Chapter 2

Propagation of proton solitons in one-dimensional hydrogen bonded chains
2.1 Introduction

There has recently been substantial interest in the study of possible collective proton motion in hydrogen bonded (HB) chains. The transport of energy and charge along one-dimensional HB chains is an extremely important problem in bioenergetic systems, such as bacteriorhodopsin, which pumps protons to higher free energies and the ATP synthase which consumes energetic protons [191]. In addition, it may be noted that proton transport has been implicated in transhydrogenase [192, 193], cytochrome oxidase and the bc1 redox loop in the mitochondrial respiratory chains [191, 194, 195]. Indeed, one requires proton transport for long distances along the membrane not just proton transport across the membrane. It is also possible to imagine that even more extensive networks of proton pathways exist in the cell, perhaps utilizing the cytosol microstructure [196, 197]. Thus, proton transport may be a part of other bioenergetic mechanisms such as muscle action [198] or flagellum motion [199, 200]. Bioenergy transport through proton dynamics in hydrogen bonded chains still remains an intriguing phenomenon to most of the physicists and biologists. A strong motivation for studying this problem is to understand the localization of energy along one-dimensional HB chains through protons. Most of the works that mention HB chains or proton channels assume that such channels will transport fast enough and efficiently enough for bioenergetic purposes [201]. Recently, extensive theoretical investigations [23, 202-205] and also some experimental evidence [206] predicted that soliton may give some answers to the fundamental question of the transmission of energy in biological macromolecules. The proton dynamics in HB chains is often modelled by a characteristic nonlinear substrate potential with two degenerate equilibrium positions. The formation of solitons ensure the transport of energy and charges in bioenergetics: e.g. mitochondrial adenosine triphosphate formation [25], photophosphorylation in chloroplast [29], anaerobic metabolism in halobacterium [30], and proton migration in ice crystals [60] and provide an explanation of some biological processes, e.g. the duplication of deoxyribonucleic acid (DNA) and the transcription of messenger ribonucleic acid (mRNA) [207],

the denaturation of DNA [208], and the elucidation of the molecular mechanism of muscle contraction [209]. As a consequence, the detailed understanding of charge transfer mechanism of HB chains finds a great thrust on localization of bioenergy in HB chains.

In the next section, we present our model with a short HB chain with nearest neighbour interactions of heavy ions in an external electric field. In this model, we consider the proton motions in the chain and derive the quasi-classical discrete nonlinear equation of motion to reveal the dynamics of protons in HB chains.

2.2 Mathematical background of proton dynamical model

We consider an idealized periodic HB chain consisting of two interacting sublattices of harmonically coupled protons. The proton motion is known to be responsible for the energy and charge transfer in many HB chains. The conduction via proton migration along the chain in HB systems appears as follows:

\[(\text{H-O-H})^* \cdots \text{O-H} \cdots \text{O-H} \cdots \text{O-H},\]

where (·) and (· · ·) stand for the covalent and the hydrogen bond respectively. The hydrogen bond bridges the system in many repetitions of the unit cell O-H···, and the system is usually considered to be a uni-dimensional macroscopic chain. Here the H\(^+\) travels from one side of the chain to another by subsequent jumps of protons from one oxygen to another and finally the system gets to

\[\text{H-O} \cdots \text{H-O} \cdots \text{H-O} \cdots (\text{H-O-H})^*.\]

By the earlier work of Tokunaga and Matsubara [210], the Hamiltonian for
the protons in one-dimensional H-bonded system in the presence of an electric field can be written in terms of spin operators as follows:

\[ H = -2\alpha - \sum_{n} S_n^x - \frac{1}{2} J_1 \sum_{n} S_n^z S_{n-1}^z + S_n^z S_{n+1}^z - \frac{1}{2} J_2 \sum_{n} S_n^x S_{n-1}^x + S_n^x S_{n+1}^x - V S_n^z. \quad (2.1) \]

Eq. (2.1) is written based on the idea of quasi-spin in hydrogen-bonded systems. One half spin is corresponding to the two possible positions of proton in the double well potential along the O-O bond (hydrogen bond). This potential is a consequence of interaction of two negative ions of oxygen or some heavy ions. Discrete changes of proton position correspond to the two projections of spin=\( \frac{1}{2} \) as represented by Fig. (2.1).

Here \( S_n = [S_n^x, S_n^y, S_n^z] \), is the spin operator with spin magnitude \( S \) associated with the proton in \( n \)-th H-bond. Its \( x \)-component \( S_n^x \) represents the tunneling of \( n \)-th proton; \( S_n^y \) makes the \( n \)-th proton jump from one of the equilibrium position \( a \) to the other equilibrium position \( b \) and vice versa (ref. Fig. (2.2)).

\( S_n^z \) represents the polarization of \( n \)-th H-bond and the two possible directions of \( S_n^z \) correspond to the two possible positions of \( n \)-th proton. The first term in the right hand side of Eq. (2.1) represents the kinetic energy. The second term represents the interaction energy between neighbouring protons. The parameter \( J_1 \) represents the strength of the interaction between protons. The terms

![Figure 2.1: The two possible orientations of the pseudospin (S) which characterized the polarization vector of the H-bonded chain.](image-url)
Figure 2.2: Schematic representation of one-dimensional H-bonded systems

proportional to \( J_2 \) represent the longitudinal interactions between a pair of tunneling protons and \( V = qE_z \).

The dimensionless spin operator satisfies the commutation relations
\[
[S^z_n, S^z_m] = 2S^z \delta_{nm}, \quad [S^z_n, S^x_m] = \pm S^z \delta_{mn} \quad \text{with} \quad S_n S_n = S[S + 1],
\]
where \( S^\pm_n = S^x_n \pm iS^y_n \). For treating the problem semiclassically, we introduce Holstein-Primakoff transformation [155] for the spin operators in terms of the bosonic operators \( a^+_n, a_n \) which satisfy the usual Bose commutation relations. At sufficiently low temperature limit, the ground-state expectation value of \( a^+_n a_n \) is small compared to 2S and therefore we can use semi-classical expansions as

\[
S^+_n = 2 \left( 1 - \frac{\epsilon^2}{4} a^+_n a_n - \frac{\epsilon^4}{32} a^+_n a_n a^+_n a_n - O(\epsilon^6) \right),
\]

\[
S^-_n = 2 \epsilon a^+_n a_n - \frac{\epsilon^2}{4} a^+_n a_n a^+_n a_n - O(\epsilon^6),
\]

\[
S^z_n = 1 - \epsilon^2 a^+_n a_n \tag{2.2}
\]

where \( \epsilon = \frac{1}{8S} \) and using Eqs. (2.2), the dimensionless Hamiltonian of Eq. (2.1) can be written as a power series in \( \epsilon \), as

\[
H = - \sqrt{2\alpha} - \epsilon a^+_n a_n + \frac{\epsilon^3}{4} a^+_n a_n a^+_n a_n + \frac{\epsilon^5}{32} a^+_n a_n a^+_n a_n a^+_n a_n
\]

\[
+ \frac{1}{2} \mathbf{J}_1 - \frac{1}{2} \epsilon^2 (a^+_n a_{n-1} + a^+_n a_{n-1} a^+_n a_{n+1} + 2a^+_n a_n) + \epsilon^4
\]

\[
(\epsilon^2 a^+_n a_{n-1} a_{n-1} + a^+_n a_n a^+_n a_{n+1}) - \frac{1}{2} \mathbf{J}_2 - \frac{1}{2} \epsilon^2 a_n a_{n+1} + a^+_n a^+_{n+1} + a^+_n
\]
\[
\begin{align*}
& a_{n+1} + a_n^\dagger a_{n+1} + a_n a_{n-1} + a_n^\dagger a_{n-1} + a_n^\dagger a_n a_{n+1} - \frac{\epsilon^4}{4} [a_n^\dagger a_n a_n a_{n+1} + \\
& + a_n^\dagger a_n a_n a_{n+1} + a_n^\dagger a_n^\dagger a_n a_{n+1} + a_n^\dagger a_n a_n a_{n+1} + a_n^\dagger a_n^\dagger a_n a_{n+1} + a_n^\dagger a_n^\dagger a_n a_{n+1} + a_n^\dagger a_n^\dagger a_n a_{n+1}] \\
& a_{n-1} a_{n-1} + a_n^\dagger a_n a_{n-1} a_{n-1} - qE_z - \epsilon^2 a_n^\dagger a_n.
\end{align*}
\] (2.3)

The Hamiltonian of Eq. (2.3) characterizes the low-energy nonlinear property of hydrogen bonded chains in an oblique electric field. The dynamics of the spins can be expressed in terms of the Heisenberg equation of motion for the Bose operator \( a_n \),

\[
\frac{i\hbar}{\partial t} \frac{\partial u_n}{\partial t} = a_n, \quad H.
\] (2.4)

We then introduce the Glauber’s coherent-state representation (\( p \)-representation) [164] defined by the product of the multimode coherent states \( |u \rangle = \Pi_n |u(n) \rangle \), with \( \langle u \circ u \rangle = 1 \). Each component \( |u(n) \rangle \) is an eigenstate of the annihilation operator \( a_n \) i.e., \( a_n |u \rangle = u_n |u \rangle \), where \( u_n^\dagger (n) \rangle \) is the coherent-state eigenvector for the operator \( a_n^\dagger \) and \( u_n \) is the coherent amplitude in this representation. Since coherent states are normalized and overcompleted, the field operators sandwiched by \( |u(n) \rangle \) can be represented only with their diagonal elements. The \( p \)-representation of nonlinear equation reads

\[
\begin{align*}
& \frac{i}{\hbar} \frac{\partial u_n}{\partial t} = -\frac{\sqrt{2\hbar}}{\lambda} - \epsilon - \epsilon^3 n^2 + 2|u_n|^2 - \frac{\epsilon^5}{32} 2|u_n|^2 u_n^2 + 3|u_n|^4 - J_1 + \\
& - 2\epsilon^2 u_n + \epsilon^4 u_n |u_{n-1}|^2 + u_n |u_{n+1}|^2 - 2J_2 - \epsilon^2 u_{n+1} + u_{n-1} + \\
& + u_{n+1}^\dagger u_{n-1} - \frac{\epsilon^4}{4} 2|u_n|^2 + u_n^2 u_{n+1} + u_{n-1} + u_{n+1}^\dagger u_{n-1} + |u_{n-1}|^2 \\
& (u_{n-1} + u_{n-1}^\dagger) + |u_{n+1}|^2 (u_{n+1} + u_{n+1}^\dagger) + qE_z \epsilon^2 u_n.
\end{align*}
\] (2.5)

The above discrete equation contains various nonlinear couplings and they lead to different nonlinear phases which are represented by various types of
nonlinear excitations. Eq. (2.5) is difficult to solve due to its nonlinearity and discreteness. In the next section, through the Jacobian elliptic function method, we investigate a set of exact solutions for this model.

2.3 Exact soliton solutions of proton dynamics

Seeking exact soliton solutions to nonlinear partial differential equations (Pde's) which describes many complex systems in the field of condensed matter systems, plasma physics, astrophysics, biological systems etc., is one of the fundamental study of nonlinear science. The exact solutions of nonlinear partial differential equations help us to understand the mechanism of complicated phenomena of the natural systems. Nowadays, several powerful methods have been proposed to solve such nonlinear equations and to obtain exact solutions to the nonlinear partial differential equations. One can think of homogeneous balance method [211-213], the trial function method [214, 215], nonlinear transform method [216, 217], exp-function method [218] and inverse scattering method [219], the tangent hyperbolic function method [220-222], the Jacobian elliptic function method [223, 224] and so on. In order to study the dynamics of Eq. (2.5), we substitute the rotating wave approximation [119] to the discrete equation of motion and is given by,

$$u_n(t) = \frac{-\infty}{\infty} \phi_n(t)e^{-i\omega t}.$$  

(2.6)

Upon substitute the RWA to the discrete equation of motion, we get,

$$i\dot{\phi}_n + w_0\phi_n - 2J_1\epsilon^2 - \phi_n + J_1\epsilon^4 - \left(2|\phi_{n-1}|^2\phi_n + \phi_n^2\phi_n^* + 2|\phi_{n+1}|^2\phi_n^*\right)$$

$$+ \phi_n^2\phi_{n+1}^* + 2J_2\epsilon^2 - \phi_{n+1} + \phi_{n-1} - J_2\frac{\epsilon^4}{2} - \left(4|\phi_n|^2\phi_{n+1}^* + 4|\phi_n|^2\phi_{n-1}\right)$$

$$+ 2\phi_n^2\phi_{n+1}^* + 2\phi_n^2\phi_{n-1}^* + 3|\phi_{n-1}|^2\phi_{n-1}^* + 3|\phi_{n+1}|^2\phi_{n+1}^* + 2|\phi_n|^2\phi_{n-1}^*$$

$$+ 2|\phi_n|^2\phi_{n+1}^* + \phi_n^2(\phi_{n+1}^* + \phi_{n-1}^*) - qE_2\epsilon^2\phi_n = 0.$$  

(2.7)
In addition, to obtain some exact soliton solutions of equation (2.7), we use the Jacobian elliptic function method. First, we make the transformations

\[
\phi_n = e^{i\theta_n}(\xi_n), \quad \theta_n = p_n + \omega t + \zeta_n, \quad \xi_n = kn + ct + \chi,
\]

which replacing \( \phi_n \) in Eq. (2.7), and separating the real from the imaginary part we get the following set of equations:

\[
\begin{align*}
-\omega \psi_n + \omega_0 \psi_n - 2J1\epsilon^2 \psi_n + J_1 \epsilon^4 \cdot 2\psi_n(\psi_n^2 + \psi_{n+1}^2) &+ \psi_n(\psi_{n-1}^2 + \psi_{n+1}^2) \cos 2p - 2J_2 \epsilon^2 (\psi_{n+1} + \psi_{n-1}) \cos p - J_2 \epsilon^4 \cdot 4\psi_n^2(\psi_{n+1} + \psi_{n-1}) \cos p \\
+ 2\psi_n^2(\psi_{n+1} + \psi_{n-1}) \cos p + 3(\psi_{n-1}^3 + \psi_{n+1}^3) \cos p + 2\psi_n^2(\psi_{n+1} + \psi_{n+1}) \cos p &- Q \epsilon^2 \psi_n = 0, \\
&\quad (2.9)
\end{align*}
\]

\[
\begin{align*}
\psi_n + J_1 \epsilon^4 \cdot \psi_n(\psi_n^2 + \psi_{n+1}^2) \sin 2p &+ 2J_2 \epsilon^2 (\psi_{n+1} + \psi_{n-1}) \sin p - J_2 \epsilon^4 \\
&\quad \cdot 4\psi_n^2(\psi_{n+1} - \psi_{n-1}) \sin p + 2\psi_n^2(\psi_{n+1} - \psi_{n-1}) \sin p + 3(\psi_{n-1}^3 + \psi_{n+1}^3) \sin p \\
&\quad + 2\psi_n^2(\psi_{n+1} - \psi_{n-1}) \sin p + \psi_n^2(\psi_{n-1} - \psi_{n+1}) \sin p = 0. \\
&\quad (2.10)
\end{align*}
\]

With the properties of the Jacobian elliptic function [225], it is possible to expand and balance the linear term of the highest order with the highest nonlinear terms in Eqs. (2.9) and (2.10), i.e.

\[
\begin{align*}
\psi_n(\xi_n) &= a_0 + a_1 \text{sn}(\xi_n), \\
\psi_{n+1}(\xi_n) &= a_0 + a_1 \frac{\text{sn}(\xi_n) \text{cn}(k) \text{dn}(k) + \text{sn}(\xi_n) \text{cn}(\xi_n) \text{dn}(\xi_n)}{1 - m^2 \text{sn}(\xi_n)^2 \text{sn}(k)^2}, \\
\psi_{n-1}(\xi_n) &= a_0 + a_1 \frac{\text{sn}(\xi_n) \text{cn}(k) \text{dn}(k) - \text{sn}(k) \text{cn}(\xi_n) \text{dn}(\xi_n)}{1 - m^2 \text{sn}(\xi_n)^2 \text{sn}(k)^2}. \\
&\quad (2.11)
\end{align*}
\]

Now, we substitute the above equations into Eqs. (2.9) and (2.10). This leads us to a set of algebraic equations with \( a_0, a_1, c \) and \( \omega \) to be determined,

\[
\text{sn}(\xi_n)^6: a_1 \cdot 3J_2 \epsilon^4 \text{sn}(k) \text{cn}(\xi_n) \text{dn}(\xi_n) \sin p a_0^3 m^2 \text{sn}(k)^4 + c \text{cn}(\xi_n) \text{dn}(\xi_n)
\]
\( m^6 \text{sn}(k)^6 = 0, \)
\[
\text{sn}(\xi_n)^5 : a_1 e^4 \text{sn}(k) \text{cn}(\xi_n) \text{dn}(\xi_n) \sin \, p a_0 a_1 m^4 \text{sn}(k)^4 - 4 J_1 \epsilon^4 \text{sn}(k) \\
\text{cn}(\xi_n) \sin(2p) a_0 a_1 m^4 \text{sn}(k)^4 = 0, \\
\text{sn}(\xi_n)^4 : a_1 e^4 - 3 c \text{cn}(\xi_n) \text{dn}(\xi_n) m^4 \text{sn}(k)^4 - 4 J_2 \epsilon^2 \text{sn}(k) \text{cn}(\xi_n) \text{dn}(\xi_n) \sin(2p) m^4 \\
\text{sn}(k)^4 - 4 J_1 \epsilon^4 \text{sn}(k) \text{cn}(\xi_n) \text{dn}(\xi_n) \sin(2p) a_0^2 m^4 \text{sn}(k)^4 + 12 J_2 \epsilon^4 \text{sn}(k) \\
\text{cn}(\xi_n) \text{dn}(\xi_n) \sin(2p) a_0^2 m^4 \text{sn}(k)^4 - 6 J_2 \epsilon^4 \text{sn}(k) \text{cn}(\xi_n) \text{dn}(\xi_n) \sin(2p) a_0^2 m^2 \\
\text{sn}(k)^2 + 4 J_1 \epsilon^4 \text{sn}(k) \text{cn}(\xi_n) \text{dn}(\xi_n) \sin(2p) a_0^2 \text{cn}(k) \text{dn}(k) m^2 \text{sn}(k)^2 = 0, \\
\text{sn}(\xi_n)^3 : a_1 e^4 - 18 J_2 \epsilon^4 \text{sn}(k) \text{cn}(\xi_n) \text{dn}(\xi_n) \sin \, p a_0 m^2 \text{sn}(k)^2 a_1 \text{cn}(k) \text{dn}(k) - 12 J_2 \\
\epsilon^4 \text{sn}(k) \text{cn}(\xi_n) \text{dn}(\xi_n) \sin \, p a_0 a_1 m^2 \text{sn}(k)^2 + 4 J_1 \epsilon^4 \text{sn}(k) \text{cn}(\xi_n) \text{dn}(\xi_n) \\
\sin \, 2p a_0 m^2 \text{sn}(k)^2 a_1 \text{cn}(k) \text{dn}(k) + 8 J_1 \epsilon^4 \text{sn}(k) \text{cn}(\xi_n) \text{dn}(\xi_n) \sin \, 2p a_0 \\
a_1 m^2 \text{sn}(k)^2 = 0, \\
\text{sn}(\xi_n)^2 : a_1 e^4 \text{sn}(k) \text{cn}(\xi_n) \text{dn}(\xi_n) \sin \, p a_0 a_1 m^2 \text{sn}(k)^2 \text{dn}(k)^2 + 8 J_2 \epsilon^4 \text{sn}(k) \text{cn}(\xi_n) \\
\text{dn}(\xi_n) \sin \, p m^2 \text{sn}(k)^2 + 3 J_2 \epsilon^4 \text{sn}(k) \text{cn}(\xi_n) \text{dn}(\xi_n) \sin \, p a_1 + 3 c \text{cn}(\xi_n) \\
\text{dn}(\xi_n) m^2 \text{sn}(k)^2 + 8 \epsilon^4 \text{sn}(k) \text{cn}(\xi_n) \text{dn}(\xi_n) \sin \, 2p a_0 m^2 \text{sn}(k)^2 - 4 J_1 \epsilon^4 \\
\text{sn}(k) \text{cn}(\xi_n) \text{dn}(\xi_n) \sin \, 2p a_0^2 \text{cn}(k) \text{dn}(k) - 24 J_2 \epsilon^4 \text{sn}(k) \text{cn}(\xi_n) \text{dn}(\xi_n) \\
\sin \, 2p a_0^2 m^2 \text{sn}(k)^2 = 0, \\
\text{sn}(\xi_n)^1 : a_1 e^4 \text{sn}(k) \text{cn}(\xi_n) \text{dn}(\xi_n) \sin \, p a_0 a_1 \text{cn}(k) \text{dn}(k) - 18 J_2 \epsilon^4 \text{sn}(k) \text{cn}(\xi_n) \text{dn}(\xi_n) \sin \, p \\
a_0 a_1 \text{cn}(k) \text{dn}(k) - 4 J_1 \epsilon^4 \text{sn}(k) \text{cn}(\xi_n) \text{dn}(\xi_n) \sin \, 2p a_0 a_1 \text{cn}(k) \text{dn}(k) = 0, \\
\text{sn}(\xi_n)^0 : a_1 e^4 - 4 J_2 \epsilon^2 \text{sn}(k) \text{cn}(\xi_n) \text{dn}(\xi_n) \sin \, p + 12 J_2 \epsilon^4 \text{sn}(k) \text{cn}(\xi_n) \text{dn}(\xi_n) \sin \, p a_0^2 \\
+ 3 J_2 \epsilon^4 \text{sn}(k)^3 \text{cn}(\xi_n)^3 \text{dn}(\xi_n)^3 \sin \, p a_1 - 4 J_1 \epsilon^4 \text{sn}(k) \text{cn}(\xi_n) \text{dn}(\xi_n) \sin \, 2p a_0^2 \\
- \text{ccn}(\xi_n) \text{dn}(\xi_n) = 0. \tag{2.12}
\]

\[
\text{sn}(\xi_n)^8 : -9 J_2 \epsilon^4 a_0^2 \cos(p) a_0 m^6 \text{sn}(k)^6 = 0, \\
\text{sn}(\xi_n)^7 : 18 J_2 \epsilon^4 \cos(p) a_0^2 a_1 m^6 \text{sn}(k)^6 + 9 J_2 \epsilon^4 \cos(p) a_1^3 \text{cn}(k) \text{dn}(k) m^4 \\
\text{sn}(k)^4 + 2 J_1 \epsilon^4 a_1 \cos(2p) a_0^2 m^6 \text{sn}(k)^6 - \omega a_1 m^6 \text{sn}(k)^6 + 4 J_1 \epsilon^4 a_0^2 a_1
\]
\[ m^6 \text{sn}(k)^6 - 2J_1 \epsilon^2 a_1 m^6 \text{sn}(k)^6 - q E_Z \epsilon^2 a_1 m^6 \text{sn}(k)^6 + \omega_0 a_1 m^6 \text{sn}(k)^6 = 0, \]

\[ \text{sn}(\xi_n)^6 : 2J_1 \epsilon^4 \cos(2p) a_0^3 m^6 \text{sn}(k)^6 + 4J_2 \epsilon^2 \cos(p) a_0 m^6 \text{sn}(k)^6 - q E_Z \epsilon^2 \]

\[ a_0 m^6 \text{sn}(k)^6 - 4J_1 \epsilon^4 a_1^2 \cos(2p) a_0 m^6 \text{cn}(k) \text{dn}(k) + \omega_0 a_0 m^6 \text{sn}(k)^6 - 2J_1 \epsilon^2 a_0 m^6 \text{sn}(k)^6 - \omega a_0 m^6 \text{sn}(k)^6 - 12J_2 \epsilon^4 \cos(p) a_0^3 m^6 \]

\[ \text{sn}(k)^6 + 27J_2 \epsilon^4 \cos(p) a_0^2 a_0 m^4 \text{sn}(k)^4 + 18J_2 \epsilon^4 \cos(p) a_0 a_1^2 \text{cn}(k) \text{dn}(k)^4 \text{sn}(k)^4 + 4J_1 \epsilon^4 a_0^3 m^6 \text{sn}(k)^6 - 8J_1 \epsilon^4 a_0 a_1^2 \text{cn}(k) \text{dn}(k) m^4 \]

\[ \text{sn}(k)^4 = 0, \]

\[ \text{sn}(\xi_n)^5 : -4J_1 \epsilon^4 \cos(2p) a_0^2 m^4 \text{sn}(k)^4 a_1 \text{cn}(k) \text{dn}(k) + 3q E_Z \epsilon^2 a_1 m^4 \text{sn}(k)^4 \]

\[ - 4J_2 \epsilon^2 \cos(p) a_1 \text{cn}(k) \text{dn}(k) m^4 \text{sn}(k)^4 - 18J_2 \epsilon^4 \cos(p) a_0^3 \text{cn}(k) \text{dn}(k) m^2 \text{sn}(k)^2 - 8J_1 \epsilon^4 a_0^2 m^4 \text{sn}(k)^4 a_1 \text{cn}(k) \text{dn}(k) + 2J_1 \epsilon^4 a_1^3 \cos(2p) \text{cn}(k) \text{dn}(k)^2 m^2 \text{sn}(k)^2 - 12J_1 \epsilon^4 a_0 a_1 m^4 \text{sn}(k)^4 + 54J_2 \epsilon^4 \cos(p) a_0^2 a_1 m^4 \text{sn}(k)^4 + 6J_1 \epsilon^2 a_1 m^4 \text{sn}(k)^4 - 3\omega_0 a_1 m^4 \text{sn}(k)^4 + 6J_1 \epsilon^4 a_1 \cos(2p) a_0^2 m \text{sn}(k)^4 + 18J_2 \epsilon^4 \cos(p) a_0^2 m^4 \text{sn}(k)^4 a_1 \text{cn}(k) \text{dn}(k) = 0, \]

\[ \text{sn}(\xi_n)^4 : 16J_1 \epsilon^4 a_0 a_1^2 \text{cn}(k) \text{dn}(k) m^2 \text{sn}(k)^2 + 2J_1 \epsilon^4 a_0 \cos(2p) a_1^2 \text{cn}(k)^2 \]

\[ \text{dn}(k)^2 m^2 \text{sn}(k)^4 + 4J_1 \epsilon^4 a_0 m^2 \text{sn}(k)^2 a_1^2 \text{cn}(k)^2 \text{dn}(k)^2 + 3\omega a_0 m^4 \text{sn}(k)^4 + 3q E_Z \epsilon^2 a_0 m^4 \text{sn}(k)^4 - 3\omega_0 a_0 m^4 \text{sn}(k)^4 - 36J_2 \epsilon^4 \cos(p) a_0 a_1^2 \text{cn}(k) \text{dn}(k) m^2 \text{sn}(k)^2 - 12J_2 \epsilon^2 \cos(p) a_0 m^4 \text{sn}(k)^4 - 12J_1 \epsilon^4 a_0^3 \text{m}^4 \text{sn}(k)^4 + 8J_1 \epsilon^4 a_0^2 \cos(2p) a_0 m^2 \text{sn}(k)^2 \text{cn}(k) \text{dn}(k) + 6J_1 \epsilon^2 a_0^2 m^4 \text{sn}(k)^4 - 27J_2 \epsilon^4 \cos(p) a_0^2 a_1^2 \text{sn}(k)^2 + 36J_2 \epsilon^4 \cos(p) a_0^2 m^4 \text{sn}(k)^4 + 9J_2 \epsilon^4 \cos(p) a_0^2 m^2 \text{sn}(k)^2 a_1^2 \text{cn}(k)^2 \text{dn}(k)^2 - 6J_1 \epsilon^4 \cos(2p) a_0^2 m^4 \text{sn}(k)^4 = 0, \]

\[ \text{sn}(\xi_n)^3 : 3J_2 \epsilon^4 \cos(p) a_0^3 \text{cn}(k)^3 \text{dn}(k)^3 - 2J_1 \epsilon^4 a_1^3 \cos(2p) a_0^2 \text{cn}(k)^2 \text{dn}(k)^2 \]

\[ + 12J_1 \epsilon^4 a_0^2 a_1 m^2 \text{sn}(k)^2 - 3\omega a_1 m^2 \text{sn}(k)^2 - 6J_1 \epsilon^2 a_1 m^2 \text{sn}(k)^2 - 4J_1 \epsilon^4 a_1^2 \text{cn}(k)^2 \text{dn}(k)^2 + 8J_2 \epsilon^2 \cos(p) a_1 \text{cn}(k) \text{dn}(k) m^2 \text{sn}(k)^2 + 6J_1 \epsilon^4 \]
\[ a_1 \cos(2p) a_0^2 m^2 \text{sn}(k)^2 + 9 J_2 \epsilon^4 \cos(p) a_1^3 \text{cn}(k) \text{dn}(k) + 4 J_1 \epsilon^4 a_1^3 \text{sn}(k)^2 \]
\[ \text{cn}(\xi_n) \text{dn}(\xi_n) m^2 \text{sn}(k)^2 - 54 J_2 \epsilon^4 \cos(p) a_0^2 \text{m}^2 \text{sn}(k)^2 + 2 J_1 \epsilon^4 a_1^3 \]
\[ \cos(2p) \text{sn}(k)^2 \text{cn}(\xi_n)^2 \text{dn}(\xi_n)^2 \text{m}^2 \text{sn}(k)^2 + 3 \omega_0 a_1^2 \text{m}^2 \text{sn}(k)^2 + 8 J_1 \epsilon^4 \cos(2p) a_0^3 \text{m}^2 \text{sn}(k)^2 a_1 \text{cn}(k) \]
\[ \text{dn}(k) - 36 J_2 \epsilon^4 \cos(p) a_0^2 m^2 \text{sn}(k)^2 a_1 \text{cn}(k) \text{dn}(k) - 3 q E_Z \epsilon^2 a_1 m^2 \text{sn}(k)^2 = 0, \]
\[ \text{sn}(\xi_n) = 9 J_2 \epsilon^4 \cos(p) a_0^2 a_0 + 3 \omega_0 a_0 m^2 \text{sn}(k)^2 - 4 J_1 \epsilon^4 a_0 a_1^2 \text{cn}(k)^2 \text{dn}(k)^2 \]
\[ - 3 q E_Z \epsilon^2 a_0 m^2 \text{sn}(k)^2 - 9 J_2 \epsilon^4 \cos(p) a_0 m^2 \text{sn}(k)^2 a_1^2 \text{sn}(k)^2 \text{cn}(\xi_n)^2 \]
\[ \text{dn}(\xi_n) - 2 J_1 \epsilon^4 a_0 \cos(2p) a_1^2 \text{cn}(k)^2 \text{dn}(k)^2 - 36 J_2 \epsilon^4 \cos(p) a_0 a_1^2 m^2 \text{sn}(k)^2 \]
\[ + 12 J_2 \epsilon^4 \cos(p) a_0 m^2 \text{sn}(k)^2 + 2 J_1 \epsilon^4 a_0 \cos(2p) a_1^2 \text{sn}(k)^2 \text{cn}(\xi_n)^2 \text{dn}(\xi_n)^2 \text{m}^2 \text{sn}(k)^2 + 9 J_2 \epsilon^4 \cos(p) a_0 a_1^2 \text{cn}(k)^2 \text{dn}(k)^2 + 18 J_2 \epsilon^4 \cos(p) a_0 a_1^2 \text{cn}(k) \]
\[ \text{dn}(k) + 6 J_1 \epsilon^4 \cos(2p) a_0 a_1^2 \text{sn}(k)^2 - 8 J_1 \epsilon^4 a_0 a_1 \text{cn}(k) \text{dn}(k) + 12 J_1 \epsilon^4 a_0^3 \]
\[ \text{m}^2 \text{sn}(k)^2 - 6 J_1 \epsilon^4 a_0 m^2 \text{sn}(k)^2 + 4 J_1 \epsilon^4 a_0 m^2 \text{sn}(k)^2 a_1 \text{sn}(k)^2 \text{cn}(\xi_n)^2 \]
\[ \text{dn}(\xi_n)^2 - 2 J_1 \epsilon^4 a_1 \cos(2p) a_0^2 - 2 J_1 \epsilon^4 a_1^3 \cos(2p) \text{sn}(k)^2 \text{cn}(\xi_n)^2 \]
\[ \text{dn}(\xi_n)^2 - 4 J_1 \epsilon^4 a_1 \text{cn}(k) \text{dn}(k) - 3 \omega_0 m^2 \text{sn}(k)^2 = 0, \]
\[ \text{sn}(\xi_n)^1 = -8 J_1 \epsilon^4 a_0^2 a_1 \text{cn}(k) \text{dn}(k) + \omega_1 + 2 J_1 \epsilon^2 a_1 - 4 J_1 \epsilon^4 \cos(2p) a_0^2 a_1 \text{cn}(k) \]
\[ \text{dn}(k) + 18 J_2 \epsilon^4 \cos(p) a_0^2 a_1 \text{cn}(k) \text{dn}(k) - 4 J_1 \epsilon^4 a_0^3 \text{sn}(k)^2 \text{cn}(\xi_n)^2 \]
\[ \text{dn}(\xi_n)^2 - 4 J_1 \epsilon^4 a_0^2 a_1 + q E_Z \epsilon^2 a_1 + 18 J_2 \epsilon^4 \cos(p) a_0^2 a_1 + 9 J_2 \epsilon^4 \cos(p) a_1^3 \]
\[ \text{cn}(k) \text{dn}(k) \text{sn}(k)^2 \text{cn}(\xi_n)^2 \text{dn}(\xi_n)^2 - 4 J_2 \epsilon^2 \cos(p) a_1 \text{cn}(k) \text{dn}(k) \]
\[ - 2 J_1 \epsilon^4 a_1 \cos(2p) a_0^2 - 2 J_1 \epsilon^4 a_1^3 \cos(2p) \text{sn}(k)^2 \text{cn}(\xi_n)^2 \]
\[ \text{dn}(\xi_n)^2 - \omega_0 a_1 = 0, \]
\[ \text{sn}(\xi_n)^0 = 2 J_1 \epsilon^4 a_0 \cos(2p) a_1 \text{sn}(k)^2 \text{cn}(\xi_n)^2 \text{dn}(\xi_n)^2 - 2 J_1 \epsilon^4 \cos(2p) a_0^3 \]
\[ - 4 J_2 \epsilon^2 \cos(p) a_0 + 12 J_2 \epsilon^4 \cos(p) a_0^3 + q E_Z \epsilon^2 a_0 - 4 J_1 \epsilon^4 a_0 a_1^2 \text{sn}(k)^2 \]
\[ \text{cn}(\xi_n)^2 \text{dn}(\xi_n)^2 + \omega_0 - \omega_0 a_0 + 9 J_2 \epsilon^4 \cos(p) a_0 a_1^2 \text{sn}(k)^2 \text{cn}(\xi_n)^2 \]
\[ \text{dn}(\xi_n)^2 + 2 J_1 \epsilon^2 a_0 - 4 J_1 \epsilon^4 a_0^3 = 0. \]
After a lengthy algebraic calculations, the following solutions of Eq. (2.7):

\[
\begin{align*}
a_0 &= a_0, \ a_1 = a_1, \ c = -\frac{3J_2 \epsilon^4 \text{sn}(k) \ \text{dn}(\xi_n) \ \text{sin}(p) a_1^2}{m^2 \text{sn}(k)^2}, \\
\omega &= -\frac{1}{m^2 \text{sn}(k)^2} 3J_2 \epsilon^2 \cos p \ 6e^2 a_0^2 m^2 \text{sn}(k)^2 - 3a_0^2 \text{cn}(k) \text{dn}(k) + 2J_1 \epsilon^2 m^2 \text{sn}(k)^2 \\
&\quad - 2\epsilon^2 a_0^2 \cos(p)^2 + (1 - \epsilon^2 a_0^2) + m^2 \text{sn}(k)^2 qE_z \epsilon^2 - \omega_0.
\end{align*}
\]  

(2.14)

and hence the function \( \psi_n \) and \( \phi_n \) becomes

\[
\begin{align*}
\psi_n &= a_0 + a_1 \times \text{sn} \cdot k \cdot n - \frac{3J_2 \epsilon^4 \text{sn}(k) \ \text{dn}(\xi_n) \ \text{sin}(p) a_1^2}{m^2 \text{sn}(k)^2} \cdot t + \chi, \\
\phi_n &= a_0 + a_1 \times \text{sn} \cdot k \cdot n - \frac{3J_2 \epsilon^4 \text{sn}(k) \ \text{dn}(\xi_n) \ \text{sin}(p) a_1^2}{m^2 \text{sn}(k)^2} \cdot t + \chi \times \exp i \cdot p \cdot n \\
&\quad + -\frac{1}{m^2 \text{sn}(k)^2} 3J_2 \epsilon^2 \cos p \ 6e^2 a_0^2 m^2 \text{sn}(k)^2 - 3a_0^2 \text{cn}(k) \text{dn}(k) + 2J_1 \epsilon^2 m^2 \\
&\quad \text{sn}(k)^2 - 2\epsilon^2 a_0^2 \cos(p)^2 + (1 - \epsilon^2 a_0^2) + m^2 \text{sn}(k)^2 qE_z \epsilon^2 - \omega_0 \cdot t + \zeta.
\end{align*}
\]  

(2.16)

The general solution of equation Eq. (2.5) gives the dynamics of protons in HB chain, i.e., \( u_n(t) \) takes the form

\[
\begin{align*}
u_n(t) &= a_0 + a_1 \times \text{sn} \cdot k \cdot n - \frac{3J_2 \epsilon^4 \text{sn}(k) \ \text{dn}(\xi_n) \ \text{sin}(p) a_1^2}{m^2 \text{sn}(k)^2} \cdot t + \chi \times \exp i \cdot p \cdot n \\
&\quad + -\frac{1}{m^2 \text{sn}(k)^2} 3J_2 \epsilon^2 \cos p \ 6e^2 a_0^2 m^2 \text{sn}(k)^2 - 3a_0^2 \text{cn}(k) \text{dn}(k) + 2J_1 \epsilon^2 m^2 \\
&\quad \text{sn}(k)^2 - 2\epsilon^2 a_0^2 \cos(p)^2 + (1 - \epsilon^2 a_0^2) + m^2 \text{sn}(k)^2 qE_z \epsilon^2 - \omega_0 \\
&\quad - \omega_0 \cdot t + \zeta.
\end{align*}
\]  

(2.17)
The graphical representation of Fig. (2.3) for the above exact solution presents the profiles of periodically propagating solitons for various values of $J_2$ with the modulus of the Jacobian elliptic functions $m = 1$. As the value of $J_2$ increases the evolution of solitonic profile emerges with minimum amplitude which can be seen through the snapshots of Fig. (2.3). Furthermore, the propagation of proton soliton suffers with damping at its hump, but preserving the periodic pattern of the profiles.

### 2.4 Perturbed Soliton excitations

Short hydrogen-bonded chains are important elements of the proton channel in proton conducting membranes and have a great polarizability that can fluctuate between two opposite directions [226]. In a short hydrogen bonded chain, the spins can coherently interact between several directions of the minimum anisotropy energy. This remarkable evidence enables us to investigate the nature of proton conduction under this perturbative environment. To illustrate the feasibility of such interactions we make use of the anisotropic interactions [227] and after the inclusion, the Eq. (2.5) becomes,

$$
\frac{\partial u_n}{\partial t} = -\sqrt{2\lambda} \epsilon - \frac{\epsilon^3}{4} u_n^2 + 2|u_n|^2 - \frac{\epsilon^5}{32} 2|u_n|^2u_n^2 + 3|u_n|^4 - J_1
$$

$$
-2\epsilon^2 u_n + \epsilon^4 u_n|u_{n-1}|^2 + u_n|u_{n+1}|^2 - 2J_2 - \epsilon^2 u_{n+1} + u_{n-1}
$$

$$
+ u_{n+1}^* u_{n-1}^* - \frac{\epsilon^4}{4} 2|u_n|^2 + u_n^2 u_{n+1} + u_{n-1} + u_{n+1}^* u_{n-1}^* + |u_{n-1}|^2
$$

$$
(u_{n-1} + u_{n-1}^*) + |u_{n+1}|^2(u_{n+1} + u_{n+1}^*) + qEz\epsilon^2 u_n - 2A\epsilon^4 |u_n|^2 u_n
$$

$$
-2A\epsilon^2 u_n - A' (12\epsilon^4 |u_n|^2 u_n - 4\epsilon^2 u_n - 12\epsilon^6 |u_n|^4 u_n).
$$

(2.18)

where, $A$, $A'$ are the anisotropic parameters corresponding to lower and higher orders respectively. However, it is difficult to solve Eq. (2.18) in its natural form because of it high nonlinearity and discreteness. Hence we take the continuum limit which is a valid approximation in the low temperature and long
wavelength limit. For this, we define $u_n(t)$ as $u(x, t)$, where $x = ny$ in which $\gamma$ is lattice parameter. We expand

$$u_{n\pm 1} = u(x, t) \pm \gamma u_x + \frac{\gamma^2}{2!} u_{xx} \pm \frac{\gamma^3}{3!} u_{xxx} + \frac{\gamma^4}{4!} u_{xxxx} \pm O(\gamma^5).$$ (2.19)

Using this in Eq. (2.18) and rescaling $x$ and $t$ as $x \to \frac{1}{j_1} x$ and $t \to \frac{1}{j_1} t$ respectively, the continuum equation of motion at $O(\gamma^4)$ when $\epsilon = \gamma$ can be written as,

$$iu_t + u_{xx} + 2|u|^2 u + \lambda_1 |u|^2 u + \lambda_2 |u|^2 u_{xx} = 0.$$ (2.20)

Here the suffixes $t$ and $x$ represent partial derivatives with respect to $t$ and $x$ respectively. Where,

$$\lambda = \frac{1}{J_1}, \delta_1 = \frac{2A + 12A'}{J_1}, \delta_2 = \frac{J_2}{2}.$$ (2.21)

Eq. (2.20) is a generalised form of NLS equation when $\lambda = 0$. Here we treat cubic NLS equation as the unperturbed part and rest as perturbation. We treat the terms proportional to $\lambda$ as weak perturbation by considering $\lambda$ as a perturbation parameter. Now we use multiple scale perturbation method [166] to find the perturbed soliton to Eq. (2.20). When $\lambda = 0$, Eq. (2.20) reduces to the completely integrable cubic NLS equation which admits the envelope one-soliton solution in the form

$$u = \eta \sech \eta(\theta - \theta_0) \exp i \xi(\theta - \theta_0) + i(\sigma - \sigma_0),$$ (2.22)

where $\theta_t = -2\xi, \theta_x = 1, \sigma_t = \eta^2 + \xi^2$ and $\sigma_x = 0$. Now we assume the parameters $\xi, \eta, \theta_0$ and $\sigma_0$ are the functions of the long time scale $T = \lambda t$. The quasi stationary solution of Eq. (2.20) is assumed to take the form

$$u = \hat{u}(\theta, T; \lambda) \exp i \xi(\theta - \theta_0) + i(\sigma - \sigma_0),$$ (2.23)

we then expand $\hat{u}$ in terms of $\lambda$ as

$$\hat{u}(\theta, T; \lambda) = u_0(\theta, T) + \lambda \hat{u}_1(\theta, T) + \cdots,$$ (2.24)
The above assumption is appropriate for explicit calculations. Where \( u_0 = \eta \sech \eta (\theta - \theta_0) \) and making use of Eq. (2.23) in Eq. (2.20) at \( O(\lambda) \) we get,

\[
-\eta^2 \dot{u}_1 + \dot{u}_{198} + 4u_0^2 \dot{u}_1 + 2u_0^2 \dot{u}_1 = \hat{F}_1,
\]

where,

\[
\dot{F}_1 = i - u_{0T} - 2\delta_2 \xi_0^2 u_{08} - i u_0 \xi_T (\theta - \theta_0) - \xi \theta_{0T} - \sigma_{0T} - \delta_1 u_0^2 - \delta_2 (u_0 u_{08} - u_0^2 \xi^2).
\]

After substituting \( u_1 = \hat{\phi}_1 + i \hat{\psi}_1 \) in Eq. (2.25), where \( \hat{\phi}_1 \) and \( \hat{\psi}_1 \) are real functions we obtain

\[
L_1 \phi_1 = -\eta^2 \phi_1 + \phi_{198} + 6u_0^2 \phi_1,
\]

\[
L_2 \psi_1 = -\eta^2 \psi_1 + \psi_{198} + 2u_0^2 \psi_1.
\]

Where \( L_1 \) and \( L_2 \) are self-adjoint operators. As \( u_{08} \) and \( u_0 \) are the solutions of the homogeneous parts of Eqs. (2.26) and (2.27) for \( \hat{\phi}_1 \) and \( \hat{\psi}_1 \) respectively, the secularity conditions yield

\[
\int_{-\infty}^{+\infty} \dot{u}_{08} \Re \hat{F}_1 d\theta = 0,
\]

and

\[
\int_{-\infty}^{+\infty} \dot{u}_0 \Im \hat{F}_1 d\theta = 0,
\]

where,

\[
\Re \hat{F}_1 = u_0 \xi_T (\theta - \theta_0) - \xi \theta_{0T} - \sigma_{0T} - \delta_1 u_0^2 - \delta_2 (u_0 u_{08} - u_0^2 \xi^2),
\]

\[
\Im \hat{F}_1 = -u_{0T} - 2\delta_2 \xi_0^2 u_{08}.
\]

On explicitly evaluating the integrals of Eq. (2.28) and (2.29) respectively, we obtain the time evolution of the quantities \( \xi_T = 0 \) and \( \eta_T = 0 \). From this, we observed that the amplitude and velocity of the solution remain unchanged during the propagation of the soliton in HB chains. The perturbed soliton solution can be constructed by solving Eq. (2.26) for \( \hat{\phi}_1 \) and Eq. (2.27) for
\[ \hat{\psi}_1 \]. The homogeneous part of Eq. (2.26) admits the following two particular solutions,

\[
\phi_{11} = \text{sech} \, \eta(\theta - \theta_0) \, \tanh \, \eta(\theta - \theta_0),
\]

\[
\phi_{12} = \frac{3}{2\eta} \eta(\theta - \theta_0) \sech \eta(\theta - \theta_0) \tanh \eta(\theta - \theta_0) + \frac{1}{2\eta} \tanh \eta(\theta - \theta_0) \sinh \eta(\theta - \theta_0) - \frac{1}{\eta} \sech \eta(\theta - \theta_0).
\]

Knowing the two particular solutions, the general solution can be then obtained using the formula,

\[
\phi = c_1 \phi_{11} + c_2 \phi_{12} \equiv \phi_{11} \rightarrow -\infty \phi_{12} \rightarrow -\infty \text{Re}F_1d\theta' + \phi_{12} \rightarrow -\infty \phi_{11} \text{Re}F_1d\theta'.
\]

where \( c_1 \) and \( c_2 \) are the arbitrary constants. Using \( \phi_{11}, \phi_{12} \) and \( \text{Re}F_1 \) in Eq. (2.34) and after evaluating the integrals with lengthy algebra, we obtain

\[
\phi_{11} \rightarrow -\infty \left[ \phi_{12} \rightarrow \infty \text{Re}F_1d\theta' = \text{sech} \, \eta(\theta - \theta_0) \, \tanh \, \eta(\theta - \theta_0) \frac{3}{4\eta} (\xi \theta_{OT} + \sigma_{OT}) \right.
\]

\[
- \text{tanh} \, \eta(\theta - \theta_0) - \frac{1}{2} \eta(\theta - \theta_0) \sech^2 \eta(\theta - \theta_0) + 1 - \frac{5}{12} \delta_1 \eta + \frac{1}{4} \delta_2 \eta \xi^2
\]

\[
- \frac{31}{60} \delta_2 \eta^3 \tanh \eta(\theta - \theta_0) + \frac{1}{6} \eta \tanh^3 \eta(\theta - \theta_0)(-\delta_1 + \delta_2 \xi^2) + \eta(\theta - \theta_0) \sech^4 \eta(\theta - \theta_0) - \frac{3}{8} \delta_1 \eta + \frac{3}{8} \delta_2 \eta \xi^2 + \frac{5}{21} \delta_1 \eta + \frac{1}{8} \delta_2 \eta \xi^2 - \frac{8}{8} \delta_2 \eta^3
\]

\[
\text{tanh} \, \eta(\theta - \theta_0) \sech^2 \eta(\theta - \theta_0) + \tanh^3 \eta(\theta - \theta_0) \sech^2 \eta(\theta - \theta_0) - \frac{1}{15} \delta_2 \eta \xi^2
\]

\[
+ \frac{1}{3} \delta_2 \eta^3 \cosh 2 \eta(\theta - \theta_0) + \frac{8}{15} \delta_2 \eta^3 - 8 \delta_2 \eta \xi^2 - \frac{1}{10} \delta_2 \eta^3 \tanh \eta(\theta - \theta_0) \sech^4 \eta(\theta - \theta_0) \sech^6 \eta(\theta - \theta_0) - \frac{1}{10} (\xi \theta_{OT} + \sigma_{OT}) \eta(\theta - \theta_0)
\]

\[
- \frac{1}{10} \delta_2 \eta^3 \tanh^5 \eta(\theta - \theta_0) + \frac{5}{12} \delta_1 \eta - \frac{37}{60} \delta_2 \eta^3 + \frac{5}{12} \eta \xi^2.
\]
and

\[
\phi_{12} = \phi_{11} \Re F_1 e^{i \Delta_1} = \frac{3}{2 \eta} \eta(\theta - \theta_0) \sech \eta(\theta - \theta_0) \tanh \eta(\theta - \theta_0) + \frac{1}{2 \eta} \tanh \eta(\theta - \theta_0) \sinh \eta(\theta - \theta_0) - \frac{1}{\eta} \sech \eta(\theta - \theta_0) \frac{1}{2} (\xi_{\theta_0} + \sigma_{\theta_0}) \sech^2 \eta(\theta - \theta_0) + \sech^4 \eta(\theta - \theta_0) \frac{\delta_1 \eta^2}{4} + \frac{\delta_2 \eta^4}{4} - \frac{\delta_2 \eta^2 \xi}{4} - \frac{\delta_2 \eta^4}{3} \sech^6 \eta(\theta - \theta_0). \tag{2.36}
\]

After simplification and making use of the boundary conditions,

\[
\phi_1(0)|_{\theta_0=0} = 0, \\
\phi_1(0)|_{\theta_0=0} = 0, \tag{2.37}
\]

we obtain \( c_1 \) and \( c_2 \) as

\[
c_1 = \frac{5}{12} \delta_2 \xi^2 + \frac{37}{60} \delta_2 \eta^3 + \frac{5}{12} \delta_1 \eta, \tag{2.38}
\]

\[
c_2 = \frac{1}{2} (\xi_{\theta_0} + \sigma_{\theta_0}) + \frac{\delta_1 \eta^2}{4} + \frac{7 \delta_2 \eta^4}{12} - \frac{\delta_2 \eta^2 \xi}{4}. \tag{2.39}
\]

Therefore \( \phi_1 \) reads as

\[
\phi_1 = \sech \eta(\theta - \theta_0) \tanh \eta(\theta - \theta_0) \frac{5}{12} \delta_2 \xi^2 + \frac{37}{60} \delta_2 \eta^3 + \frac{5}{12} \delta_1 \eta \\
+ \frac{3}{2} (\theta - \theta_0) \frac{1}{2} (\xi_{\theta_0} + \sigma_{\theta_0}) + \frac{\delta_1 \eta^2}{4} + \frac{7 \delta_2 \eta^4}{12} - \frac{\delta_2 \eta^2 \xi}{4} - \frac{3}{4 \eta} (\xi_{\theta_0} + \sigma_{\theta_0}) + 1 - \frac{5}{12} \delta_1 \eta \\
+ \frac{1}{4} \delta_2 \eta^3 - \frac{31}{60} \delta_2 \eta^3 \tanh \eta(\theta - \theta_0) - \frac{1}{6} \eta \tanh^3 \eta(\theta - \theta_0) (\delta_2 \xi^2 - \delta_1) \\
- \eta(\theta - \theta_0) \sech^4 \eta(\theta - \theta_0) \frac{3}{8} \delta_1 \eta + \frac{3}{8} \delta_2 \eta^3 - \frac{3}{8} \delta_2 \xi^2 \eta - \frac{5}{2} \delta_1 \eta + \frac{1}{8} \delta_2 \eta^2 \\
+ \frac{1}{8} \delta_2 \eta^3 \tanh \eta(\theta - \theta_0) \sech \eta(\theta - \theta_0) + \frac{1}{10} \delta_2 \eta^3 \tanh \eta(\theta - \theta_0) \\
\sech^4 \eta(\theta - \theta_0) + \frac{1}{2} \delta_2 \eta^3 \eta(\theta - \theta_0) \sech^6 \eta(\theta - \theta_0) + \frac{1}{2 \eta} (\xi_{\theta_0} + \sigma_{\theta_0})
\]
\[
\begin{align*}
\eta(\theta - \theta_0) + \frac{1}{10} \delta_2 \eta^3 \tanh^6 \eta(\theta - \theta_0) + \frac{5}{12} \delta_1 \eta + \frac{37}{60} \delta_2 \eta^3 - \frac{5}{12} \delta_2 \eta^2 \\
+ \frac{3}{2} (\theta - \theta_0) - \frac{1}{2} (\xi \theta_{ot} + \sigma_{ot}) \text{sech}^2 \eta(\theta - \theta_0) + \text{sech}^4 \eta(\theta - \theta_0) (\frac{\delta_1 \eta^2}{4} \\
+ \frac{\delta_2 \eta^4}{4} - \frac{\delta_2 \eta^2 \xi}{4}) - \frac{\delta_2 \eta^4}{3} \text{sech}^6 \eta(\theta - \theta_0) - \frac{1}{2 \eta} \tanh \eta(\theta - \theta_0) \\
\sinh \eta(\theta - \theta_0) - \frac{1}{\eta} \text{sech} \eta(\theta - \theta_0) - \frac{1}{2} (\xi \theta_{ot} + \sigma_{ot}) + \frac{\delta_1 \eta^2}{4} + \frac{7}{12} \delta_2 \eta^4 \\
- \frac{\delta_2 \eta^2 \xi^2}{4} + \frac{1}{2} (\xi \theta_{ot} + \sigma_{ot}) \text{sech}^2 \eta(\theta - \theta_0) + \text{sech}^4 \eta(\theta - \theta_0) (\frac{\delta_1 \eta^2}{4} + \frac{\delta_2 \eta^4}{4} \\
- \frac{\delta_2 \eta^2 \xi^2}{4} - \frac{\delta_2 \eta^4}{3} \text{sech}^6 \eta(\theta - \theta_0) .
\end{align*}
\]

(2.40)

In the similar way, \( \psi_1 \) can also be evaluated using the two particular solutions corresponding to the homogeneous part of Eq. (2.27) for \( \psi_1 \) which are of the form,

\[
\psi_{11} = \text{sech} \eta(\theta - \theta_0),
\]

(2.41)

\[
\psi_{12} = \frac{1}{2 \eta} \eta(\theta - \theta_0) \text{sech} \eta(\theta - \theta_0) + \sinh \eta(\theta - \theta_0).
\]

(2.42)

Knowing the two particular solutions, the general solution can then be obtained using the formula,

\[
\psi_1 = c_3 \hat{\psi}_{11} + c_4 \hat{\psi}_{12} - \hat{\psi}_{11} \int_{-\infty}^{\theta} \text{Im} \hat{f}_1 d\theta + \hat{\psi}_{12} \int_{-\infty}^{\theta} \text{Im} \hat{f}_1 d\theta,
\]

(2.43)

where \( c_3 \) and \( c_4 \) are the arbitrary constants. Using \( \psi_{11}, \psi_{12} \) and \( \text{Im} \hat{f}_1 \) in Eq. (2.43) and after evaluating the integrals with lengthy algebra, we get

\[
\begin{align*}
\hat{\psi}_{11} \int_{-\infty}^{\theta} \text{Im} \hat{f}_1 d\theta &= \frac{1}{4} (\theta - \theta_0) \tanh \eta(\theta - \theta_0) \text{sech} \eta(\theta - \theta_0) \\
- \frac{1}{4} (\theta - \theta_0) \eta(\theta - \theta_0) \text{sech}^3 \eta(\theta - \theta_0) + \frac{1}{2} (\theta - \theta_0) \eta(\theta - \theta_0) \\
\text{sech} \eta(\theta - \theta_0) - \frac{1}{2} (\theta - \theta_0) \tanh \eta(\theta - \theta_0) \text{sech} \eta(\theta - \theta_0) - \frac{1}{4} (\theta - \theta_0) \tanh \eta(\theta - \theta_0) \\
\text{sech} \eta(\theta - \theta_0) + \delta_2 \eta^2 + \frac{1}{6} \text{sech} \eta(\theta - \theta_0) \tanh \eta(\theta - \theta_0) - \frac{1}{4} \eta(\theta - \theta_0) \\
\text{sech}^5 \eta(\theta - \theta_0) + \frac{1}{12} \tanh \eta(\theta - \theta_0) \text{sech}^3 \eta(\theta - \theta_0) + \frac{1}{3} \tanh^3 \eta(\theta - \theta_0) \\
\text{sech} \eta(\theta - \theta_0) + \frac{1}{2} \text{sech} \eta(\theta - \theta_0) .
\end{align*}
\]

(2.44)
and

$$\hat{\psi}_{12} \overset{\theta}{\sim} \psi_{11} \text{Im} \int_{-\infty}^{\theta} d\theta = -\frac{1}{4} \eta(\theta - \theta_0) \sech^3 \eta(\theta - \theta_0) - \frac{1}{4} \eta^2 \eta \sech \eta(\theta - \theta_0) \sech \eta(\theta - \theta_0)$$

$$- \frac{1}{4} \delta \xi \eta^3(\theta - \theta_0) \sech \eta(\theta - \theta_0) - \frac{1}{4} \delta \xi \eta^2 \sech \eta(\theta - \theta_0)$$

By using the boundary conditions

$$\psi_1(0)|_{\theta_0=0} = 0,$$
$$\psi_{19}(0)|_{\theta_0=0} = 0,$$}

we can write the general solution for $\psi_1$ as

$$\psi_1 = \frac{1}{2} + \frac{1}{4} \eta(\theta - \theta_0) \sech \eta(\theta - \theta_0) + \frac{1}{4} \eta^2 \eta \sech \eta(\theta - \theta_0) + \frac{1}{4} \delta \xi \eta^3(\theta - \theta_0)$$

$$\frac{1}{2 \eta}[\eta(\theta - \theta_0) \sech \eta(\theta - \theta_0) + \eta \sech \eta(\theta - \theta_0)] - \frac{1}{4} \eta^2 \eta \sech \eta(\theta - \theta_0)$$

$$\tanh \eta(\theta - \theta_0) \sech \eta(\theta - \theta_0) - \frac{1}{2} \eta(\theta - \theta_0) \sech \eta(\theta - \theta_0) - \frac{1}{2} \eta^2 \eta \sech \eta(\theta - \theta_0)$$

$$\frac{1}{2 \eta}[\eta(\theta - \theta_0) \sech \eta(\theta - \theta_0) + \eta \sech \eta(\theta - \theta_0)] - \frac{1}{4} \eta^2 \eta \sech \eta(\theta - \theta_0)$$

$$\tanh \eta(\theta - \theta_0) - \frac{1}{4} \eta(\theta - \theta_0) \sech \eta(\theta - \theta_0) + \frac{1}{12} \tanh \eta(\theta - \theta_0)$$

$$\sech \eta(\theta - \theta_0) + \frac{1}{2} \sech \eta(\theta - \theta_0) \sech \eta(\theta - \theta_0) + \frac{1}{2} \sech \eta(\theta - \theta_0)$$

$$- \frac{1}{4} \eta(\theta - \theta_0) \sech \eta(\theta - \theta_0) \sech \eta(\theta - \theta_0) - \frac{1}{4} \eta^2 \eta \sech \eta(\theta - \theta_0)$$

$$\sech \eta(\theta - \theta_0) - \frac{1}{4} \delta \xi \eta^3(\theta - \theta_0) \sech \eta(\theta - \theta_0) - \frac{1}{4} \delta \xi \eta^2 \sech \eta(\theta - \theta_0)$$

$$\sech \eta(\theta - \theta_0),$$

with arbitrary constants,

$$c_3 = \frac{1}{2} + \frac{1}{4} \eta(\theta - \theta_0),$$

$$c_4 = \frac{1}{4} \eta(\theta - \theta_0) \sech \eta(\theta - \theta_0) - \frac{1}{4} \delta \xi \eta \sech \eta(\theta - \theta_0).$$
Having obtained the explicit form of $\xi$, $\eta$, $\hat{\phi}_1$ and $\hat{\psi}_1$, we can easily construct the perturbed soliton solution $\hat{u}_1$ through the relation $u_1 = \hat{\phi}_1 + i\hat{\psi}_1$. The solution for $\hat{u}_1$ is

\[
\hat{u}_1 = \text{sech} \eta(\theta - \theta_0) \tanh \eta(\theta - \theta_0) \cdot \frac{5}{12} \delta_2 \xi^2 + \frac{37}{60} \delta_2 \eta^3 + \frac{5}{12} \delta_1 \eta
\]

\[
+ \frac{3}{2} (\theta - \theta_0) \cdot \frac{1}{2} (\xi_{\theta \theta_0} + \sigma_{\theta \theta_0}) + \frac{\delta_1 \eta^2}{4} + \frac{7}{12} \delta_2 \eta^4 - \frac{\delta_2 \eta^2 \xi^2}{4} - \frac{3}{4 \eta} (\xi_{\theta \theta_0}
\]

\[
+ \sigma_{\theta \theta_0}) \cdot \tanh \eta(\theta - \theta_0) - \frac{1}{2} \eta(\theta - \theta_0) \text{sech}^2 \eta(\theta - \theta_0) + \frac{1}{12} \delta_1 \eta
\]

\[
+ \frac{1}{4} \delta_2 \eta^2 - \frac{31}{60} \delta_2 \eta^3 \cdot \tanh \eta(\theta - \theta_0) - \frac{1}{6} \eta \tanh^3 \eta(\theta - \theta_0)(\delta_2 \xi^2 - \delta_1)
\]

\[
- \eta(\theta - \theta_0) \text{sech}^4 \eta(\theta - \theta_0) \cdot \frac{3}{8} \delta_1 \eta + \frac{3}{8} \delta_2 \eta^3 - \frac{3}{8} \delta_2 \xi^2 \cdot - \frac{5}{2} \delta_1 \eta + \frac{1}{8} \delta_2 \eta^2
\]

\[
- \frac{1}{8} \delta_2 \eta^3 \cdot \tanh \eta(\theta - \theta_0) \text{sech} \eta(\theta - \theta_0) + \frac{1}{10} \delta_2 \eta^3 \tanh \eta(\theta - \theta_0)
\]

\[
\text{sech}^4 \eta(\theta - \theta_0) + \frac{1}{2} \delta_2 \eta^3 \eta(\theta - \theta_0) \text{sech} \eta(\theta - \theta_0) + \frac{1}{2 \eta} (\xi_{\theta \theta_0} + \sigma_{\theta \theta_0})
\]

\[
\eta(\theta - \theta_0) + \frac{1}{10} \delta_2 \eta^3 \tanh^6 \eta(\theta - \theta_0) + \frac{5}{12} \delta_1 \eta + \frac{37}{60} \delta_2 \eta^3 - \frac{5}{12} \delta_2 \eta^2
\]

\[
+ \frac{3}{2} (\theta - \theta_0) \cdot \frac{1}{2} (\xi_{\theta \theta_0} + \sigma_{\theta \theta_0}) \text{sech}^2 \eta(\theta - \theta_0) + \text{sech}^4 \eta(\theta - \theta_0)(\frac{\delta_1 \eta^2}{4}
\]

\[
+ \frac{\delta_2 \eta^4}{4} - \frac{\delta_2 \eta^2 \xi^2}{4} - \frac{\delta_2 \eta^4}{3} \text{sech}^6 \eta(\theta - \theta_0) \cdot + \frac{1}{2} \eta \tanh \eta(\theta - \theta_0)
\]

\[
\text{sinh} \eta(\theta - \theta_0) - \frac{1}{\eta} \text{sech} \eta(\theta - \theta_0) \cdot + \frac{1}{2} (\xi_{\theta \theta_0} + \sigma_{\theta \theta_0}) + \frac{\delta_1 \eta^2}{4} + \frac{7}{12} \delta_2 \eta^4
\]

\[
- \frac{\delta_2 \eta^2 \xi^2}{4} + \frac{1}{2} (\xi_{\theta \theta_0} + \sigma_{\theta \theta_0}) \text{sech}^2 \eta(\theta - \theta_0) + \text{sech}^4 \eta(\theta - \theta_0)(\frac{\delta_1 \eta^2}{4}
\]

\[
+ \frac{\delta_2 \eta^4}{4} - \frac{\delta_2 \eta^2 \xi^2}{4} - \frac{\delta_2 \eta^4}{3} \text{sech}^6 \eta(\theta - \theta_0) \cdot + i \cdot \frac{1}{2} + \frac{1}{4} (\theta - \theta_0) \cdot
\]

\[
\text{sech} \eta(\theta - \theta_0) + \frac{1}{4} (\theta - \theta_0) \cdot (3 \eta - 1) + \frac{1}{2} \delta_2 \xi^3 \cdot \frac{1}{2 \eta} \eta(\theta - \theta_0)
\]

\[
\text{sech} \eta(\theta - \theta_0) + \text{sinh} \eta(\theta - \theta_0) \cdot - \frac{1}{4} (\theta - \theta_0) \cdot \tanh \eta(\theta - \theta_0)
\]

\[
\text{sech} \eta(\theta - \theta_0) - \frac{1}{4} (\theta - \theta_0) \cdot \eta(\theta - \theta_0) \cdot \text{sech}^3 \eta(\theta - \theta_0) + \frac{1}{2} (\theta - \theta_0)
\]

\[
\eta(\theta - \theta_0) \text{sech} \eta(\theta - \theta_0) - \frac{1}{2} (\theta - \theta_0) \cdot \tanh \eta(\theta - \theta_0) \cdot \text{sech} \eta(\theta - \theta_0)
\]

\[
- \frac{1}{4} (\theta - \theta_0) \cdot \text{sech} \eta(\theta - \theta_0) + \delta_2 \xi^2 \cdot \frac{1}{6} \text{sech} \eta(\theta - \theta_0) \cdot \tanh \eta(\theta - \theta_0)
\]
\[-\frac{1}{4} \eta(\theta - \theta_0) \mathrm{sech}^5 \eta(\theta - \theta_0) + \frac{1}{12} \tanh \eta(\theta - \theta_0) \mathrm{sech}^3 \eta(\theta - \theta_0) + \frac{1}{3} \]
\[\tanh^3 \eta(\theta - \theta_0) \mathrm{sech} \eta(\theta - \theta_0) + \frac{1}{2} \mathrm{sech} \eta(\theta - \theta_0) - \frac{1}{4} \eta(\theta - \theta_0) \mathrm{sech}^2 \eta(\theta - \theta_0) \mathrm{sech} \eta(\theta - \theta_0) - \frac{1}{4} \delta_2 \eta^3 \]
\[(\theta - \theta_0) \mathrm{sech}^5 \eta(\theta - \theta_0) - \frac{1}{4} \delta_2 \eta^2 \mathrm{sech}^4 \eta(\theta - \theta_0) \mathrm{sech} \eta(\theta - \theta_0) \].

Thus, we have constructed the perturbed soliton solution \(\hat{u}_1 = \hat{\phi}_1 + i \psi_1\) as represented in Eq. (2.50). We have also shown the graphical representations for the perturbed soliton solutions. The real part of perturbed the soliton solution is portrayed in Fig. (2.4) for various values of \(\eta\). As increasing the values of \(\eta\), the evolution of soliton solution exhibits anti-solitonic profile and also the profile transforms into anti-kink in shape with damped tail regime. While varying values of \(\xi\), the coherent structure possesses anti-soliton pattern having some fluctuations in its tail portion which is illustrated in Fig. (2.5). Similarly, the imaginary part of the perturbed soliton solutions is depicted in Fig. (2.6). We have obtained the corresponding proton-soliton profiles for various values of \(\eta\) and \(\xi\) respectively, which are shown in Figs. (2.6) and (2.7). In Fig. (2.7) the propagation of proton-soliton emerges with the humps suffered by damping.

We have also plotted the perturbed soliton solution \(\hat{u} = u_0 + \lambda \hat{u}_1\) and for various values of perturbation parameter \(\lambda\), we observe bell-shaped soliton evolutions which have small damping in its tail region. While increasing the values of \(\lambda\), we get the proton-soliton with larger amplitude but retaining the shape intact.

### 2.5 Conclusions

In this chapter, we have studied the nonlinear dynamics of protons in one-dimensional short HB chains. Initially, we consider an idealized periodic HB chain consisting of two interacting sublattices of harmonically coupled protons. We have formulated a model hamiltonian for this system using quasi spin analogy. Under H-P transformation, a discrete dynamical equation for proton
transfer has been derived. Using the Jacobian elliptic function method, we have derived a set of exact solutions of the model under study. These solutions include the Jacobi periodic solution which depends on the values of the modulus of the Jacobi function. We have found that in an external field, the propagation of proton-soliton is periodic in nature with damping at its hump. Further, we have analysed the system under anisotropic interactions as perturbation through multiple scale perturbation method. As a result of this analysis, we have obtained shape changing solitons from anti-solitonic to anti-kink profiles. As the introduction of perturbative environment, the propagation of protons in a short HB chain is explained through bell-shaped solitons. Thus, we remarkably conclude that the coupling between the proton motion and lattice deformations plays an vital role and seems to be important for proton mobility in a short hydrogen bonded chain. Therefore, for the propagation of solitons in soft HB chains, it might be concluded that the role play of $J_1$ is more adequate, to support lossless transport of energy.
2.5 Conclusions

![Graphs showing the evolution of different functions over time and iteration.]
Figure 2.3: Propagation of the Jacobi solution for Eq. (2.17) with m=1, k=1, c=0.002, p=1, \( \chi = 10^{-30} (\text{ms}^2)^{-1} \), \( \epsilon = 1 \), \( E_z = 10 \times 10^{-19} \text{Vm}^{-1} \) and \( \sigma = 1 \).
Figure 2.4: Real part of perturbed soliton solution for varying the value of $\eta$. 
Figure 2.5: Real part of perturbed soliton solution for varying the value of $\xi$. 

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Figure 2.6: Imaginary part of perturbed soliton solution for varying the value of $\eta$. 
Figure 2.7: Imaginary part of perturbed soliton solution for varying the value of $\xi$. 
Figure 2.8: Snapshots of propagation of perturbed proton soliton for various values of $\lambda$. 