuum approximation as in the previous section we transform Eqs. (5.63) and (5.64) for a single phonon mode to

\[
\nonumber
ih \dot{\hat{A}} = (E_0 - 2J)A + (2E_1 + 4J_1)|A|^2A + \hbar \omega \left( \frac{1}{2} \\
+ (A + 2|A|^2A)(b^* \exp(-i\omega t) + \beta \exp(i\omega t) \\
+ v^2 + B(\beta^* + \beta) + 2v \cos(\omega t)) \right) + \epsilon^2[-J A_{zz} \\
+ 4J_1 A^* A^2 z + 4J_1 |A|^2 A_{zz}^2 + \epsilon^4 \left( -\frac{J}{12} A_{zzzz} \\
+ J_1 A^* A^2 z + \frac{4}{3} J_1 A^* A_{zz} + \frac{1}{3} J_1 |A|^2 A_{zzz} \right) \\
+ \frac{1}{3} J_1 |A|^2 A_{zzz} \}
\] (5.65)

and

\[
\nonumber
ih \dot{\beta} = \hbar \omega K |A|^2 + \hbar \omega K |A|^4. \] (5.66)
After rescaling $A \rightarrow \epsilon A$, $\beta \rightarrow \epsilon \beta$ and neglecting higher powers of $\epsilon$, Eqs. (5.65) and (5.66) become

$$\epsilon \hbar \dot{A} = \epsilon [(E_0 - 2J + \frac{1}{2} + v^2)A] + \epsilon^2 \hbar \omega (\beta + \beta^*) 2v \cos(\omega t) + \beta \exp(i\omega t)$$

$$+ \beta^* \exp(-i\omega t) + \epsilon^3 [-JA_{zz}] + \epsilon^4 \hbar \omega (2\beta + 2v \cos(\omega t)) + \beta \exp(i\omega t)$$

$$+ \beta^* \exp(-i\omega t) |A|^2 A + \epsilon^5 \hbar \omega \frac{-J}{12} A_{zzzz} + 4J_1 |A|^2 A_{zz}, \quad (5.67)$$

$$\epsilon \hbar \dot{\beta} = \epsilon^2 \hbar \omega K |A|^2 + \epsilon^4 \hbar \omega K |A|^4. \quad (5.68)$$

Assuming plane wave solution to $\beta$, $\beta = \beta_0 \exp(i\nu t)$ where $\nu$ is the frequency of the wave we get $\beta = \gamma |A|^2$. Using this in Eq. (5.67), we obtain

$$i \hbar \dot{A}_n = a_0 A + a_1 A_{zz} + a_2 |A|^2 A + a_3 A_{zzzz}$$

$$+ a_4 |A|^4 A + a_5 A^* A_z^2 + a_6 |A|^2 A_{zz}, \quad (5.69)$$

where $a_0 = \epsilon(E_0 - 2J + v^2 + 1/2 + 2\hbar \omega K \cos(\omega t))$, $a_1 = \epsilon^3 J$, $a_2 = (2E_1 + 4J_1 + \hbar \omega (2K + v \cos(\omega t)))$, $a_3 = \epsilon^5 \frac{J}{12}$, $a_4 = a_5 = \epsilon^5 \hbar \omega 2B |A|^4 A + 4J_1$, $a_6 = \epsilon^7 J_1$.

Making similar transformation as in $|\psi_1\rangle$ ansatz case, Eq. (5.69) reduces to

$$i \dot{q} + q_{zz} + 2|q|^2 q + \alpha_1 q_{zzzz} + \alpha_2 |q|^4 q$$

$$+ \alpha_3 q^* q_z^2 + \alpha_4 |q|^2 q_{zz} = 0, \quad (5.70)$$
5.4 Site Independent Dynamics, $|\psi_2\rangle$ Ansatz

where

$$\alpha_1 = \frac{-48\hbar^3 \omega(1 + 2K)}{J(2E_1 + 4J_1 + \hbar \omega 2K \cos(\omega t))^2}; \quad (5.71)$$

$$\alpha_2 = \alpha_3 = \frac{8\hbar J_1}{2E_1 + 4J + \hbar \omega 2K \cos(\omega t)}. \quad (5.72)$$

Eq. (5.70) describes the dynamics of alpha-helical proteins in the continuum limit. It is a perturbed NLS equation which may be rewritten as

$$iq_t + q_{zz} + 2|q|^2 q + \gamma q_{zzzz} + \delta_1 |q|^4 q + \delta_2 q^* q^2_z + \delta_2 |q|^2 q_{zz} = 0, \quad (5.73)$$

where $\gamma = \alpha_1$, $\delta_1 = \alpha_2 / \alpha_1$, $\delta_2 = \alpha_3 / \alpha_1$. When $\gamma = 0$, Eq. (5.73) becomes the completely integrable cubic NLS equation which admits soliton solutions.

The multiple scale parametric perturbation method is employed here to solve Eq. (5.73). Using the leading order solution and on evaluating the integrals, we get $\xi_r = 0$ and $\eta_r = 0$ which imply that the velocity and amplitude of the soliton remain unchanged from their unperturbed values. The solution in this case becomes

$$\hat{q}_1 = sech\eta(\theta - \theta_0)\tanh\eta(\theta - \theta_0)[h_1 sech^2\eta(\theta - \theta_0)$$

$$+ h_2 sech^6\eta(\theta - \theta_0) + h_3 \tanh\eta(\theta - \theta_0) + h_4 \tanh^3\eta(\theta - \theta_0)$$

$$+ h_5 \tanh^5\eta(\theta - \theta_0) + h_6 \tanh^6\eta(\theta - \theta_0) + h_7 \log(sech\eta(\theta - \theta_0)))]$$

$$+ \frac{3}{2} \eta(\theta - \theta_0) sech\eta(\theta - \theta_0) \tanh\eta(\theta - \theta_0)$$

$$+ \frac{1}{2\eta} \tanh\eta(\theta - \theta_0)\sinh\eta(\theta - \theta_0) - \frac{1}{\eta} \text{sech}\eta(\theta - \theta_0) \times$$
\[ h_8 \text{sech}^2 \eta (\theta - \theta_0) + h_9 \text{sech}^4 \eta (\theta - \theta_0) + h_{10} \text{sech}^6 \eta (\theta - \theta_0) \]

\[ + i \{ \text{sech} \eta (\theta - \theta_0) [g_1 \text{sech}^2 \eta (\theta - \theta_0) + g_2 \text{sech}^4 \eta (\theta - \theta_0)] + \frac{1}{2} \eta (\theta - \theta_0) \text{sech} \eta (\theta - \theta_0) \]

\[ + g_3 \text{tanh}^3 \eta (\theta - \theta_0) + g_5 \text{tanh}^4 \eta (\theta - \theta_0) \]

\[ + g_7 \text{sech}^4 \eta (\theta - \theta_0) + g_8 \text{tanh}^4 \eta (\theta - \theta_0) \}, \quad (5.74) \]

where

\[ h_1 = \frac{-3}{4} (\xi \theta_0 + \sigma + \xi^4)(\theta - \theta_0), \quad h_2 = \frac{5}{4} \eta^4 - \frac{3}{4} \delta_2 \eta^4 (\theta - \theta_0), \quad (5.75) \]

\[ h_3 = \left( \frac{3}{4} + \frac{3}{\eta} \right) (\xi \theta_0 + \sigma o + \xi^4) + \eta^3 \left( \frac{9}{4} \delta_1 - \frac{65}{4} - \frac{1}{3} \delta_2 \right) - \frac{5}{4} \delta_2 (\theta - \theta_0) + \xi^2 \eta \left( -\frac{21}{8} \delta_2 - 3 \right) + \frac{21}{4} \xi \eta - \frac{1}{2} \delta_2 \eta^4 - 6 \xi \eta^2, \quad (5.76) \]

\[ h_4 = \eta^3 \left( -\frac{1}{3} \delta_3 - \frac{1}{4} \frac{3}{2} \delta_2 - \frac{2}{3} \delta_1 \right) + \frac{1}{8} \xi^2 \eta \delta_2 + \xi \eta^2 \left( 3(\theta - \theta_0) + 1 \right) + \frac{7}{4} \xi \eta^3 \frac{5}{3} \eta^4, \quad (5.77) \]

\[ h_5 = \eta^3 \left( \frac{9}{2} + \frac{\delta_1}{20} + \frac{\delta_2}{4} \right) + \eta^4 \left( 10 + \frac{2}{5} \delta_2 \right) - \frac{3}{10} \xi \eta, \quad h_6 = \frac{3}{2} \eta^4 (\theta - \theta_0) \quad (5.78) \]

\[ h_7 = \xi \theta_0 + \sigma + \xi^4 - \frac{\eta^2}{2} - 3 \xi \eta^2, \quad h_8 = h_9 = \frac{9}{2} \eta^5 + \frac{1}{4} \eta^2 - \frac{\delta_2}{4} \eta^4 \quad (5.79) \]

\[ h_{10} = \left( \frac{2}{3} + \frac{1}{3} \delta_2 \right) \eta^4 - 3 \eta^5 + \frac{1}{6} \eta^2, \quad (5.80) \]

and

\[ g_1 = -\frac{\eta}{4} \eta (\theta - \theta_0) + \xi^2 \eta, \quad (5.82) \]
5.4 Site Independent Dynamics, $|\psi_2\rangle$ Ansatz

![Figure 5.7: Evolution of $|q|^2$ at temperature 150K.](image)

![Figure 5.8: Evolution of $|q|^2$ at temperature 300K.](image)

\begin{align*}
g_2 &= \frac{5}{2} \xi \eta^2 \eta (\theta - \theta_0) - \xi \eta^3, \\
g_3 &= \frac{5}{2} \xi \eta^2 - \frac{1}{2} \eta^2 \xi^2, \\
g_4 &= -\frac{5}{6} \xi \eta^2 + \frac{1}{12 \eta^2}, \\
g_5 &= -\frac{\eta^2}{8} (\theta - \theta_0), \\
g_6 &= \frac{\eta}{2} (\theta - \theta_0) - 4 \xi \eta^3, \\
g_7 &= -\frac{9}{2} \xi \eta^3, \\
g_8 &= -5 \xi \eta^3.
\end{align*}

The time evolution of $|q(t)|^2$ for the same parameters as in the case of $|\psi_1\rangle$ ansatz state are shown in Fig. (5.7) and Fig. (5.8) at 150K and 300K respectively.
5.5 Conclusions

We have found qualitatively very similar behaviour as in the $|\psi_1\rangle$ case. The formation of the solitary wave in this case is again shown to be a clear temperature effect. At $T = 150K$, we observe a clear solitary wave which remains qualitatively unchanged up to $300K$. The velocity and amplitude of the soliton are found to be not varying with time.

5.5 Conclusions

We studied the effect of temperature on two exciton states in alpha-helical proteins in the continuum level. In our study we proposed a model Hamiltonian which includes internal molecular excitations, dipole-dipole interactions and nonlinear coupling between exciton and phonon. In order to study the nature of two exciton states and the soliton excitations along the hydrogen bonding spines in the alpha helical proteins, new higher order excitations, interactions and nonlinear couplings between higher order molecular excitations and interactions have also been included. The dynamics was studied by constructing the Lagrange’s equation of motion using two types of wave functions $|\psi_1\rangle$ and $|\psi_2\rangle$. The lattice model was also treated in the continuum limit which is a valid approximation in the low temperature, long wavelength limit. The resulting equation was found to be a perturbed NLS equation which shows the transfer of two exciton energy in the form of solitons. A multiple scale perturbation analysis to study the effect of two excitons showed that for $|\psi_1\rangle$ ansatz as time passes on the velocity and
amplitude of the soliton increase and when reaching a maximum value a phase change occurs and the soliton moves in the opposite direction. We see that the formation of the solitary wave is a clear temperature effect, the solitary wave starts to form at $250K$. Higher temperatures reduce the stability of the solitons. For $|\psi_2\rangle$ ansatz the formation of the solitary wave is also found to be temperature dependent. At $T = 150K$, we observe a clear solitary wave which remains qualitatively unchanged upto $300K$. The velocity and amplitude of the soliton are found to be not varying with time. It was found that the energy of the soliton is larger than that of Davydov soliton which comes from its two exciton nature. Thus we conclude that there exists two exciton states in alpha helical proteins that can support solitons, the stability of which depends mainly on temperature.