Energy transport mechanism in the form of proton soliton in a one-dimensional hydrogen-bonded polypeptide chain

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Abstract The dynamics of protons in a one-dimensional hydrogen-bonded (HB) polypeptide chain (PC) is investigated theoretically. A new Hamiltonian is formulated with the inclusion of higher-order molecular interactions between peptide groups (PGs). The wave function of the excitation state of a single particle is replaced by a new wave function of a two-quanta quasi-coherent state. The dynamics is governed by a higher-order nonlinear Schrödinger equation and the energy transport is performed by the proton soliton. A non-linear multiple-scale perturbation analysis has been performed and the evolution of soliton parameters such as velocity and amplitude is explored numerically. The proton soliton is thermally stable and very robust against these perturbations. The energy transport by the proton soliton is more appropriate to understand the mechanism of energy transfer in biological processes such as muscle contraction, DNA replication, and neuro-electric pulse transfer on biomembranes.

Keywords Hydrogen bond · Proton transfer · Solitons

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1 Introduction

In living organisms, many biological processes such as muscle contraction, DNA replication, neuro-electric pulse transfer on membranes of neurocytes as well as work of the calcium pump and sodium pump and so on, are directed by and associated with energy transport. Energies that are needed for biological processes in bio-tissues are provided by the energy released during the hydrolysis of adenosine triphosphate (ATP) [1]. Thus, there are always biological processes of energy transport from a production location to an absorption location in living systems. In general, this energy transport is carried out by means of protein molecules. Proteins are crucial molecular components of biological systems and the biological function of any protein is intimately linked to its three-dimensional structure. Major research efforts have been mounted to develop a variety of energy transfer prediction methods to complement the array of experimental methods. However, proteins are often composed of thousands of amino acid residues, with which their size precludes a rigorous treatment and significantly smaller systems are used as models when computational techniques are to be employed. For this reason, peptides have served as valuable models for larger biomolecules and proteins. A special property of PGs is their ability to form HBs [2] with each other, and with water and other molecules in the environment. The study of HB chains [3–5] can lead to insight regarding how local interactions can dictate global features of PCs and proteins. Basically, PCs of protein structures [6] are the major workers within the cells, and carry out the functions described by the genetic codes: providing structural support, transmitting signals, catalyzing reactions, and transporting molecules. In general, all protein molecules are composed of a linear polymerization of 20 different amino acids and represent very long PCs with periodic repetition of PGs that contain H, C, N, and O atoms. When two amino acids join together, they release one water molecule and form a peptide bond. In this way, the PC has been formed and can be folded into a variety of complex three-dimensional conformations [7, 8]. In alpha helical proteins, the PCs are coiled into long helices, stabilized by HBs between neighboring carbon atoms within the primary PC, and the PGs are situated along three chains of HBs equidistant from one another, forming periodic structures. The energy of HBs in these PCs is approximately of an order of magnitude less than that of ordinary chemical bonds. Therefore, the displacements of PGs from their equilibrium positions along the chains of HBs occur much more readily than their displacements along the main PC [9]. Obviously, both acetanilide (ACN) and *N*-methylacetamide (NMA) crystals have an orthorhombic structure, with parallel chains of intermolecular HBs connecting the peptide units. They are very simple model systems for polypeptides. In this acetanilide organic crystal, the amide groups have bond distances comparable to those in protein molecules. As a result, it may be studied easily instead of a more complex protein and still provide useful polypeptide dynamical information. Hence, large interest has been focused on these peptide substances due to unusual properties of vibrations of the O–C–N–H atoms (also called amide–I modes) [10, 11]. These vibrations are assigned to coherent nonlinear excitations called Davydov solitons and polarons [12, 13]. This thought to be one of the driving mechanisms for transferring this vibrational energy in biomolecules. According to Davydov's idea, the best candidate for storing this vibrational energy in polypeptide molecules is the amide-I vibration, which is essentially of C=O stretch type because one quantum of this vibration has an energy of 0.205 eV, roughly half of the energy released by ATP hydrolysis. This quantum of vibrational energy is formed as a soliton. The main feature of solitons appealing to

biology is their property of dispersiveless transport; if a soliton-like packet of energy forms in a biomolecule, it may propagate without losses and enable long-range coherent energy transfer. This feature could be critical in the internal energetics of proteins where energy deposited on given sites produces large effects at relatively distant locations. Various studies have been made in recent years to examine the possibility of energy transport [14] via soliton mechanisms in proteins [15–17]. The so-called Davydov soliton and the vibron soliton [18–21], which involve the coupling of amide-I vibrations of PGs, have received particular attention over the past two decades. However, these theories are still being subjected to discussion and alternative explanations are invoked for the energy transport mechanism.

In α -helical protein molecules [22], the C=O groups of a turn in the helix form HBs to the N-H groups in the next turn. As indicated in the following sketch (Fig. 1), these HBs are coupled harmonically to each other in chains parallel to the helical axis and perpendicular to the covalent backbone and form a hydrogen-bonded PC. These linearly coupled HBs develop a phonon system, since the excitation energy of amide-I oscillators is naturally dependent on the length of the HB in which the C=O group takes part in the system of the HB chain. This makes the system nonlinear and thus it could be possible that an initially localized excitation would not disperse, but travel in the chain as a solitary wave. The conventional Davydov and vibron soliton [23] models are characterized by the nonlinearity in interactions between vibrational excitons. Here, the inherent presence of soft nonlinearity due to mobile protons of hydrogen-bonded PCs is overlooked. Even though many theoretical models [24–26] have been proposed to elucidate the energy transfer in biological systems, the proton transfer through HB PCs remains questionable. The charge-transport process in proteins is a fundamentally important process in a biological system. The charge-transport process in a real protein has been investigated experimentally for alpha helix. The charge transport in a polypeptide chain at room temperature has been described by Schlag et al. [27] by using a bifunctional model. This model shows a fast electronic charge transport rate combined with dynamic effects. A protein dynamic effect is not included in typical network theory, although, in general, dynamic effects on charge transport are known and have been recently invoked for DNA. Moreover, electronic transport plays a well-known and fundamental role in many biological processes, such as nervous conduction, photosynthesis, cellular respiration, and redox reactions. The electron motion is described by a tight-binding system. It is assumed that the electron motion is predominantly influenced by vibrational modes of the double helix. The nonlinear interaction between the electron and the vibrational modes causes the formation of polarons or electron-vibron breathers supporting charge localization and transport. Recently, the sequence-dependent twisting between adjacent base pairs and torsional elasticity of the double helix in DNA–DNA interaction has been analyzed by many investigators [28, 29]. Their results show that pairing and counterion-induced aggregation of nonhomologous DNA is accompanied by considerable torsional deformation. The deformation tunes negatively charged phosphate strands and positively charged grooves on opposing molecules to stay “in register”, essentially reducing nonideality of the helical structure of DNA. The purpose of the present work is to explore some possible mechanisms by which protons may move successively through HB PCs with a clear picture of peptide molecular structure as shown in Fig. 1. Also, this paper explores a study on energy transfer and propagation of solitons during the migration of protons between neighboring peptide groups of HB PCs. These solitons can arise due to interaction of amide-I excitation with anacoustic phonon and the interaction of PGs with its

Fig. 1 Schematic representation of hydrogen-bonded peptide groups

local environment chosen in the form of nonlinear interactions. Thus, to describe an efficient solitonic transport of amide-I energy along the chains of HB PGs, it is essential to consider the interpeptide proton displacements with higher-order molecular interactions and excitations.

In the present work, we focus our attention to bring out the energy transport in the form of proton-solitons in PCs with higher-order molecular excitations. In Section 2, we formulate an appropriate model Hamiltonian incorporating the higher-order molecular excitations in PCs and equations of motion are derived by invoking a quasi-coherent state method. We perform a nonlinear multiple-scale perturbation analysis along the lines of Kodama–Ablowitz in Section 3. The evolution equations for soliton parameters are solved using the fourth-order Runge–Kutta method and the perturbed soliton solutions are constructed in Section 4. We carry out molecular dynamics simulation studies in Section 5. The results are concluded in Section 6.

2 The nonlinear dynamics of protons in PCs

Following Davydov’s idea [8], Scott proposed a self-trapping theory that is closely related to that of Davydov, and explains the salient experimental facts of spectral measurements in the amide-I region of crystalline acetanilide or acetanilide (ACN) [12]. The soliton model of energy transport seems to be surely a competing picture for the dissipation free transport mechanism and consequently has been a subject of a large body of work [9, 12, 13]. Many problems related to Davydov’s model have been extensively studied. Pouthier et al. [15] modified the Davydov model with the influence of intramolecular anharmonicity and strong vibron-phonon coupling using the small-polaron approach. Takeno [21] has shown that the vibrational solitons (amide-I solitons) thus formed are governed by the nonlinear Schrödinger equation, which arises from modulations of vibrational excitations by nonlinear coupling with acoustic phonons propagating along the chain. Yomosa [32] regarded the one-dimensional HB chain of PGs in the α -helical protein molecule as a Toda nonlinear lattice, since the potential of the hydrogen-bonding interaction between PGs has a remarkably nonlinear character. Recently, Daniel et al. [24] investigated the effect of higher-order molecular excitations and interactions on the soliton dynamics of alpha-helical proteins for the first time and found that the results were in favor of soliton propagation through the chains. They improved and extended the Davydov model by incorporating the internal molecular excitations of different orders and nonlinear couplings with nearest and next-nearest neighboring peptide units assuming that the left and right interactions with the nearest neighboring peptide units are unequal in general. At different orders of continuum approximation, the generalized model describing molecular excitations reduces to completely integrable models of the nonlinear Schrödinger family for specific parametric choices. On the other hand, Pang et al. [1] studied the propagating properties of soliton-transporting energy excited in the α -helix protein molecules with three channels in the cases of the short-time and

long-time motions and its features of collision at biological temperature $T = 300$ K by the dynamic equations in the improved Davydov theory using a fourth-order Runge–Kutta method. They suggested that motion of the proton between a pair of heavy ions crossed over the barrier in the intrabond, which results in a change of relative position between the protons and neighboring heavy ions, mainly determined by the double-well potential. In this context, we would like to improve the Pang model by making an attempt to construct an entirely new Hamiltonian incorporating higher-order molecular excitations with quadrupole–quadrupole interaction and higher-order nonlinear coupling, which characterizes the new nonlinear coupling coefficient due to higher-order molecular excitations. It is therefore imperative to reexamine, both analytically and numerically, the proton dynamics in polypeptides by including the higher-order molecular excitations, interactions, and discreteness. Thus, we model a new Hamiltonian for the PCs with the inclusion of higher-order molecular excitations,

$$\begin{aligned}
 H = \sum_n \bigg\{ & B_n^\dagger [(2E_0 + W)B_n + J(B_{n+1} + B_{n-1})] - \frac{\hbar\omega_1^2}{4\omega_0} (B_n^\dagger + B_n) (B_{n+1}^\dagger + B_{n+1}) \\
 & + U_0 \left[1 - \frac{\hbar}{m\omega_0 r_0^2} (B_n + B_n^\dagger)^2 + \frac{\hbar^2}{4m^2\omega_0^2 r_0^4} (B_n + B_n^\dagger)^4 \right] \\
 & + \chi [B_n^\dagger B_n (u_{n+1} + u_{n-1})] + \chi_1 [B_n^\dagger B_n B_n^\dagger B_n (u_{n+1} - u_{n-1})] + E_1 B_n^\dagger B_n B_n^\dagger B_n \\
 & - J_1 [B_n^\dagger B_{n+1} B_n^\dagger B_{n+1} + B_n^\dagger B_{n-1} B_n^\dagger B_{n-1}] \bigg\}, \quad (1)
 \end{aligned}$$

where $W = \frac{1}{2} \sum_n \left[\frac{1}{M} v_n^2(t) + k(b_n - b_{n-1})^2 \right]$ is the deformation energy of the chain. Here, E_0 represents the excitation energy of each PG in the hydrogen bonding spine including the resonant interaction energy between neighboring PGs. J represents the dipole–dipole coupling coefficient between adjacent PGs along the spine and the parameter χ is a nonlinear coupling coefficient representing the change in energy of the amide-I bond caused by stretching of the chain between two neighboring PGs. The parameter E_1 characterizes the higher-order excitation energy of the PG and J_1 corresponds to the higher-order coupling coefficient. Further, χ_1 is the new nonlinear coupling coefficient due to higher-order molecular excitations. The operator b_n is the displacement operator of a lattice oscillator at site n , v_n is its conjugate momentum operator, M is the mass of a peptide molecule, k is the elasticity constant of polypeptide chains, U_0 is the height of the barrier of the double-well potential, ω_0 are the diagonal elements of the dynamic matrix of the proton and also the Einstein resonant frequency of the protonic sublattice, r_0 is the distance between the central maximum and one of the minima of the double well and m is the mass of the proton. The real experimental values for the above parameters are as follows [1] $J = 1.55 \times 10^{-22} J$, $W = (1.3 - 19.5)N/m$, $m = (1.77 - 19.1) \times 10^{-25} Kg$, $\chi_1 = 62 \times 10^{-2}$, $E_0 = 0.205 eV$, $U_0 = 0.22 eV$, $\omega_0 = (1 - 1.5) \times 10^{14} s^{-1}$, $\omega_1 = (4 - 5) \times 10^3 s^{-1}$.

All biological processes are directed and regulated by specific interactions between biomolecules. Prediction and experimental confirmations of these interactions are the major challenges in the process of energy transfer in PCs, especially since the wealth of information now available has revealed that the most significant role of proton transport is to enable the complete energy transfer necessary for a given specific interaction between peptide molecules. An inspection of α -helical structure reveals three channels of HB PGs situated approximately in the longitudinal direction with sequence $O = C - N - H - - - O =$

$C - N - H - \cdots - O = C - N - H$ etc., where the dashed lines represent HBs. Also, the maintenance of the helical structure of PCs depends upon the HBs. To illustrate the present work, in comparison with previous theories [30–32], we consider our model as the highly idealized case of one molecule (peptide group) per unit cell as shown in Fig. 1. The peptide chain consists of the repeated structure, in which the repeated unit is the PG made up of H, N, C, and O four atoms as shown in Fig. 1.

Despite the many contributions to understanding the serial transport of protons in HB chains, to the best of our knowledge, no previous study of these important molecules has considered all possible combinations of residues. Instead, the approach has invariably been to focus on a small subset of HB polypeptides either because there is a specific interest in the subset or because the full set would exceed the scope of the study. In order to explain the dynamics of protons, it is necessary to consider a co-operative proton migration through the HB between each peptide group. Every proton [33] that affects the HB is connected with nitrogen atoms by a covalent bond on one hand and with an oxygen atom by a HB on the other hand. The local contraction of the chain, formed by the non-linear lattice distortion, may serve as a potential well for proton transfer. This vibration allows a comparatively easy compression of HBs. In this case, the HB length varies, i.e., when the proton in the hydrogen bridges goes over the local potential barrier, this alters the HB length. The potential energy for mobile protons is well established by the double-well potential created virtually by the pair of nearest-neighbor peptide molecules. The flexible proton transfer along the PCs is subjected to a stepwise mechanism. In each step, only one proton jumps along the HB, which is schematically indicated in Fig. 2. Owing to the fact that the proton motion and amide-I vibrations are all quantized, we utilize a quantum mechanical approach to analyze the dynamics. Furthermore, the proton motion in PCs is a nonlinear problem, which is caused by the double-well potential and nonlinear coupling between the protons and the excitons. In such systems, collective excitations arising from these nonlinear interactions have coherence. Therefore, we adopt the coherent states to express these collective excitations. Thus, we choose a wave function which may be in the form [24]

$$\Psi_n(t) = \sum_n a_n(t) \exp[\sigma(t)] B_n^\dagger |0\rangle, \quad (2)$$

where $|0\rangle$ represents a vacuum state with $|0\rangle = |0\rangle_{pr} |0\rangle_{ex} |0\rangle_{ph}$ and

$$\sigma(t) = -\frac{i}{\hbar} \sum_n b_n(t) p_n - v_n(t) u_n. \quad (3)$$

Fig. 2 Stepwise mechanism of proton transfer in polypeptide chain

In this framework, we have considered that the state of motion of the proton and exciton lie in the same state. Thus, $B_n(B_n^\dagger)$ corresponds to creation (annihilation) operator for exciton and proton. The parameters b_n and v_n correspond to the coherent states of the displacements and conjugate momenta of the unit cells in the state given by $\Psi(t)$, where $b_n(t)$ and $v_n(t)$ are given as

$$b_n(t) = \langle \Psi_n(t) | u_n | \Psi_n(t) \rangle, \quad (4)$$

$$v_n(t) = \langle \Psi_n(t) | p_n | \Psi_n(t) \rangle. \quad (5)$$

The position and momentum operators satisfy the commutation relations

$$[u_n, p_n] = i\hbar\sigma_n n', \quad (6)$$

and the coherent state representation for the operators B_n and $B_n^\dagger$ are given by

$$a_n(t) = \langle \Psi_n(t) | B_n | \Psi_n(t) \rangle, \quad (7)$$

$$a_n^*(t) = \langle \Psi_n(t) | B_n^\dagger | \Psi_n(t) \rangle, \quad (8)$$

where $|a_n(t)|^2$ characterizes the probability of excitation of the n^{th} PG and the normalization condition for the wavefunction $\Psi_n(t)$ yields

$$\sum_n |a_n(t)|^2 = 1. \quad (9)$$

In order to obtain the equations of motion, (2) can be used to form the expectation value of the total energy, which is then used as the Hamiltonian for constructing the equations of motion for a_n and b_n , which are assumed to evolve as classical variables. Now the Hamiltonian can be written as

$$H = \langle \Psi(t) | H | \Psi(t) \rangle, \quad (10)$$

Using (1) and (2) in (10), we can again recast the Hamiltonian as

$$\begin{aligned} H = \sum_n \bigg\{ & a_n^* [(2E_0 + W) a_n - J (a_{n+1} + a_{n-1})] + \chi [a_n^* a_n (b_{n+1} - b_{n-1})] \\ & + \chi_1 [a_n^* a_n a_n^* a_n (b_{n+1} - b_{n-1})] + E_1 a_n^* a_n a_n^* a_n \\ & - J_1 [a_n^* a_{n+1} a_n^* a_{n+1} + a_n^* a_{n-1} a_n^* a_{n-1}] \\ & - \frac{\hbar\omega_1^2}{4\omega_0} (a_n^* a_{n+1}^* + a_n a_{n+1}^* + a_n^* a_{n+1} + a_n a_{n+1}) \\ & + U_0 \left[1 - \frac{\hbar}{m\omega_0 r_0^2} (a_n^* + a_n)^2 + \frac{\hbar^2}{4m^2\omega_0^2 r_0^4} (a_n^* + a_n)^4 \right] \bigg\}. \quad (11) \end{aligned}$$

Having developed the Hamiltonian, we can write the equations of motion using the Heisenberg equation for the polypeptide chain,

$$i\hbar \frac{\partial a_n}{\partial t} = [a_n, H]. \quad (12)$$

By using (12), we write the equations of motion as follows,

$$\begin{aligned} i\hbar a_{nt} = & \left[(2E_0 + W) + \chi (b_{n+1} - b_{n-1}) + 2E_1 |a_n|^2 \right] a_n - J (a_{n+1} + a_{n-1}) \\ & - 2J_1 a_n^* (a_{n+1}^2 + a_{n-1}^2) + 2\chi_1 \left[|a_n|^2 a_n (b_{n+1} - b_{n-1}) \right] \\ & - \frac{\hbar\omega_1^2}{4\omega_0} (a_{n+1}^* + a_{n-1}^* + a_{n-1} + a_{n+1}) - 2jU_0 (a_n^* + a_n) \\ & + U_0 \left(\frac{j'}{2} \right)^2 \left[4a_n^{*3} + 4a_n^3 + 12|a_n|^2 a_n + 12|a_n|^2 a_n^* \right], \end{aligned} \quad (13)$$

$$\begin{aligned} mb_{ntt} = & k [b_{n+1} + b_{n-1} - 2b_n] - \chi \left[|a_{n+1}|^2 - |a_{n-1}|^2 \right] \\ & + \chi_1 \left[|a_{n+1}|^4 - |a_{n-1}|^4 \right]. \end{aligned} \quad (14)$$

The equations of motion describe the energy transfer during the process of ATP hydrolysis through large amide-I vibrations along the hydrogen spine of PCs.

3 Governing dynamical equations in continuum limit

In order to understand the proton dynamics, we have to solve the discrete (13–14). However, it is very difficult to solve (13–14) as such due to its high nonlinearity and discreteness. Therefore it is quite reasonable to go to continuum approximation in the low-temperature and long-wavelength limit, by the way of assuming that the lattice constant is very small when compared to the length of the lattice. Thus, we introduce the following series expansions for $a_{n+1}(t)$ and $b_{n+1}(t)$ by expressing $a_n(t)$ and $b_n(t)$, respectively, as $a(x)$ and $b(x)$, where x is a continuous variable.

$$\begin{aligned} a_{n+1}(t) = & \left[1 \pm \varepsilon \frac{\partial}{\partial x} + \frac{\varepsilon^2}{2!} \frac{\partial^2}{\partial x^2} \pm \frac{\varepsilon^3}{3!} \frac{\partial^3}{\partial x^3} + \frac{\varepsilon^4}{4!} \frac{\partial^4}{\partial x^4} \pm \dots \right] a(x, t), \\ b_{n+1}(t) = & \left[1 \pm \varepsilon \frac{\partial}{\partial x} + \frac{\varepsilon^2}{2!} \frac{\partial^2}{\partial x^2} \pm \dots \right] b(x, t). \end{aligned}$$

Using the above expansions in the discrete equations of motion (13–14), we obtain the following continuous equations of motion written to $O(\varepsilon^4)$.

$$\begin{aligned} i\hbar a_t = & \left[(2E_0 + W - 2J) + (2E_1 - 4J_1) |a|^2 \right] a - J\varepsilon^2 \left[(a_{xx}) + \frac{\varepsilon^2}{12} (a_{xxx}) \right] \\ & - 2J_1\varepsilon^2 \left[2|a|^2 (a_{xx}) + 2a^* (a_x)^2 + \frac{\varepsilon^2}{6} |a|^2 (a_{xxx}) + \frac{\varepsilon^2}{2} a^* (a_{xx})^2 + \frac{2}{3} \varepsilon^2 a^* (a_x) (a_{xxx}) \right] \\ & + 2\varepsilon \left(\chi + 2\chi_1 |a|^2 \right) a (b_x) + U_0 \left[2j' (a + a^*) + (j')^2 (a^3 + a^{*3} + 3|a|^2 a + 3|a|^2 a^*) \right] \\ & - \frac{\hbar\omega_1^2}{4\omega_0} \left[2(a + a^*) + \varepsilon^2 (a_{xx}^* + a_{xx}) + \frac{\varepsilon^4}{12} (a_{xxx}^* + a_{xxx}) \right], \end{aligned} \quad (15)$$

$$\begin{aligned} mb_{tt} = & k\varepsilon^2 (b_{xx}) + 2\chi\varepsilon \left[\left(|a|^2 \right)_x + \frac{\varepsilon^2}{6} (aa_{xxx}^* + a^* a_{xxx}) + \frac{\varepsilon^2}{2} (a_x q_x^*) \right] \\ & + 2\chi_1\varepsilon \left[\left(|a|^4 \right)_x + \frac{\varepsilon^2}{3} |a|^2 (aa_{xxx}^* + a^* a_{xxx}) + \varepsilon^2 a^2 (a_x^*) (a_{xx}^*) \right. \\ & \left. + \varepsilon^2 a^{*2} (a_x) (a_{xx}) + 2\varepsilon^2 \left(|a|^2 (a_x) (a_x^*) \right)_x \right]. \end{aligned} \quad (16)$$

Now, defining the terms $\lambda' = 2E_0 + W - 2J$, $C_0^2 = \frac{k}{m}$, $\rho(x, t) = -\varepsilon \frac{\partial b(x, t)}{\partial x}$ and after differentiating (16) with respect to x once and introducing the wave variable $\xi = x - ct$ integrating (16) twice, we obtain

$$\begin{aligned} \rho(\xi) = & \frac{1}{k(1-s^2)} \left\{ 2\chi \left[|a|^2 + \frac{\varepsilon^2}{6} (aa_{xx}^* + a^* a_{xx}) + \frac{\varepsilon^2}{3} (a_x) (a_x^*) \right] + \frac{2}{3} \chi_1 \left(\varepsilon^2 \left\{ |a|^2 [aa_{xx}^* \right. \right. \right. \\ & \left. \left. \left. + a^* a_{xx} - 2(a_x) (a_x^*) \right\] + a^2 (a_x^*)^2 + a^{*2} (a_x)^2 + 6|a|^2 (a_x) (a_x^*) \right\} + 3|a|^4 \right) \right\}. \end{aligned} \quad (17)$$

Choosing $\lambda' = 0$, $J = \hbar = 1$, $\chi_1 = \frac{\chi}{4}$, $J_1 = \frac{\chi^2}{2k(1-s^2)}$, $E_1 = \frac{-4\chi^2}{k(1-s^2)}$ and substituting (17) in (15), we obtain the following higher-order perturbed NLS equation, after making the transformation $a = \sqrt{\frac{k(1-s^2)}{4\chi^2}} q$ and $t = \frac{t}{\varepsilon^3}$.

$$\begin{aligned} iq_t + q_{xx} + 2|q|^2 q + \lambda \left[q_{xxx} + 8|q|^2 q_{xx} + 2q^2 q_{xx}^* + 4q|q_x|^2 + 6q^* q_x^2 + 6|q|^4 q \right] \\ + \alpha \left\{ |q|^2 \left[\frac{1}{2} q_{xxx} + \frac{3}{2} |q|^2 q_{xx} + 4q^2 q_{xx}^* + 5|q_x|^2 q \right] + q^* q_x^2 + \frac{3}{2} q^* q_{xx}^2 + 2q^* q_x q_{xxx} + q^3 q_x^{*2} \right\} \\ + \beta |q|^2 \left\{ |q|^4 q_{xx} + |q|^2 q^2 q_{xx}^* + q^3 q_x^{*2} + |q|^2 q^* q_x^2 + 3|q|^4 q + 4|q|^2 |q_x|^2 q \right\} + b_1 (q + q^*) \\ + b_2 (q^3 + q^{*3}) + 3b_2 (|q|^2 q + |q|^2 q^*) - b_3 \frac{\varepsilon^2}{2} (q_{xx} + q_{xx}^*) - b_3 \frac{\varepsilon^4}{24} (q_{xxx} + q_{xxx}^*) \Big] = 0 \end{aligned} \quad (18)$$

where $\lambda = \frac{\varepsilon^2}{12}$, $\alpha = \frac{k(1-s^2)}{4\chi^2\varepsilon^2}$, $\beta = \frac{1}{4} \left[\frac{k(1-s^2)}{4\chi^2} \right]^2$, $b_1 = \left[\frac{24U_0 j' \alpha}{\varepsilon^2} - \frac{12\hbar\alpha}{\omega_0\varepsilon^2} \right]$, $b_2 = \frac{12j'^2\alpha^3}{\varepsilon^2}$ and $b_3 = \frac{12\hbar\omega_1^2\alpha}{\omega_0\varepsilon^2}$. In the above equation, the subscript denotes the partial derivative with respect to x , where α, β, λ , are different parameters as defined above. The equations of motion

representing the dynamics of proton transfer in polypeptide chains leads to the higher-order nonlinear Schrödinger (NLS) equation, which contain a soliton solution. Solving (18) analytically is very difficult due to its mathematical complexity, which arises because of the high degree of nonlinearity. This equation is a perturbed higher-order NLS equation and contains two integrable models. For example, when $\lambda = 0$, the equation reduces to the integrable cubic nonlinear Schrödinger equation,

$$iq_t + q_{xx} + 2|q|^2q = 0.$$

When $\alpha = \beta = 0$, $\lambda \neq 0$ (18) reduces to the integrable higher-order (fourth order) nonlinear Schrödinger equation

$$iq_t + q_{xx} + 2|q|^2q + \lambda \left[q_{xxxx} + 8|q|^2q_{xx} + 2q^2q_{xx}^* + 4q|q_x|^2 + 6q^*q_x^2 + 6|q|^4q \right] = 0.$$

This implies that the coupled interactions between the proton and PG play the leading role for determining the properties of protons and it makes the proton dynamics governed by solitons shift over the barriers in the interbonds by the mechanism of quasi-self trapping whereas the double-well potential plays only a minor role. In general, the evolution of a quantum particle subjected to a time-dependent asymmetric bistable potential and affected by environmental noise has been analyzed by the Caldeira–Leggett model, which allows to derive a quantum mechanical analogue of the generalized Langevin equation [34–36]. More recently, one of the present authors reported breather-like protonic quantum tunneling in a discrete hydrogen-bonded chain with heavy-ionic interactions [4]. Kavitha et al. also reported the solitonic dynamics of the chain polarization in HB systems, when tunnel processes prevail over the thermal activation and analyzed the tunneling between two opposite directions governed by a bistable potential system at low temperature [2, 5]. They suggested a possible coherent tunneling mechanism of spontaneous polarization oscillations of HB chain. This mechanism is similar to coherent quantum tunneling, which was observed in small magnetic grains. For a macroscopic system, however, the quantum-mechanical tunneling rate is suppressed by dissipation. Caldeira and Leggett showed that the dissipation inherent in macroscopic systems reduces the quantum escape rate below the predictions for the frictionless system. Tomchuk [37] already reported that at low temperatures the protons are tightly bound with the ions, the vibrations reduce the coherent tunnel rate, and the protons are localized near the potential barrier.

4 Effect of discreteness on proton soliton

It is a standard feature of nonlinear systems that exact analytic solutions are possible only in exceptional cases. We now carry out the multiple scale perturbations analysis [38] laid down by Kodama and Ablowitz [39–41] by treating terms proportional to λ in (18) as perturbations when $\beta = 0$. In what follows, we apply the multiple scaling analysis to (18) when $\beta = 0$. The envelope one soliton solution of (18) can be written as

$$q = \eta \operatorname{sech} \eta (\theta - \theta_0) \exp [i\xi(\theta - \theta_0) + i(\sigma - \sigma_0)], \quad (19)$$

where $\theta_t = -2\xi$, $\theta_x = 1$, $\sigma_t = \eta^2 + \xi^2$ and $\sigma_x = 0$. We write η , ξ , θ , θ_0 and σ_0 as functions of the new time scale $T = \lambda t$. Hence the soliton solution of (18) can be written as

$$q = \hat{q}(\theta, T : \lambda) \exp [i\xi(\theta - \theta_0) + i(\sigma - \sigma_0)]. \quad (20)$$

The above assumption of quasi-stationarity seems to be a conceptually simple generalization of the unperturbed form and is appropriate for explicit calculations. Upon substituting (20) in (18), we obtain

$$-\eta^2 \hat{q} + \hat{q}_{\theta\theta} + 2\hat{q}^2 \hat{q}^* = \lambda F(\hat{q}) \quad (21)$$

where

$$\begin{aligned} F(\hat{q})v = & - \left\{ \hat{q}_{\theta\theta\theta\theta} - 6\hat{q}_{\theta\theta}\xi^2 + \hat{q}_\xi^4 + 10\hat{q}^2\hat{q}_\theta - 20\hat{q}^3\xi^2 + 20\hat{q}^2\hat{q}_{\theta\theta} + 10\hat{q}\hat{q}_\theta^2 + 20\hat{q}\hat{q}_\theta^2 + 60\hat{q}^5 \right. \\ & + \frac{1}{2}\alpha\hat{q}^2\hat{q}_{\theta\theta\theta\theta} - 3\alpha\hat{q}^2\hat{q}_{\theta\theta}\xi^2 + \frac{\alpha}{2}\hat{q}^2\xi^4 + \alpha\hat{q}^2\hat{q}_{\theta\theta\theta\theta} - 15\alpha\hat{q}^2\hat{q}_{\theta\theta}\xi^2 + \frac{7}{2}\alpha\hat{q}^3\xi^4 + 33\alpha\hat{q}^4\hat{q}_{\theta\theta} \\ & - 40\alpha\hat{q}^5\xi^2 + 22\alpha\hat{q}^4\hat{q}_{\theta\theta} + 21\alpha\hat{q}^3\hat{q}_\theta^2 + 6\alpha\hat{q}^3\hat{q}_\theta^2 + 42\alpha\hat{q}^3\hat{q}_\theta^2 + 3\hat{q}\alpha\hat{q}_{\theta\theta}^2 + 6\alpha\hat{q}\hat{q}_\theta^2\xi^2 \\ & - 3\alpha\hat{q}^2\hat{q}_{\theta\theta}\xi^2 + \frac{3}{2}\alpha\hat{q}\hat{q}_{\theta\theta}^2 - 12\alpha\hat{q}\hat{q}_\theta^2\xi^2 - 3\alpha\hat{q}^2\hat{q}_{\theta\theta}\xi^2 + 2\alpha\hat{q}\hat{q}_\theta\hat{q}_{\theta\theta\theta} + 2\alpha\hat{q}\hat{q}_\theta\hat{q}_{\theta\theta\theta} \\ & - 6\alpha\hat{q}_\theta^2\hat{q}_\theta^2 + 2\alpha\hat{q}\hat{q}_\theta\hat{q}_{\theta\theta\theta} + 6\alpha\hat{q}^2\xi^2\hat{q}_{\theta\theta} + 6\alpha\hat{q}^2\xi^2\hat{q}_{\theta\theta} - \hat{q}\xi_T(\theta - \theta_0) + 2b_1\hat{q} + 24b_2\hat{q}^3 \\ & - b_3\varepsilon^2\hat{q}_{\theta\theta} - b_3\varepsilon^2\xi^2\hat{q} - \frac{b_3\varepsilon^4}{12}\hat{q}_{\theta\theta\theta\theta} + \frac{b_3\varepsilon^4}{2}\xi^2\hat{q}_{\theta\theta} - \frac{b_3\varepsilon^4}{12}\xi^4\hat{q} - \frac{12}{\varepsilon^2}\omega_0\hat{q} + \frac{48}{\varepsilon^2}\hat{q}^3 \left. \right\} \\ & - i \left\{ 4\xi\hat{q}_{\theta\theta\theta} - 4\xi^3\hat{q}_\theta + 40\xi\hat{q}^2\hat{q}_\theta - 2\alpha\hat{q}^2\xi\hat{q}_{\theta\theta\theta} + 2\alpha\hat{q}^2\hat{q}_\theta\xi^3 + 4\alpha\xi\hat{q}^2\hat{q}_{\theta\theta\theta} - 22\alpha\xi^3\hat{q}^2\hat{q}_\theta \right. \\ & + 66\alpha\xi\hat{q}^4\hat{q}_\theta - 14\alpha\xi\hat{q}^2\hat{q}^2\hat{q}_\theta + 6\alpha\xi^3\hat{q}^2\hat{q}_\theta - 8\alpha\xi^3\hat{q}^2\hat{q}_\theta + \hat{q}_T - 2b_3\varepsilon^2\xi\hat{q}_\theta + 12\alpha\xi\hat{q}\hat{q}_{\theta\theta}\hat{q}_{\theta\theta} \\ & \left. + 2\alpha\xi\hat{q}^2\hat{q}_{\theta\theta\theta} + 6\alpha\xi^3\hat{q}^2\hat{q}_\theta - \frac{b_3\varepsilon^4}{3}\xi\hat{q}_{\theta\theta\theta} + \frac{b_3\varepsilon^4}{3}\xi^3\hat{q}_\theta \right\}. \quad (22) \end{aligned}$$

Expanding $\hat{q}$ in terms of λ as

$$\hat{q}(\theta, T; \lambda) = \hat{q}_0(\theta, T) + \lambda\hat{q}_1(\theta, T) + \dots, \quad (23)$$

where $\hat{q}_0 = \eta \operatorname{sech} \eta(\theta - \theta_0)$ and substituting (23) in (21) at $O(\lambda)$ we get

$$-\eta^2 \hat{q}_1 + \hat{q}_{1\theta\theta} + 2\hat{q}_0^2 \hat{q}_1^* + 4\hat{q}_0^2 \hat{q}_1 = F_1(\hat{q}_0). \quad (24)$$

The right-hand side of (24) is of the form

$$\begin{aligned} F_1(\hat{q}_0) = & - \left\{ \hat{q}_{0\theta\theta\theta\theta} - 6\hat{q}_{0\theta\theta}\xi^2 + \hat{q}_0\xi^4 + 10\hat{q}_0^2\hat{q}_{0\theta} - 20\hat{q}_0^3\xi^2 + 20\hat{q}_0^2\hat{q}_{0\theta\theta} + 30\hat{q}_0\hat{q}_0^2 + 60\hat{q}_0^5 \right. \\ & + \frac{3}{2}\alpha\hat{q}_0^2\hat{q}_{0\theta\theta\theta\theta} + \frac{\alpha}{2}\hat{q}_0^2\xi^4 + \frac{3}{2}\alpha\hat{q}_0^2\hat{q}_{0\theta\theta\theta\theta} + \frac{7}{2}\alpha\hat{q}_0^3\xi^4 + 55\alpha\hat{q}_0^4\hat{q}_{0\theta\theta} - 40\alpha\hat{q}_0^5\xi^2 \\ & + 69\alpha\hat{q}_0^3\hat{q}_{0\theta}^2 + 3\hat{q}_0\alpha\hat{q}_{0\theta\theta}^2 - 12\alpha\hat{q}_0\hat{q}_{0\theta}^2\xi^2 - 24\alpha\hat{q}_0^2\hat{q}_{0\theta\theta}\xi^2 + \frac{3}{2}\alpha\hat{q}_0\hat{q}_{0\theta}^2 + 6\alpha\hat{q}_0\hat{q}_{0\theta}\hat{q}_{0\theta\theta\theta} \\ & + 6\alpha\hat{q}_0^2\xi^2\hat{q}_{0\theta\theta} + 6\alpha\hat{q}_0^2\xi^2\hat{q}_{0\theta\theta} - \hat{q}_0\xi_T(\theta - \theta_0) + 2b_1\hat{q}_0 + 24b_2\hat{q}_0^3 - b_3\varepsilon^2\hat{q}_{0\theta\theta} \\ & - b_3\varepsilon^2\xi^2\hat{q}_0 - \frac{b_3\varepsilon^4}{12}\hat{q}_{0\theta\theta\theta\theta} + \frac{b_3\varepsilon^4}{2}\xi^2\hat{q}_{0\theta\theta} - \frac{b_3\varepsilon^4}{12}\xi^4\hat{q}_0 - \frac{12}{\varepsilon^2}\omega_0\hat{q}_0 + \frac{48}{\varepsilon^2}\hat{q}_0^3 \left. \right\} \\ & - i \left\{ 4\xi\hat{q}_{0\theta\theta\theta} - 4\xi^3\hat{q}_{0\theta} + 40\xi\hat{q}_0^2\hat{q}_{0\theta} - 16\alpha\hat{q}_0^2\hat{q}_{0\theta}\xi^3 + 66\alpha\xi\hat{q}_0^4\hat{q}_{0\theta} - 14\alpha\xi\hat{q}_0^2\hat{q}_{0\theta}\hat{q}_{0\theta\theta} \right. \\ & \left. + \hat{q}_{0T} - 2b_3\varepsilon^2\xi\hat{q}_{0\theta} + 12\alpha\xi\hat{q}_0\hat{q}_{0\theta}\hat{q}_{0\theta\theta} - \frac{b_3\varepsilon^4}{3}\xi\hat{q}_{0\theta\theta\theta} + \frac{b_3\varepsilon^4}{3}\xi^3\hat{q}_{0\theta} \right\}. \quad (25) \end{aligned}$$

Substituting $\hat{q}_1 = \hat{\Phi}_1 + i\hat{\Psi}_1$ (Φ_1 and Ψ_1 are real) in (23), we obtain

$$L_1 \hat{\Phi}_1 = \left[-\eta^2 \hat{\Phi}_1 + \hat{\Phi}_{1\theta\theta} + 6\hat{q}_0^2 \hat{\Phi}_1 \right] = \text{Re} \hat{F}_1(\hat{q}_0), \quad (26)$$

and

$$L_2 \hat{\Psi}_1 = \left[-\eta^2 \hat{\Psi}_1 + \hat{\Psi}_{1\theta\theta} + 2\hat{q}_0^2 \hat{\Psi}_1 \right] = \text{Im} \hat{F}_1(\hat{q}_0). \quad (27)$$

where $\text{Re} F_1(\hat{q}_0)$ and $\text{Im} F_1(\hat{q}_0)$ are the real and imaginary parts of $F_1(\hat{q}_0)$ given by (25) and L_1 and L_2 are self-adjoint operators. On solving (26) and (27), we obtain the perturbed soliton solution.

4.1 Evolution of amplitude and velocity of the soliton

As $\hat{q}_{0\theta}$ and $\hat{q}_0$ are solutions of the homogeneous parts of (26) and (27), respectively, we have the secularity conditions

$$\int_{-\infty}^{+\infty} \hat{q}_{0\theta} \text{Re}(\hat{F}_1) d\theta = 0, \quad \int_{-\infty}^{+\infty} \hat{q}_0 \text{Im}(\hat{F}_1) d\theta = 0. \quad (28)$$

Upon substituting the values of $\hat{q}_0$, $\hat{q}_{0\theta}$, $\text{Re}(F_1)$ and $\text{Im}(F_1)$ into the above integrals and after evaluation, we finally obtain

$$\xi_T = \left(-\frac{b_3 \epsilon^4}{2} + 6 \right) \eta^5 + \left(\frac{b_3 \epsilon^2}{2} - 3\xi^2 + \frac{b_3 \epsilon^4}{4} \right) \eta^3; \quad \eta_T = \left(\frac{b_3 \epsilon^4}{6} - 2\xi \right) \eta^4. \quad (29)$$

Equation (29) represents the evolution of soliton parameters, such as velocity (ξ) and amplitude (η). We attempt to solve these evolution equations numerically using the fourth-order Runge–Kutta method and investigate the proton dynamics in PCs under the influence of higher-order molecular excitations and the effect of discreteness. We have investigated the evolution of soliton parameters by solving the amplitude $\eta(t)$ and the velocity $\xi(t)$ of the soliton by choosing the initial value of $\eta(t) = \eta(0) = 0.3$ and $\xi(t) = \xi(0) = -1$ with the step size $h = 0.1$. In Fig. 3a and b, we have plotted the amplitude and the velocity of the soliton when $\eta_0 = 0.3$ and $\xi_0 = -1$. From Fig. 3a and b, it is evident that the amplitude of proton soliton decelerates with the increase in the value of ϵ . It could be inferred from the above result that when the HB length increases, the amplitude of the proton soliton decelerates very fast along the PCs. On the other hand, when ϵ increases, the velocity of soliton shoots up, as shown in Fig. 3b and in this case, an amide-1 excitation propagates from one peptide group to the next because of the higher-order molecular excitations. An excitation initially located at one PG will induce a distortion of the associated HB which, in turn, will decrease the energy of the corresponding amide-1 state.

4.2 Perturbed proton solitons

In order to construct the perturbed proton soliton, we need to solve (26) and (27) for ϕ_1 and ψ_1 . The homogeneous part of (26) admits the following two particular solutions [42, 43]:

Fig. 3 **a** Amplitude of the soliton. **b** Velocity of the soliton

$\hat{\phi}_{11} = \text{sech} \tau \tanh \tau$, $\hat{\phi}_{12} = -\frac{1}{\eta} \left[\text{sech} \tau - \frac{3}{2} \tau \text{sech} \tau \tanh \tau - \frac{1}{2} \tanh \tau \sinh \tau \right]$, and $\hat{\psi}_{11} = \text{sech} \tau$, $\hat{\psi}_{12} = \frac{1}{2\eta} [\tau \text{sech} \tau + \sinh \tau]$, where $\tau = \eta (\theta - \theta_0)$, with two particular solutions known for both (26) and (27), the general solutions of the second-order inhomogeneous (26) and (27), respectively, can be written as

$$\hat{\phi}_1 = \delta_1 \phi_{11} + \delta_2 \phi_{12} - \phi_{11} \int_{-\infty}^{\theta} \phi_{12} \text{Re } \hat{F}_1 d\theta' + \phi_{12} \int_{-\infty}^{\theta} \phi_{11} \text{Re } \hat{F}_1 d\theta', \quad (30)$$

$$\hat{\psi}_1 = \delta_3 \psi_{11} + \delta_4 \psi_{12} - \psi_{11} \int_{-\infty}^{\theta} \psi_{12} \text{Im } \hat{F}_1 d\theta' + \psi_{12} \int_{-\infty}^{\theta} \psi_{11} \text{Im } \hat{F}_1 d\theta', \quad (31)$$

where δ_1 , δ_2 , δ_3 and δ_4 are arbitrary integration constants. The construction of explicit forms of the general solutions of ϕ_{11} , ϕ_{12} requires evaluation of the integrals in the last two terms in (30). In order to find the general solution

Fig. 4 Real part of the perturbed soliton

of $\hat{\phi}_1$ as given in (A1) in Appendix, we remove the secular terms using the boundary conditions $\hat{\phi}_1(0)|_{\theta_0=0} = 0$ and $\hat{\phi}_{1\theta}(0)|_{\theta_0=0} = 0$, and choosing $\delta_1 = 2.15\alpha\eta^5 - 15.4\left(\frac{b_3\varepsilon^4}{12} - 1\right)\eta^3 + 0.45(12\alpha\xi^2 - 20)\eta^3 - 0.1(40\alpha\xi^2 - 60)\eta^5 - \frac{5}{8}\left(6\xi^2 + b_3\varepsilon^2 - \frac{b_3\varepsilon^4\xi^2}{2}\right)\eta + \frac{7}{8}\left(20\xi^2 - \frac{7\alpha\xi^4}{2} - 24b_2 + \frac{48}{\xi^2}\right)\eta - 14.65\alpha\eta^2 - 4\eta^2 - 0.12\tan^{-1}\left(\frac{1}{2}\right)\xi^4\eta^2 + \frac{16}{15}(12\alpha\xi^2 - 20) - \frac{4}{15}(6\alpha\xi^2 - 10) + \frac{3.15\alpha}{\eta} + \frac{1}{4}\tan^{-1}\left(\frac{1}{2}\right)\alpha\xi^4 + \frac{3}{4}\left(\xi_T(\theta - \theta_0) - 2b_1 + b_3\varepsilon^2\xi^2 + \frac{b_3\varepsilon^4\xi^4}{12} + \frac{12\omega_0}{\varepsilon^2}\right)\eta + \left(\frac{5}{2} - \frac{5}{24}b_3\varepsilon^4\right)\eta^3$ and $\delta_2 = \left(\frac{353}{8}\alpha - \frac{2b_3\varepsilon^4}{3} + \frac{17}{4}\right)\eta^6 + \left(\frac{40}{3}\alpha\xi^2 + \frac{85}{3}\right)\eta^4 + \left(\frac{b_3\varepsilon^2}{2} - \frac{55}{4}\alpha - \frac{9\xi^4}{20} + 3\xi^2 - \frac{b_3\varepsilon^4\xi^2}{8}\right)\eta^3 + \left(10\xi^2 - 12b_2 - 2\xi_T(\theta - \theta_0) + 4b_1 - 2b_3\varepsilon^2\xi^2 - \frac{b_3\varepsilon^4\xi^4}{6} - \frac{24\omega_0}{\varepsilon^2}x - \frac{b_3\varepsilon^4\xi^2}{2}\right)\eta^2 + \left(4\alpha\xi^2 - \frac{\alpha\xi^4}{3} - \frac{20}{3}\right)\eta + \left(\frac{3\xi^2}{2} + \frac{b_3\varepsilon^2}{4} - \frac{b_3\varepsilon^4\xi^2}{8} + \frac{7b_3\varepsilon^4}{12} - 7\right)\frac{1}{\eta} - \frac{9\alpha}{16}$. We have plotted the real part of the perturbed solution (A1) in the Appendix for various values of η , ranging from ($\eta = 0.55, 1.87$) in Fig. 4. From Fig. 4a–b, we observe that when the amplitude of soliton η is tuned gradually, the anti-kink excitation of the proton soliton transforms to anti-solitonic excitation as predicted. Thus, it is evident that the real part of the perturbed proton soliton is quite stable and retains its shape, and remains very robust against these perturbations. Following the same analogy, $\hat{\psi}_1$ can also be constructed as given in (A2) in the Appendix by solving (31) and removing the secular terms upon imposing the boundary conditions $\hat{\psi}_1(0)|_{\theta_0=0} = 0$ and $\hat{\psi}_{1\theta}(0)|_{\theta_0=0} = 0$, and choosing $\delta_3 = \left[\frac{b_3\varepsilon^4\xi}{3} - 2\alpha + 2\alpha\xi\right]\eta^2 - \xi\lambda + \frac{5b_3\varepsilon^4\xi\eta^2}{9} - \frac{80\xi\eta^2}{3} + \frac{53}{45}\alpha\xi\eta^4 - 2\xi^3 + 8\alpha\xi^3\eta^2 + b_3\varepsilon^2 + 2b_3\varepsilon^2\xi - \frac{2b_3\varepsilon^4\xi^3}{3}$ and $\delta_4 = \left[32\xi - \frac{5}{2}b_3\varepsilon^4\xi + 6\alpha\xi - 8\alpha\xi^3\right]\eta^3 + \frac{1728}{135}\alpha\xi\eta^5 + \left[\frac{b_3\varepsilon^4\xi^3}{3} - 4\xi^3 - 2b_3\varepsilon^2\xi\right]\eta - \frac{2\eta_T}{\eta}$. The imaginary part of the perturbed solution is plotted in Fig. 5. It can be noticed from the figures that as the value of η increases, the shape of the proton soliton gains its increasing amplitude as it moves along the PC without any dispersion despite the perturbation

Fig. 5 Imaginary part of the perturbed soliton

existing along the system. This lossless propagation of the proton soliton may explain many biological phenomena. One can conclude that the nonlinear dynamics of the soliton can undoubtedly proceed in understanding the mechanism of information transduction from the exterior to the interior of a cell. A class of molecules, utilized as intravenous anesthetics, form hydrogen bonds with protein molecules situated inside and outside the cytoplasmic membrane. The binding of anesthetic molecules to proteins inhibits the normal function of a cell. One of the possible mechanisms of such an inhibition by the binding of anesthetic molecules, barbiturates to protein, was proposed by Layne in 1984 on the basis of a soliton model. Molecules of barbiturates contain the H-N-C=O group of atoms, which are very similar to the peptide groups in proteins. When a barbiturate molecule attaches to a protein, the hydrogen bonds between neighboring peptide groups in protein molecules are broken and new hydrogen bonds are produced with the oxygen and hydrogen atoms of the barbiturates molecule. At a site of dissociating hydrogen bonds of the protein molecule, the interpeptide separation increases, and this results in the violation of the free motion of a soliton and hence interferes with of the process of transduction of information and energy along the protein molecule. Layne suggested that a decrease of efficiency of the transduction of energy and information by solitons under the binding of barbiturates to proteins is important in helical proteins of the inner mitochondrial membranes which appear to participate in ATP synthesis, and in membrane helical proteins responsible for chemical reception and transduction of signals inside a cell.

5 Molecular dynamic simulation studies of PCs

In this section, in order to analyze the effect of temperature on the evolution of solitons, we carry out molecular dynamics simulation studies for the discrete equations

$$\begin{aligned}
 i\hbar a_{nt} = & \left[(2E_0 + W) + \chi (b_{n+1} - b_{n-1}) + 2E_1 |a_n|^2 \right] a_n - J (a_{n+1} + a_{n-1}) \\
 & - 2J_1 a_n^* (a_{n+1}^2 + a_{n-1}^2) + 2\chi_1 \left[|a_n|^2 a_n (b_{n+1} - b_{n-1}) \right] \\
 & - \frac{\hbar\omega_1^2}{4\omega_0} (a_{n+1}^* + a_{n-1}^* + a_{n-1} + a_{n+1}) - 2jU_0 (a_n^* + a_n) + U_0 \left(\frac{j'}{2} \right)^2 \\
 & \times \left[4a_n^{*3} + 4a_n^3 + 12|a_n|^2 a_n + 12|a_n|^2 a_n^* \right], \quad (32)
 \end{aligned}$$

$$\begin{aligned}
 mb_{nt} = & k [b_{n+1} + b_{n-1} - 2b_n] - \chi \left[|a_{n+1}|^2 - |a_{n-1}|^2 \right] \\
 & + \chi_1 \left[|a_{n+1}|^4 - |a_{n-1}|^4 \right] - M\Gamma q_{nt} + F_n, \quad (33)
 \end{aligned}$$

where Γ is the damping coefficient of the medium, which is about $0.3 \times 10^8 s^{-1}$ for peptide chains. In (33), a decay term $M\Gamma\dot{q}_n$ and random noise term $F_n(t)$, resulting from the interaction between the environment at finite temperature T and the peptide chain, have been added to the displaced equation of heavy ions along the lines of the Lomdahl and Kerr method [44]. The explicit representation for the correlation function of the random noise force is $\langle F(x, t)F(0, 0) \rangle = 2M\Gamma k_B T \delta(x) \delta(t) \frac{1}{\tau}$, where τ' is a damping constant. In our algorithm, we use an ensemble of Gaussian forces F_n with variance equal to $\sigma = 2Mk_B\Gamma\frac{T}{\tau'}$ and we also assume that the deviation of the random noise satisfies the normal distribution and has zero expectation value expressed by $N(F_n) = (\frac{1}{\sqrt{2\pi}\sigma}) \exp(\frac{-F_n^2}{2\sigma^2})$. The above choice of Gaussian width is highly compatible with the fluctuation–dissipation theorem and time discretization. In order to analyze the effects of temperature and random thermal noise forces of the medium, we numerically solve (32) and (33), with the above decay term and random noise force by the fourth-order Runge–Kutta method. The evolution of soliton for different temperatures (273, 300, and 320 K) are depicted in Fig. 6 in the case of the long time of 300 ps for the parametric values $J = 1.55 \times 10^{-22} J$, $W = (1.3 - 19.5) N/m$,

Fig. 6 Snapshots of soliton evolution for **a** $T = 273$ K **b** $T = 300$ K and **c** $T = 320$ K

$m = (1.77 - 19.1) \times 10^{-25} \text{ Kg}$, $\chi_1 = 62 \times 10^{-2}$, $E_0 = 0.205 \text{ eV}$, $U_0 = 0.22 \text{ eV}$, $\omega_0 = (1 - 1.5) \times 10^{14} \text{ s}^{-1}$, $\omega_1 = (4 - 5) \times 10^3 \text{ s}^{-1}$. In Fig. 6, the top panels represent the evolution of soliton for $T = 273 \text{ K}$, the middle panels represent $T = 300 \text{ K}$ and the bottom panels represent the evolution for $T = 320 \text{ K}$. It should also be noted that the first column of Fig. 6 represents the evolution of the soliton for zero nonlinear coupling coefficients representing the change in energy of the amide-I bond caused by stretching of the chain between two neighboring peptide groups, i.e., $\chi_1 = 0$. The other two columns in the Fig. 6 represent the evolution of the soliton for $\chi_1 = 0.5$ and $\chi = 3.5$, respectively. It is clear from Fig. 6a and b that the soliton moves along the peptide chains without dispersion, though it suffers significant damping, as depicted for both $T = 273 \text{ K}$ and $T = 300 \text{ K}$. However, at higher temperature, $T = 320 \text{ K}$, it could be observed from Fig. 6c that though there is a larger thermal perturbation, the nonlinear coupling interaction between the neighboring peptide groups is still able to stabilize the soliton, and the soliton is very robust against the thermal perturbation of the environment with a lifetime of 300 ps, which is same with the numerical results in uniform chains [45].

6 Conclusions

In this paper, we proposed an entirely new improved model for the molecular dynamics of polypeptide chains. Considering Davydov's model as the basis for our analysis, we incorporated the relative change in the displacement of neighboring peptide groups, resulting from the dipole–dipole interaction of amide-I vibrations along with higher-order molecular excitations with quadrupole–quadrupole interaction and higher-order nonlinear coupling, which characterizes the change in energy of the amide-I bond caused by stretching of the chain between two neighboring peptide groups. The Davydov wave function of the excitation state of single particle is now replaced by the quasi-coherent state with two excitons and a coherent phonon state, which can represent the coherent features of the collective excitation of the excitons. The dynamics of the proton transport along the peptide chain is governed by a higher-order nonlinear Schrödinger equation and the energy transport is performed by the proton soliton. The proton soliton in the peptide chains is formed as a result of the dynamical balance between the dispersion due to the resonant interaction of intrapeptide dipole vibrations and the nonlinearity provided by the higher-order molecular interaction of these vibrations with the local displacements of the equilibrium positions of the peptide groups.

In order to study the effect of discreteness, we performed a nonlinear multiple-scale perturbation analysis along the lines of Kodama and Ablowitz. We employ the fourth-order Runge–Kutta method to solve the coupled equations for the soliton parameters such as amplitude and velocity. The perturbed proton soliton solution is constructed and the proton soliton still regains its shape and is robust against the perturbation. We performed molecular dynamics simulation studies and the proton soliton was found to be thermally stable up to 320 K. Furthermore, we have investigated the impact of thermal perturbations on the soliton propagation and hence the robustness of the soliton. For this purpose, the peptide chain is brought into contact with a heat bath that is mimicked by a Gaussian white noise with zero mean and delta-function correlations. The corresponding damping constant is related to the temperature via the fluctuation-dissipation theorem. Altogether,

the evolution of the proton soliton virtually does not change under the impact of thermal and structural perturbations. The experimental world became interested in the Davydov soliton model because of the intriguing infrared (IR) temperature dependence of molecular crystals of the amino acid analog ACN [46] for the coherent energy flow in peptides. ACN, a metabolic precursor to the commercial pain reliever Tylenol, has a far simpler structure than a globular protein, and forms a molecular crystal. This led Alywn Scott to conjecture that indeed the interactions between the acetanilide molecules in the molecular crystal formed by ACN had the right parameters to form a self-trapped Davydov soliton at low temperatures upon absorbing an IR photon at around 6 μm . Myoglobin (a highly alpha-helical protein) thus has a long wavelength-shifted band that has a similar temperature dependence and binding energy (with soliton model) to ACN. Hence, we believe that this solitonic model of higher-order molecular interactions might have some relevance to biology and help to explain the energy flow in peptides at least in the near future.

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Appendix

$$\begin{aligned}
 \hat{\phi}_1 = & \delta_1 S \Delta T \Delta + \frac{\delta_2}{2\eta} (3\Delta S \Delta T \Delta + T \Delta \sinh \Delta) - \frac{\delta_2}{\eta} S \Delta - \alpha \eta^5 \left[\left(\frac{49}{10} \right) S \Delta T^2 \Delta - \left(\frac{14}{5} \right) \cosh(2\Delta) S^3 \right. \\
 & \times \Delta T^4 \Delta - \left(\frac{56}{5} \right) S^3 \Delta T^4 \Delta + \left(\frac{21}{2} \right) \Delta S^7 \Delta T \Delta - \left(\frac{63}{4} \right) \Delta S^5 \Delta T \Delta - \left(\frac{21}{10} \right) S^5 \Delta T \Delta + \left(\frac{49}{20} \right) S^3 \Delta T^2 \Delta \\
 & + \left(\frac{49}{10} \right) S \Delta T \Delta + \left(\frac{21}{5} \right) S \Delta T^6 + \left(\frac{21}{5} \right) S \Delta T \Delta \Delta - \left(\frac{36}{35} \right) \cosh(2\Delta) S^3 \Delta T^6 \Delta + \left(\frac{216}{35} \right) S^3 \Delta T^6 \Delta \\
 & - \left(\frac{87}{35} \right) S \Delta T^2 \Delta + \left(\frac{27}{4} \right) \Delta S^9 \Delta T \Delta - 18 \Delta S^7 \Delta T \Delta + \left(\frac{27}{2} \right) \Delta S^5 \Delta T \Delta - \left(\frac{27}{28} \right) S^7 \Delta T^2 \Delta + \left(\frac{171}{70} \right) \\
 & S^5 \Delta T^2 \Delta - \left(\frac{87}{70} \right) S^3 \Delta T^2 \Delta - \left(\frac{87}{35} \right) S \Delta T \Delta - \left(\frac{18}{7} \right) S \Delta T^8 \Delta - \left(\frac{18}{7} \right) S \Delta T \Delta + \left(\frac{5}{2} \right) S^3 \Delta T^2 \Delta \\
 & + 10 S \Delta T \Delta - \left(\frac{15}{8} \right) S \Delta T^2 \Delta + \left(\frac{45}{16} \right) \Delta S^5 \Delta T \Delta - \left(\frac{45}{8} \right) S^3 \Delta T^2 \Delta - \left(\frac{15}{8} \right) S \Delta T \Delta - \left(\frac{5}{4} \right) S \Delta T^4 \Delta \\
 & - \left(\frac{5}{4} \right) S \Delta T \Delta + \left(\frac{88}{21} \right) S \Delta T^2 \Delta - \left(\frac{55}{7} \right) S^7 \Delta T^2 \Delta - \left(\frac{55}{7} \right) S^7 \Delta T^2 \Delta + \left(\frac{11}{7} \right) S^5 \Delta T^2 \Delta + \left(\frac{44}{21} \right) S^3 \Delta \\
 & T^2 \Delta + \left(\frac{88}{21} \right) S \Delta T \Delta + \left(\frac{44}{21} \right) \Delta S \Delta T^2 \Delta + \left(\frac{55}{48} \right) S^9 \Delta T \Delta - \left(\frac{275}{126} \right) S^7 \Delta T \Delta + \left(\frac{11}{56} \right) S^5 \Delta T \Delta + \left(\frac{11}{21} \right) \\
 & S^3 \Delta T \Delta + \left(\frac{11}{14} \right) \Delta S^5 \Delta T^2 \Delta + \left(\frac{11}{14} \right) \cosh(2\Delta) S^3 \Delta T^6 \Delta + \left(\frac{22}{21} \right) \Delta S^3 \Delta T^2 \Delta + \left(\frac{11}{14} \right) S^3 \Delta T^6 \Delta \\
 & + \left(\frac{36}{35} \right) S^3 \Delta T^6 \Delta + \left(\frac{6}{35} \right) \cosh(2\Delta) S^3 \Delta T^6 \Delta - \left(\frac{29}{70} \right) S \Delta T^2 \Delta - 3 \Delta S^7 \Delta T \Delta + \left(\frac{9}{8} \right) \Delta S^9 \Delta T \Delta \\
 & + \left(\frac{9}{4} \right) \Delta S^5 \Delta T \Delta - \left(\frac{9}{56} \right) S^7 \Delta T^2 \Delta + \left(\frac{57}{140} \right) S^5 \Delta T^2 \Delta - \left(\frac{29}{140} \right) S^3 \Delta T^2 \Delta - \left(\frac{29}{70} \right) S \Delta T \Delta
 \end{aligned}$$

$$\begin{aligned}
& -\left(\frac{3}{7}\right)S\Delta T^8\Delta - \left(\frac{3}{7}\right)S\Delta T\Delta - \left(\frac{16}{7}\right)S\Delta T^2\Delta + \left(\frac{30}{7}\right)S^7\Delta T^2\Delta - \left(\frac{6}{7}\right)S^5\Delta T^2\Delta - \left(\frac{8}{7}\right)S^3\Delta T^2\Delta \\
& - \left(\frac{16}{7}\right)S\Delta T\Delta + \left(\frac{10}{7}\right)S\Delta T^2\Delta + \left(\frac{45}{8}\right)\Delta S^9\Delta T\Delta - \left(\frac{15}{2}\right)\Delta S^7\Delta T\Delta - \left(\frac{45}{56}\right)S^7\Delta T^2\Delta - \left(\frac{10}{7}\right) \\
& S\Delta T^2\Delta + \left(\frac{45}{8}\right)\Delta S^9\Delta T\Delta - \left(\frac{15}{2}\right)\Delta S^7\Delta T\Delta - \left(\frac{45}{56}\right)S^7\Delta T^2\Delta + \left(\frac{15}{28}\right)S^5\Delta T^2\Delta + \left(\frac{5}{7}\right)S^3\Delta T^2\Delta \\
& + \left(\frac{10}{7}\right)S\Delta T\Delta + \left(\frac{3}{7}\right)\cosh(2\Delta)S^3\Delta T^6\Delta + \left(\frac{18}{7}\right)S^3\Delta T^6\Delta + \left(\frac{184}{35}\right)\Delta T^2\Delta - \left(\frac{69}{7}\right)S^7\Delta T^2\Delta \\
& + \left(\frac{69}{35}\right)S^5\Delta T^2\Delta + \left(\frac{92}{35}\right)S^3\Delta T^2\Delta + \left(\frac{184}{105}\right)S\Delta T\Delta - \left(\frac{23}{7}\right)S\Delta T^2\Delta - \left(\frac{207}{4}\right)\Delta S^9\Delta T\Delta \\
& + \left(\frac{69}{4}\right)\Delta S^7\Delta T\Delta + \left(\frac{207}{112}\right)S^7\Delta T^2\Delta - \left(\frac{69}{56}\right)S^5\Delta T^2\Delta - \left(\frac{69}{42}\right)S^3\Delta T^2\Delta - \left(\frac{23}{7}\right)S\Delta T\Delta \\
& - \left(\frac{69}{70}\right)\cosh(2\Delta)S^3\Delta T^6\Delta + \left(\frac{9}{70}\right)\cosh(2\Delta)S^3\Delta T^6\Delta - \left(\frac{207}{35}\right)S^3\Delta T^6\Delta + \left(\frac{27}{35}\right)S^3\Delta T^6\Delta \\
& - \left(\frac{87}{280}\right)S\Delta T^2\Delta + \left(\frac{27}{32}\right)\Delta S^9\Delta T\Delta - \left(\frac{9}{4}\right)\Delta S^7\Delta T\Delta + \left(\frac{27}{16}\right)\Delta S^5\Delta T\Delta - \left(\frac{27}{224}\right)S^7\Delta T^2\Delta \\
& + \left(\frac{1071}{560}\right)S^5\Delta T^2\Delta - \left(\frac{1071}{1680}\right)S\Delta T\Delta - \left(\frac{87}{280}\right)S\Delta T\Delta - \left(\frac{9}{28}\right)S\Delta T^8\Delta - \left(\frac{9}{28}\right)S\Delta T\Delta \Big] \\
& - \left(\frac{b_3\varepsilon^4}{12} - 1\right)\eta^3 \left[\left(\frac{28}{3}\right)S\Delta T^4\Delta + \left(\frac{28}{3}\right)S\Delta T\Delta - 14S\Delta T^2\Delta - \left(\frac{21}{2}\right)\Delta S^5\Delta T\Delta + 21\Delta S^3\Delta T\Delta \right. \\
& + \left(\frac{14}{4}\right)S^3\Delta T\Delta - 14S\Delta T\Delta - 14\Delta S\Delta T\Delta + \left(\frac{56}{3}\right)S\Delta T^2\Delta - \left(\frac{14}{3}\right)S^3\Delta T^2\Delta + \left(\frac{56}{3}\right)S\Delta T\Delta \\
& + 6S\Delta T^5\Delta + 6S\Delta T\Delta + 23S\Delta T^2\Delta - 6\Delta S^7\Delta T\Delta + 18\Delta S^5\Delta T\Delta - 18\Delta S^3\Delta T\Delta + \left(\frac{6}{5}\right)S^5\Delta T\Delta \\
& - \left(\frac{33}{5}\right)S^3\Delta T^2\Delta + \left(\frac{46}{5}\right)S\Delta T\Delta + 12\Delta S\Delta T\Delta - \left(\frac{52}{5}\right)S\Delta T^2\Delta - \left(\frac{12}{5}\right)S^5\Delta T\Delta + \left(\frac{44}{5}\right)S^3\Delta T^2\Delta \\
& - \left(\frac{92}{5}\right)S\Delta T\Delta - 5S\Delta T^2\Delta - 5S\Delta T\Delta + \left(\frac{15}{4}\right)S\Delta T^2\Delta - \left(\frac{15}{4}\right)\Delta S^3\Delta T\Delta + \left(\frac{15}{2}\right)S\Delta T\Delta + \left(\frac{5}{2}\right) \\
& \Delta S\Delta T\Delta - \left(\frac{5}{2}\right)S\Delta T^2\Delta - \left(\frac{5}{2}\right)S\Delta T\Delta \Big] - \eta \left(6\xi^2 + b_3\varepsilon^2 - \frac{b_3\varepsilon^4\xi^2}{2} \right) \left[\left(\frac{1}{3}\right)S\Delta T^4\Delta + \left(\frac{1}{3}\right)S\Delta T\Delta \right. \\
& - \left(\frac{1}{2}\right)S\Delta T^2\Delta - \left(\frac{3}{8}\right)\Delta S^5\Delta T\Delta + \left(\frac{3}{4}\right)\Delta S^3\Delta T\Delta + \left(\frac{1}{8}\right)S^3\Delta T\Delta - \left(\frac{1}{2}\right)S\Delta T\Delta - \left(\frac{1}{2}\right)\Delta S\Delta T\Delta \\
& + \left(\frac{2}{3}\right)S\Delta T^2\Delta - \left(\frac{1}{6}\right)S^3\Delta T^2\Delta - \left(\frac{2}{3}\right)S\Delta T\Delta \Big] - \left(6\xi^2 + b_3\varepsilon^2 - \frac{b_3\varepsilon^4\xi^2}{2} \right) \frac{1}{\eta} \left[\left(-\frac{1}{2}\right)S^3\Delta T^2\Delta \right. \\
& - \left(\frac{2}{3}\right)S\Delta T^2\Delta - \left(\frac{2}{3}\right)S\Delta T\Delta + \left(\frac{1}{4}\right)S\Delta T^2\Delta - \left(\frac{3}{8}\right)\Delta S^5\Delta T\Delta + \left(\frac{1}{8}\right)S^3\Delta T^2\Delta + \left(\frac{1}{4}\right)S\Delta T\Delta \\
& + \left(\frac{1}{3}\right)S\Delta T^4\Delta + \left(\frac{1}{3}\right)S\Delta T\Delta \Big] - \eta \left(12\alpha\xi^2 - 20 \right) \left[\left(\frac{1}{15}\right)\cos(2\Delta)S^3\Delta T^4\Delta + \left(\frac{4}{15}\right)S^3\Delta T^4\Delta \right. \\
& - \left(\frac{7}{60}\right)S\Delta T^2\Delta - \left(\frac{1}{4}\right)\Delta S^7\Delta T\Delta + \left(\frac{3}{8}\right)\Delta S^5\Delta T\Delta + \left(\frac{1}{60}\right)S^5\Delta T\Delta - \left(\frac{7}{120}\right)S^3\Delta T^2\Delta \\
& - \left(\frac{7}{60}\right)S\Delta T\Delta - \left(\frac{1}{10}\right)S\Delta T^6\Delta - \left(\frac{1}{10}\right)S\Delta T\Delta - \left(\frac{8}{15}\right)S\Delta T\Delta - \left(\frac{1}{5}\right)S^5\Delta T^2\Delta - \left(\frac{4}{15}\right)S^3\Delta T^2\Delta \\
& - \left(\frac{8}{15}\right)S\Delta T\Delta \Big] - \left(6\alpha\xi^2 - 10 \right) \left[\left(\frac{4}{15}\right)S\Delta T^2\Delta - \left(\frac{1}{2}\right)\Delta S^7\Delta T\Delta + \left(\frac{1}{10}\right)S^5\Delta T^2\Delta + \left(\frac{2}{15}\right)S^3\Delta T^2\Delta \right. \\
& + \left(\frac{4}{15}\right)S\Delta T\Delta + \left(\frac{1}{15}\right)\cos(2\Delta)S^3\Delta T^4\Delta + \left(\frac{4}{5}\right)S^3\Delta T^4\Delta \Big] - \alpha\eta^2 \left[\left(\frac{176}{7}\right)S\Delta T^2\Delta + \left(\frac{11}{7}\right)S^7\Delta T^2\Delta \right. \\
& + \left(\frac{66}{7}\right)S^5\Delta T^2\Delta + \left(\frac{88}{7}\right)S^3\Delta T^2\Delta + \left(\frac{176}{7}\right)S\Delta T\Delta - \left(\frac{33}{7}\right)S\Delta T^2\Delta + \left(\frac{165}{16}\right)\Delta S^9\Delta T\Delta - \left(\frac{165}{112}\right)
\end{aligned}$$

$$\begin{aligned}
& S^7 \Delta T^2 \Delta - \left(\frac{99}{56}\right) S^5 \Delta T^2 \Delta - \left(\frac{33}{14}\right) S^3 \Delta T^2 \Delta - \left(\frac{33}{7}\right) S \Delta T \Delta - \left(\frac{44}{21}\right) S \Delta T^2 \Delta + \left(\frac{55}{14}\right) S^7 \Delta T^2 \Delta \\
& - \left(\frac{11}{14}\right) S^5 \Delta T \Delta - \left(\frac{22}{21}\right) S^3 \Delta T^2 \Delta - \left(\frac{44}{21}\right) S \Delta T \Delta + \left(\frac{24}{35}\right) S \Delta T^2 \Delta - \left(\frac{9}{7}\right) S^7 \Delta T^2 \Delta + \left(\frac{9}{35}\right) S^5 \\
& \Delta T^2 \Delta + \left(\frac{24}{35}\right) S \Delta T \Delta + \left(\frac{3}{7}\right) S \Delta T^2 \Delta + \left(\frac{27}{16}\right) \Delta S^9 \Delta T \Delta - \left(\frac{9}{4}\right) \Delta S^7 \Delta T \Delta - \left(\frac{27}{112}\right) S^7 \Delta T^2 \Delta \\
& + \left(\frac{9}{56}\right) S^5 \Delta T^2 \Delta + \left(\frac{3}{14}\right) S^3 \Delta T^2 \Delta + \left(\frac{3}{7}\right) S \Delta T \Delta + \left(\frac{9}{70}\right) \cos(2\Delta) S^3 \Delta T^6 \Delta + \left(\frac{27}{35}\right) S^3 \Delta T^6 \Delta \Big] \\
& - \eta^2 \left[\left(\frac{5}{2}\right) S^5 \Delta T \Delta + \left(\frac{5}{2}\right) S \Delta T \Delta + 2 \Delta S \Delta T^2 \Delta - \left(\frac{3}{4}\right) S^5 \Delta T \Delta + \left(\frac{1}{2}\right) S^3 \Delta T \Delta - 2 \log(\cosh \Delta) S \Delta \right. \\
& \left. T \Delta - 3 \Delta S^5 \Delta T^2 \Delta - \Delta S^3 \Delta T^2 \Delta + \left(\frac{5}{4}\right) S \Delta T^5 \Delta + \left(\frac{5}{4}\right) S \Delta T \Delta \right] - \eta^3 \left(12 \alpha \xi^2 - 30 \right) \left[\left(\frac{1}{15}\right) \cos(2\Delta) \right. \\
& \left. S^3 \Delta T^4 \Delta + \left(\frac{4}{15}\right) S^3 \Delta T^4 \Delta + \left(\frac{7}{60}\right) S \Delta T^2 \Delta + \left(\frac{1}{4}\right) S^7 \Delta T \Delta - \left(\frac{3}{8}\right) \Delta S^5 \Delta T \Delta - \left(\frac{1}{20}\right) S^5 \Delta T^2 \Delta \right. \\
& \left. + \left(\frac{7}{120}\right) S^3 \Delta T^2 \Delta + \left(\frac{7}{60}\right) S \Delta T \Delta + \left(\frac{1}{10}\right) S \Delta T^6 \Delta + \left(\frac{1}{10}\right) S \Delta T \Delta \right] - \frac{\alpha}{\eta} \left[\left(\frac{72}{35}\right) S \Delta T^2 \Delta + \left(\frac{9}{14}\right) S^7 \right. \\
& \left. \Delta T^2 \Delta + \left(\frac{27}{35}\right) S^5 \Delta T^2 \Delta + \left(\frac{36}{35}\right) S^3 \Delta T^2 \Delta + \left(\frac{72}{35}\right) S \Delta T \Delta - \left(\frac{27}{70}\right) S \Delta T^2 \Delta + \left(\frac{27}{32}\right) \Delta S^9 \Delta T \Delta \right. \\
& \left. - \left(\frac{27}{224}\right) S^7 \Delta T^2 \Delta - \left(\frac{81}{560}\right) S^5 \Delta T^2 \Delta - \left(\frac{27}{140}\right) S^3 \Delta T^2 \Delta - \left(\frac{27}{70}\right) S \Delta T \Delta - \left(\frac{12}{70}\right) S \Delta T^2 \Delta \right. \\
& \left. + \left(\frac{9}{28}\right) S^7 \Delta T^2 \Delta - \left(\frac{9}{140}\right) S^5 \Delta T^2 \Delta - \left(\frac{3}{35}\right) S^3 \Delta T^2 \Delta - \left(\frac{6}{35}\right) S \Delta T \Delta \right] - \eta \left(20 \xi^2 - \frac{7}{2} \alpha \xi^4 - 24 b_2 \right. \\
& \left. + \frac{48}{\varepsilon^2} \right) \left[\left(\frac{1}{3}\right) S^3 \Delta T^2 \Delta + \left(\frac{2}{3}\right) S \Delta T^2 \Delta + \left(\frac{2}{3}\right) S \Delta T \Delta + \left(\frac{1}{4}\right) S \Delta T^2 \Delta - \left(\frac{3}{8}\right) \Delta S^5 \Delta T \Delta + 8 S^3 \Delta T^2 \Delta \right. \\
& \left. - \frac{12 \omega_0}{\varepsilon^2} \right) (S \Delta T^2 \Delta + S \Delta T \Delta) + \left(\frac{3}{2} \xi_T (\Theta - \Theta_0) - 3 b_1 + \frac{3 b_3 \varepsilon^2 \xi^2}{2} + \frac{b_3 \varepsilon^4 \xi^4}{8} + \frac{18 \omega_0}{\varepsilon^4} \right) \\
& (\Delta S \Delta T \Delta - S \Delta T^2 \Delta - S \Delta T \Delta) \Big] - \xi^4 \eta^2 \left[\left(\frac{3}{4}\right) S \Delta T \Delta \tan^{-1} \left(T \left(\frac{\Delta}{2} \right) \right) + \left(\frac{1}{4}\right) S^4 \Delta T^2 \Delta \right. \\
& + \left(\frac{3}{8}\right) S^2 \Delta T^2 \Delta + \left(\frac{3}{4}\right) S \Delta T \Delta \tan^{-1} \left(\frac{1}{2} \right) + \left(\frac{3}{10}\right) \Delta S^6 \Delta T \Delta - \left(\frac{9}{40}\right) S \Delta T \Delta \tan^{-1} \left(T \left(\frac{\Delta}{2} \right) \right) \\
& - \left(\frac{3}{40}\right) S^4 \Delta T^2 \Delta - \left(\frac{9}{80}\right) S^2 \Delta T^2 \Delta - \left(\frac{9}{40}\right) S \Delta T \Delta \tan^{-1} \left(\frac{1}{2} \right) - \left(\frac{1}{8}\right) S \Delta T \Delta \tan^{-1} \left(T \left(\frac{\Delta}{2} \right) \right) \\
& + \left(\frac{1}{8}\right) S^4 \Delta T^2 \Delta - \left(\frac{1}{16}\right) S^2 \Delta T^2 \Delta - \left(\frac{1}{8}\right) S \Delta T \Delta \tan^{-1} \left(\frac{1}{2} \right) \Big] - (40 \alpha \xi^2 - 60) \eta^3 \left[\left(\frac{8}{15}\right) S \Delta T^2 \Delta \right. \\
& + \left(\frac{1}{5}\right) S^5 \Delta T^2 \Delta + \left(\frac{4}{15}\right) S^3 \Delta T^2 \Delta + \left(\frac{8}{15}\right) S \Delta T \Delta + \left(\frac{2}{15}\right) S \Delta T^2 \Delta - \left(\frac{1}{4}\right) \Delta S^7 \Delta T \Delta \\
& + \left(\frac{1}{20}\right) S^5 \Delta T^2 \Delta + \left(\frac{1}{15}\right) S^3 \Delta T^2 \Delta + \left(\frac{2}{15}\right) S \Delta T \Delta + \left(\frac{2}{15}\right) S^3 \Delta T^4 \Delta + \left(\frac{1}{30}\right) \cos(2\Delta) S^3 \Delta T^4 \Delta \Big] \\
& - \alpha \xi^4 \left[\left(\frac{1}{4}\right) S^2 \Delta T^2 \Delta + \left(\frac{1}{4}\right) \Delta S^4 \Delta T \Delta \right] + \left[\frac{161}{6} \alpha \eta^5 + \frac{35}{3} \eta^3 + \frac{20}{3} \alpha \xi^2 \eta^3 + 2 \alpha \xi^2 - \frac{10}{3} \right] S^7 \Delta \\
& - \left[-\frac{139}{4} \alpha \eta^5 + \frac{5}{2} \eta^3 + \frac{15}{4} \eta^5 - \left(\frac{3}{2} \xi^2 + \frac{b_3 \varepsilon^2}{4} - \frac{b_3 \varepsilon^4 \xi^2}{8} \right) \frac{1}{\eta^2} - \left(5 \xi^2 - \frac{7}{8} \alpha \eta^4 - 6 b_2 + \frac{12}{\varepsilon^2} \right) \eta \right] S^5 \Delta \\
& - \left[\frac{103}{2} \alpha \eta^5 + \frac{55}{8} \alpha \eta^2 + \frac{9 \alpha}{16 \eta} \right] S^9 \Delta + \left[\frac{3 \xi^2}{2} + \frac{b_3 \varepsilon^2}{4} - \frac{b_3 \varepsilon^4 \xi^2}{8} \right] \eta S \Delta T^4 \Delta - \left(\frac{b_3 \varepsilon^4}{3} - 4 \right) \eta^3 S \Delta T^6 \Delta \\
& - \left(\frac{5}{2} - \frac{5}{24} b_3 \varepsilon^4 \right) \eta^3 S^3 \Delta T \Delta - \frac{2}{3} \eta^2 \cos(2\Delta) S^3 \Delta T^3 \Delta - \frac{8}{3} \eta^2 S^3 \Delta T^3 \Delta - \left[\xi_T (\Theta - \Theta_0) - 2 b_1 \right.
\end{aligned}$$

$$\begin{aligned}
& +b_3\varepsilon^2\xi^2 + \frac{b_3\varepsilon^4\xi^4}{12} + \frac{12\omega_0}{\varepsilon^2} \Big] \eta S^2\Delta - \frac{\xi^4\eta^2S^6\Delta}{4} - \frac{\alpha\varepsilon^4S^4\Delta}{6} + \left(\frac{7b_3\varepsilon^4}{12} - 7 \right) \frac{1}{\eta^2} S\Delta + \left[6\xi^2 + b_3\varepsilon^2 \right. \\
& \left. - \frac{b_3\varepsilon^4\xi^2}{2} \right] \frac{\eta^2}{4} S\Delta - \left(\frac{b_3\varepsilon^4\eta^5}{3} - 4\eta^5 \right) S\Delta + \left[\frac{75}{4}\alpha\eta^5 - \frac{25}{2}\eta^3 - 3\alpha\xi^2 - 10\alpha\xi^2\eta^3 + 5 \right] \Delta S^7\Delta T\Delta \\
& + \left[\frac{15}{4}\eta^3 + \frac{45}{8}\eta^5 - \frac{849}{16}\alpha\eta^5 - \frac{\xi^2}{\eta^2} - \frac{3}{8}b_3\varepsilon^2 - \frac{3}{16}\varepsilon^4\xi^2 - \frac{15\xi^2}{2\eta} - \frac{21\alpha\eta\xi^4}{16} - 9b_2\eta + \frac{18\eta}{\varepsilon^2} \right] \Delta S^5\Delta T\Delta \\
& + \left[\frac{165}{16}\alpha\eta^2 + \frac{27\alpha}{32\eta} + \frac{309}{2}\alpha\eta^5 \right] \Delta S^9\Delta T\Delta - \eta \left[\frac{9}{4}\xi^2 + \frac{3b_3\varepsilon^2}{8} - \frac{3b_3\varepsilon^4\xi^2}{16} \right] \Delta S\Delta T^5\Delta + \left(\frac{b_3\varepsilon^4}{2} - 6 \right) \\
& \eta^3 S\Delta T^7\Delta + \left[\frac{15\eta^3}{4} - \frac{5\eta^3b_3\varepsilon^4}{16} \right] \Delta S^3\Delta T\Delta + 4\eta^2 S^3\Delta T^4\Delta + \eta^2\Delta \cos(2\Delta) S^3\Delta T^4\Delta - \frac{3}{2\eta} \left[\xi_T \right. \\
& \left. (\Theta - \Theta_0) - 2b_1 + b_3\varepsilon^2\xi^2 + \frac{b_3\varepsilon^4\xi^4}{12} + \frac{12\omega_0}{\varepsilon^2} \right] \Delta S^2\Delta T\Delta + \frac{3}{10}\xi^4\eta^2\Delta S^6\Delta T\Delta + \frac{1}{4}\alpha\varepsilon^4\Delta S^4\Delta \\
& T\Delta + \left[\frac{3}{2\eta} \left(7 - \frac{7}{12}b_3\varepsilon^4 \right) - \frac{3\eta}{8} \left(6\xi^2 + b_3\varepsilon^2 - \frac{b_3\varepsilon^4\xi^2}{2} \right) + \frac{3}{2} \left(b_3\varepsilon^4\eta^3 - 4\eta^3 \right) \right] \Delta S\Delta T\Delta \\
& + \left[-\frac{125}{12}\alpha\eta^5 - \frac{35}{6}\eta^3 - \alpha\xi^2 + \frac{5}{3} - \frac{5}{3}\alpha\xi^2\eta^3 \right] S^6\Delta T\Delta s\Delta + \left[\frac{5}{4}\eta^3 - \frac{41}{2}\alpha\eta^5 - \left(\frac{3}{4}\xi^2 + \frac{b_3\varepsilon^2}{8} \right. \right. \\
& \left. \left. - \frac{b_3\varepsilon^4\xi^2}{16} \right) \frac{1}{\eta^2} - \left(\frac{5}{2}\xi^2 - \frac{7}{16}\alpha\xi^4 - 3b_2 + \frac{6}{\varepsilon^2} \right) \eta \right] S^4\Delta T\Delta s\Delta + \left[\frac{103}{2}\alpha\eta^5 + \frac{55}{16}\alpha\eta^2 + \frac{9\alpha}{32\eta} \right] \\
& S^8\Delta T\Delta s\Delta - \eta \left[\frac{3\xi^2}{4} + \frac{b_3\varepsilon^2}{8} - \frac{b_3\varepsilon^4\xi^2}{16} \right] T^5\Delta s\Delta + \left[\frac{b_3\varepsilon^4}{6} - 2 \right] \eta^3 T^7\Delta s\Delta + \left[\frac{5}{4} - \frac{5b_3\varepsilon^4}{48} \right] \\
& \eta^3 S^2\Delta T\Delta s\Delta + \frac{4}{3}\eta^2 S^2\Delta T^4\Delta s\Delta + \frac{\eta^2}{3} \cos(2\Delta) S^2\Delta T^4\Delta s\Delta - \left[\xi_T (\Theta - \Theta_0) - 2b_1 + b_3\varepsilon^2\xi^2 \right. \\
& \left. + \frac{b_3\varepsilon^4\xi^4}{12} + \frac{12\omega_0}{\varepsilon^2} \right] \frac{1}{2\eta} S\Delta T\Delta s\Delta + \frac{\xi^4\eta^2}{10} S^5\Delta T\Delta s\Delta + \frac{\alpha}{2}\varepsilon^4 S^3\Delta T\Delta s\Delta + \left[\left(7 - \frac{7b_3\varepsilon^4}{12} \right) \right. \\
& \left. \frac{1}{2\eta^2} + \frac{b_3\varepsilon^4\eta^3}{6} - 2\eta^3 - \frac{\eta}{8} \left(6\xi^2 + b_3\varepsilon^2 - \frac{b_3\varepsilon^4\xi^2}{2} \right) \right] T\Delta s\Delta. \tag{A1}
\end{aligned}$$

$$\begin{aligned}
\hat{\psi}_1 = & \left[\left(\frac{34}{3} \right) \xi\eta^2 - \left(\frac{14}{3} \right) \alpha\xi\eta^2 - \left(\frac{118}{45} \right) \alpha\xi\eta^4 - 2\xi^3 + 3\varepsilon^4\xi^3 + \left(\frac{1}{3} \right) b_3\varepsilon^4\xi\eta^3 + \left(\frac{5}{18} \right) b_3 \right. \\
& \xi\varepsilon^4\eta^2 + \left(\frac{8}{3} \right) \alpha\xi^3\eta^2 - 2b_3\varepsilon^2\xi + \frac{\theta - \theta_0}{2} \Big] S\Delta T\Delta + \left[\delta_3 - 18\xi\eta^2 - 14\alpha\xi\eta^2 \right. \\
& \left. + \left(\frac{3}{2} \right) b_3\varepsilon^4\xi\eta^2 + \left(\frac{227}{15} \right) \alpha\xi\eta^4 + 8\alpha\xi^3\eta^2 + \left(\frac{2}{3} \right) b_3\varepsilon^4\xi^3 - 2\xi^3 - 2b_3\varepsilon^2\xi + \frac{(\theta - \theta_0)_T}{2} \right] \\
& S\Delta + \left[\left(\frac{\delta_4}{2\eta} \right) + \left(\frac{1}{3} \right) b_3\varepsilon^4\xi - \left(\frac{7}{2} \right) \xi\eta^2 + 4\xi^3 + 2b_3\varepsilon^2\xi - \left(\frac{1}{3} \right) b_3\varepsilon^4\xi^3 - \left(\frac{1}{24} \right) b_3\varepsilon^4\xi\eta^2 \right. \\
& \left. - (\theta - \theta_0)_T \right] \Delta S\Delta + \left[\left(\frac{23}{3} \right) \xi\eta^2 - 3b_3\varepsilon^4\xi\eta^2 + \left(\frac{14}{3} \right) \alpha\xi\eta^2 - 2\alpha\xi^3\eta^2 - 2\alpha\xi\eta^4 \right. \\
& \left. - \left(\frac{5}{24} \right) b_3\varepsilon^4\eta^2 \right] \Delta S^5\Delta + \left[2\xi\eta^2 + 2\alpha\xi\eta^2 - \left(\frac{1}{6} \right) b_3\varepsilon^4\xi - \xi^3 - b_3\varepsilon^2 - \left(\frac{1}{2} \right) b_3\varepsilon^4\xi^3 \right.
\end{aligned}$$

$$\begin{aligned}
& + \left(\frac{1}{2} \right) b_3 \varepsilon^2 \xi - \frac{(\theta - \theta_0)T}{3} \Big] \Delta S^3 \Delta + \left[\left(\frac{-13}{3} \right) \xi \eta^2 + \left(\frac{1}{3} \right) \alpha \xi \eta^2 - \left(\frac{5}{36} \right) \varepsilon^4 \xi \eta^2 + \left(\frac{4}{3} \right) \right. \\
& \alpha \xi^3 \eta^2 - \left(\frac{59}{45} \right) \alpha \xi \eta^4 \Big] S^3 \Delta T \Delta + \left[\left(\frac{-20}{3} \right) \xi \eta^2 - \left(\frac{5}{9} \right) b_3 \varepsilon^4 \xi \eta^2 + \left(\frac{16}{3} \right) \alpha \xi^3 \eta^2 \right] S \Delta T \Delta \\
& - \left(\frac{112}{15} \right) \alpha \xi \eta^4 S^3 \Delta T^3 \Delta \left(\frac{14}{3} \right) \Delta S \Delta + \left(\frac{\eta_T}{\eta^2} \right) \Delta S \Delta T \Delta - \left(\frac{4}{3} \right) \alpha \xi \eta^4 \cos(2\Delta) S \\
& \Delta T^3 \Delta - \frac{4}{5} \alpha \xi \eta^4 S \Delta T \Delta + \left[\frac{\delta_4}{2\eta} - \left(\frac{1}{2} \right) b_3 \varepsilon^4 \xi \eta^2 + \frac{\xi \eta^2}{2} \right] s \Delta - \frac{26}{15} \alpha \xi \eta^4 S \Delta T \Delta \\
& + 2\alpha \xi \eta^4 S \Delta + 3\alpha \xi \eta^4 S \Delta T^4 \Delta + \frac{\eta_T}{2\eta^2} \Delta^2 S \Delta + \left[\frac{\xi \eta^2}{2} - \left(\frac{1}{24} \right) b_3 \varepsilon^4 \xi \eta^2 \right] \Delta S \Delta T^6 \Delta \\
& - \alpha \xi \eta^4 S^4 \Delta + \left[\left(\frac{-5}{2} \right) \xi \eta^2 - \left(\frac{5}{8} \right) b_3 \varepsilon^4 \eta^2 + \alpha \xi \eta^4 + 2\alpha \xi^3 \eta^2 \right] S^4 \Delta s \Delta + \left[\left(\frac{-1}{24} \right) b_3 \varepsilon^4 \right. \\
& \left. \xi \eta^2 + \left(\frac{1}{2} \right) \xi \eta^2 \right] \tanh^6 \Delta s \Delta - \left(\frac{7}{3} \right) \alpha \xi \eta^4 S \Delta s \Delta + \left[\xi^3 + \left(\frac{1}{2} \right) b_3 \varepsilon^2 \xi - \left(\frac{1}{12} \right) S^2 \Delta s \Delta \right]. \quad (A2)
\end{aligned}$$

where, $S\Delta = \text{sech } \Delta$, $T\Delta = \tanh \Delta$ and $s\Delta = \sinh \Delta$

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