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Soliton excitations and interaction in alpha helical protein with interspine coupling in modified nonlinear Schrödinger equation*

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The three-coupling modified nonlinear Schrödinger (MNLS) equation with variable-coefficients is used to describe the dynamics of soliton in alpha helical protein. This MNLS equation with variable-coefficients is firstly transformed to the MNLS equation with constant-coefficients by similarity transformation. And then the one-soliton and two-soliton solutions of the variable-coefficient-MNLS equation are obtained by solving the constant-coefficient-MNLS equation with Hirota method. The effects of different parameter conditions on the soliton solutions are discussed in detail. The interaction between two solitons is also discussed. Our results are helpful to understand the soliton dynamics in alpha helical protein.

Keywords: soliton, three-coupling nonlinear modified Schrödinger equation, similarity transformation

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1. Introduction

Bio-material, bio-information, and bio-energy are three essential elements in life activity. Among them, the transmission of biological information is always accompanied by the transmission of bio-energy. Therefore, the transport of biological energy is an important and basic process in life activities, and its research is one of the important research topics in biophysics.[1,2] In the living system, the energy required for most life activities is provided by the hydrolysis of Adenosine triphosphate (ATP), and the energy released by ATP hydrolysis always requires transmission media to reach the desired place. Since ATP molecules can be attached to specific sites of the protein molecules, and the transport of bio-energy released by ATP hydrolysis is always related to the conformation and configuration of protein molecules, so proteins become ideal media for transmitting biological energy. Among three conformations in proteins including α-helix, β-sheet, and globular conformation, it is generally believed that the alpha helical structure of proteins is the most stable and beneficial structure for biological energy transport.[3,4] It is of great significance to study the transmission mechanism of biological energy in alpha helical protein to understand the fundamental processes of many life activities, such as DNA reduplication, muscle contraction, neuroelectric pulse delivery on the neurolemma, and intracellular calcium pump and sodium pump, and so on. Therefore, the storage and transport of energy through alpha helical protein chains have attracted the attention of many researchers. Davydov *et al.*[5] first proposed a novel mechanism of the bio-energy transport in protein by using the soliton theory in 1973. They illustrated that the energy released by the ATP can be propagated as soltions along the alpha helical protein chain due to the precise balance between the dipole–dipole dispersion and nonlinear interaction of amide-I vibration (exciton) and protein acoustic vibration (phonon).[6,7]

The dynamic behavior of these solitons is generally governed by various nonlinear equations, which can be used to study proteins,[8] optics,[9–11] shallow water waves,[12] plasma,[13] and many other systems.[14–16] Through the study of energy-associated Hamiltonian, the nonlinear Schrödinger equation (NLSE) was usually proposed to simulate the soliton dynamics of the Davydov's model in alpha helical protein, which was first proposed by Davydov.[5] Various properties of such one-dimensional polaron-like self-trapped states have been investigated in detail both analytically and numerically. What is more, the dynamical properties of Davydov solitons have also been investigated in discrete and continuum models.[17–19] Most of these results have been obtained for a single chain.[20,21] In fact, the alpha helical protein contains three chains, each of which contains periodic peptide groups linked by hydrogen bonds, which has long been the focus of researchers. Based on the above ideas, a three-coupled model

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has been used to describe the dynamic behavior of solitons in the three-spine alpha helical protein.[22] At the same time, Daniel and Deepamala have studied the effects of high-order molecular excitation and interaction on the solitons dynamics of alpha helical protein.[23] Recently, Saravana Veni and Latha[24] obtained the three-coupled MNLS equation to describe the dynamics of alpha helical protein as follows:

$$\mathrm{i}u_{j,t}+\frac{1}{2}u_{j,xx}-\mathrm{i}\lambda\sum_{q=1}^{3}(u_j|u_q|^2)_x+\sum_{q=1}^{3}(u_j|u_q|^2)=0,\quad(j=1,2,3),\tag{1}$$

where u_j characterizes the probability amplitudes of the exciton in the j-th spine and λ is a constant.

Most of these works reported earlier focused on the nonlinear Schrödinger equations with constant-coefficients to investigate the dynamics of solitons alpha helical protein. In fact, there are some additional molecules at specific sites in the sequence, and the change of the distance between the adjacent atom can also lead to the presence of dipole–dipole interactions in the proteins, which can lead to inhomogeneity of alpha helical protein.[25,26] These inhomogeneities usually result in loss or gain, phase modulation, and variable dispersion of the alpha helical protein. When the inhomogeneity is considered, the NLS equation with variable-coefficients can describe the dynamics of soliton in inhomogeneous alpha helical protein more clearly and systematically.[27] So in this paper, the three-coupling modified nonlinear Schrödinger equation with variable-coefficient is considered as follows:

$$\mathrm{i}u_{j,t}+\frac{1}{2}\beta u_{j,xx}-\mathrm{i}\lambda\gamma_1\sum_{q=1}^{3}(u_j|u_q|^2)_x+\gamma_2\sum_{q=1}^{3}(u_j|u_q|^2)+\Gamma u=0,\quad(j=1,2,3),\tag{2}$$

where $\beta=\beta(x,t)$, $\gamma_1=\gamma_1(x,t)$, $\gamma_2=\gamma_2(x,t)$, $\Gamma=\Gamma(x,t)$ are four real functions of the distance variable x and time variable t. These parameters represent coefficients related to the dispersion terms and the nonlinear terms, and their values vary with the disturbance of protein molecular structure and the influence of environmental conditions.

Yet, to date, little is known about the periodicity of solitons and the interaction between the solitons in alpha helical protein. Actually, the periodic solitons such as breathers and their collision are very important in optics[28–30] and other systems,[31–33] especially in those systems with higher-order terms.[34] In this paper, the periodic behavior of the solitons and the effect of the parameters on the soliton profile and soliton dynamics will be investigated in detail. The interaction between two solitons will also be studied. There are many nonlinear methods can be used to study the dynamics of the soliton.[35–38] Due to the advantages of the similarity transformation and bilinear method in solving analytic soliton solutions of variable-coefficient equations, these two methods are used in combination here to solve the soliton solutions of the three-coupling MNLS equation in Section 2. In Section 3, the profile and dynamic behavior of the soliton in alpha helical protein are analyzed. The periodic oscillation dynamics of the soliton are excited in alpha helical protein. The effect of parameters on soliton is also investigated. Section 4 is devoted to the conclusion.

2. Exact soliton solutions of the three coupled MNLS equation

In order to obtain the analytical soliton solutions of Eq. (2), a similarity transformation is used in the following form:[39]

$$u_j(x,t)=\Psi_j(X,T)\rho\,\mathrm{e}^{\mathrm{i}\varphi},\tag{3}$$

where Ψ_j includes two independent variables $X=X(x,t)$ and $T=T(t)$. By substituting Eq. (3) into Eq. (2), the following equations are obtained:

$$\begin{aligned}&\mathrm{i}\rho T_t\Psi_{j,t}+\frac{1}{2}\beta\rho X_x^2\Psi_{j,XX}-\mathrm{i}\lambda\gamma_1\rho^3X_x\sum_{q=1}^{3}(\Psi_j|\Psi_q|^2)_X\\&+(-\mathrm{i}\beta\lambda(3\rho^2\rho_x+\mathrm{i}\rho^3\phi_x)+\gamma_2\rho^3)\sum_{q=1}^{3}(\Psi_j|\Psi_q|^2)\\&+\left(\mathrm{i}\rho_t-\rho\phi_t+\frac{1}{2}\beta\rho_{xx}+\mathrm{i}\beta\rho_x\phi_{xx}\right.\\&\left.+\frac{1}{2}\mathrm{i}\beta\rho\phi_{xx}-\frac{1}{2}\beta\rho\phi_x^2+\rho V\right)\Psi_j\\&+\left(\mathrm{i}\rho X_t+\frac{1}{2}\beta\rho X_{xx}+\beta X_x\rho_x+\mathrm{i}\beta X_x\rho\phi_x\right)\Psi_{j,x},\\&(j=1,2,3).\end{aligned}\tag{4}$$

By using the similarity transformation method, the following equations are obtained:

$$\rho(x,t)=\frac{1}{T_t}\beta,\quad(x,t)=\frac{T_t}{X_x^2},\quad\gamma_1=\frac{T_t^3}{X_x}\lambda,$$
$$T_t^3\varphi_x+\gamma_2X_x=0,\quad-T_{\mathrm{tt}}X_x^2+\frac{1}{2}T_t^2\varphi_{xx}=0,\tag{5}$$
$$\Gamma X_x^2-\varphi_tX_x^2-\frac{1}{2}\varphi_x^2T_t=0,$$
$$X_tX_x+T_t\varphi_x=0\frac{1}{2}T_tX_{xx}=0.\tag{6}$$

Then equation (4) can be simplified into the following equation with constant-coefficients:

$$\mathrm{i}\Psi_{j,T}+\frac{1}{2}\Psi_{j,XX}-\mathrm{i}\lambda\sum_{q=1}^{3}(|\Psi_q|^2\Psi_j)_X=0,\quad(j=1,2,3).\tag{7}$$

By solving Eq. (5), we have

$$\rho=\frac{\sqrt{m_1}}{c_1},\quad\varphi=-m_1^{3/2}\left(\frac{1}{2}(m_{1,t}x^2+m_{2,t}x)\right)\Big/c_1+m_3,$$

$$X = m_1 x + m_2, \quad \beta = \frac{c_1}{m_1^{5/2}}, \quad \gamma_2 = \frac{\lambda c_1^2 (m_{1,t} x + m_{2,t})}{m_1},$$
$$\Gamma = -\frac{1}{4c_1}(n_1 x^2 + n_2 x + n_3), \quad \gamma_1 = \frac{c1}{m_1^{5/2}},$$
$$T = c_2 + c_1 \int 1/\sqrt{m_1}\mathrm{d}t, \tag{8}$$

where

$$n_1 = 2m_1^{3/2} m_{1,tt} + 3(m_{1,t})^2 \sqrt{m_1} + 2m_{1,t}^2 c_1,$$
$$n_2 = 4m_1^{3/2} m_{2,tt} + 6m_{1,t} m_{2,t} \sqrt{m_1} + 4m_{1,t} m_{2,t} c_1,$$
$$n_3 = 2(m_{2,t})^2 c_1 - 4m_{3,t} c_1. \tag{9}$$

Here m_1, m_2, and m_3 are a functions of t, and c_1 and c_2 are constants. Then by using the following transformation formula:

$$\tau = 2T\lambda^2, \quad \xi = -2\lambda X, \tag{10}$$

and substituting Eq. (9) into Eq. (6), we obtain

$$\mathrm{i}\Psi_{j,\tau} + \Psi_{j,\xi\xi} + \mathrm{i}\sum_{q=1}^{3}(|\Psi_q|^2\Psi_j)_\xi = 0, \quad (j = 1,2,3), \tag{11}$$

we gain a concise equation which is easier to be solved by Hirota bilinear method.[40]

2.1. One-soliton solution

Ansatz of Hirota bilinear method[40] $\Psi_1 = g_1 f^*/f^2$, $\Psi_2 = g_2 f^*/f^2$, $\Psi_3 = g_3 f^*/f^2$ is used, by substituting it into Eq. (10), and then one-soliton and two-soliton solutions of Eq. (2) are obtained according to the steps of Hirota bilinear method.

The one-soliton solution reads

$$u_j(x,t) = \rho(t)\frac{g_j(1+f_2)^*}{(1+f_2)^2}\mathrm{e}^{\mathrm{i}\varphi(x,t)}, \quad (j = 1,2,3), \tag{12}$$

where

$$g_{j,1} = \zeta_j \mathrm{e}^{\theta_1}, \quad f_2 = \eta_1 \mathrm{e}^{\theta_1 + \theta_1^*},$$
$$\theta_1 = k\xi + \mathrm{i}k^*\tau, \quad \eta_1 = \frac{\mathrm{i}k\sum_{j=1}^{3}|\zeta_j|^2}{2(k+k^*)^2}. \tag{13}$$

Here ζ_j $(j = 1,2,3)$, η_1, and k are arbitrary complex parameters, and $\rho(t)$, $\varphi(t)$, ξ, and τ are given in Eqs. (9) and (7).

2.2. Two-soliton solution

The two soliton solution reads

$$u_j(x,t) = \rho(t)(g_{j,1} + g_{j,3})\frac{(1+f_2+f_4)^*}{(1+f_2+f_4)^2}\mathrm{e}^{\mathrm{i}\varphi(x,t)},$$
$$(j = 1,2,3), \tag{14}$$

where

$$\theta_1 = k_1\xi + \mathrm{i}k_1^2\tau, \quad \theta_2 = k_2\xi + \mathrm{i}k_2^2\tau,$$
$$\eta_1 = \frac{\mathrm{i}k_1(|\zeta_1^{(1)}|^2 + |\zeta_2^{(1)}|^2 + |\zeta_3^{(1)}|^2)}{2(k_1 + k_1^*)^2},$$
$$\eta_2 = \frac{\mathrm{i}k_1(\zeta_1^{(1)}\zeta_1^{(2)*} + \zeta_2^{(1)}\zeta_2^{(2)*} + \zeta_3^{(1)}\zeta_3^{(2)*})}{2(k_1 + k_2^*)^2},$$
$$\eta_3 = \frac{\mathrm{i}k_2(\zeta_1^{(1)*}\zeta_1^{(2)} + \zeta_2^{(1)*}\zeta_2^{(2)} + \zeta_3^{(1)*}\zeta_3^{(2)})}{2(k_1^* + k_2)^2},$$
$$\eta_4 = \frac{\mathrm{i}k_2(|\zeta_1^{(2)}|^2 + |\zeta_2^{(2)}|^2 + |\zeta_3^{(2)}|^2)}{2(k_2 + k_2^*)^2},$$
$$\delta_j^{(1)} = \frac{\zeta_j^{(1)}\eta_3(k_1 - k_2)}{k_1 + k_1^*} - \frac{\zeta_j^{(2)}\eta_1(k_1 - k_2)}{k_1^* + k_2},$$
$$g_{j,3} = \delta_j^{(1)}\mathrm{e}^{\theta_1 + \theta_2 + \theta_1^*} + \delta_j^{(2)}\mathrm{e}^{\theta_1 + \theta_2 + \theta_2^*},$$
$$\delta_j^{(2)} = \frac{\zeta_j^{(1)}\eta_4(k_1 - k_2)}{k_1 + k_2^*} - \frac{\zeta_j^{(2)}\eta_2(k_1 - k_2)}{k_2 + k_2^*},$$
$$g_{j,1} = \zeta_j^{(1)}\mathrm{e}^{\theta_1} + \zeta_j^{(2)}\mathrm{e}^{\theta_2},$$
$$\eta_5 = \frac{\eta_1\eta_4|k_1 - k_2|^2}{(k_2 + k_1^*)(k_1 + k_2^*)} - \frac{\eta_2\eta_3|k_1 - k_2|^2}{(k_1 + k_1^*)(k_2 + k_2^*)},$$
$$f_4 = \eta_5 \mathrm{e}^{\theta_1 + \theta_2 + \theta_1^* + \theta_2^*},$$
$$f_2 = \eta_1\mathrm{e}^{\theta_1 + \theta_1^*} + \eta_2\mathrm{e}^{\theta_1 + \theta_2^*} + \eta_3\mathrm{e}^{\theta_2 + \theta_1^*} + \eta_4\mathrm{e}^{\theta_2 + \theta_2^*},$$
$$(j = 1,2,3). \tag{15}$$

Here $\zeta_j^{(1)}$, $\zeta_j^{(2)}$ $(j = 1,2,3)$, η_1, η_2, η_3, η_4, $\eta_5 k_1$, and k_2 are arbitrary complex parameters.

3. Dynamical behaviors of solitons and discussion

In this section, by choosing a set of parameters as follows: $m_1 = 1/(0.2\sin(t) + 1)^2$, $m_2 = m_3 = 0$, $c_1 = c_2 = 1$, one of the typical types of one soliton Eq. (11) and two-soliton Eq. (13) is obtained as an example to illustrate their dynamic behavior. Then the influences of different parameters on the soliton dynamics are also studied.

Figure 1(a)–1(d) show the dynamic behavior of three different chains in the three-coupled alpha helical protein. As shown in the figure, the soliton amplitude of three chains in protein exhibits obvious periodic breathing behavior. All the solitons of the three chains have the same period of oscillation. However, the soliton amplitudes are different for the three chains when ζ_1, ζ_2, ζ_3 are different from each other. This difference may be derived from the difference between the environment and the structure of each chain in the alpha helical protein. When $\zeta_1 = \zeta_2 = \zeta_3$, the soliton amplitudes of the three chains are the same, that is $|u_1|^2 = |u_2|^2 = |u_3|^2$. So only the evolution figure of $|u_1|^2$ is shown in Fig. 1(e) to study the effect of parameter ζ_j $(j = 1,2,3)$ on the soliton. It can be found that the amplitude of the solitons $|u_1|^2$ is the same when the condition $\zeta_1 = \zeta_2 = \zeta_3$ is still satisfied but the values of ζ_j are different. However, the soliton centers are different and moves towards the positive direction of the x axis with the increase of ζ_j. Then we fixed ζ_2 and ζ_3 to obtain the effect of ζ_1 on the amplitude maximum of $|u_1|^2$, as shown in Fig. 1(f). It is found that when the value of ζ_1 increases, the amplitude maximum of $|u_1|^2$ increases, but the increasing trend of the curve decreases.

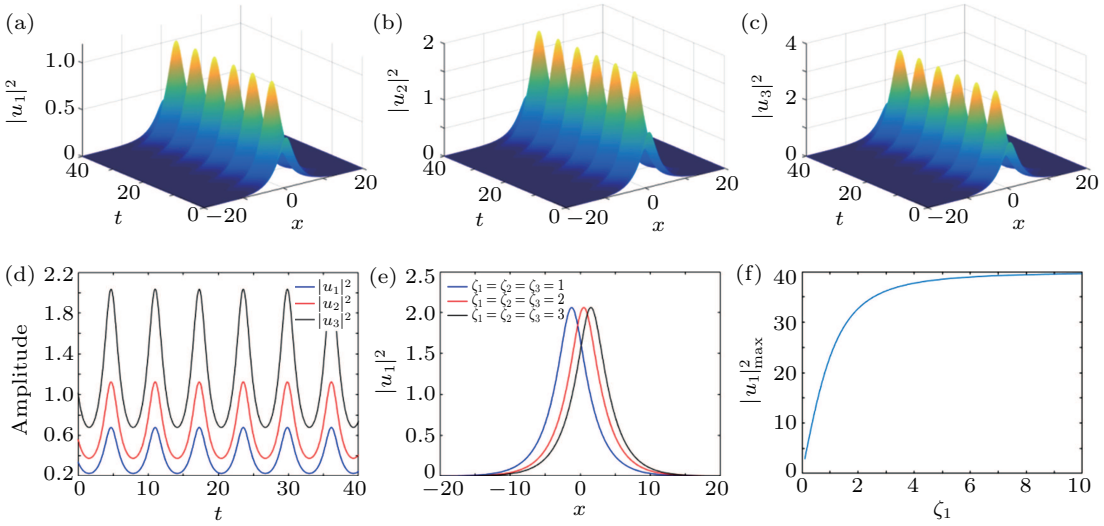


Fig. 1. The influence of ζ_j on soliton amplitude. (a)–(c) The soliton evolution figures of three chains with $\zeta_1 = 1$, $\zeta_2 = 2$, and $\zeta_3 = 3$. (d) The soliton amplitude evolution over time of panels (a)–(c) at $x = -1.2$. (e) Soliton amplitude of $|u_1|^2$ varies with x for different ζ_j at $t = 11.05$. (f) The amplitude of soliton varies with ζ_1 at $\zeta_2 = 1$, $\zeta_3 = 1$. Other parameters are $\lambda = 0.2$, $k = 1$.

In Fig. 2, the influence of parameter k on the propagation of solitons is studied. Unlike in Fig. 1, where k is real, the x coordinate of the soliton center is always the same over time. However, in Fig. 2, where k has an imaginary part, the x coordinate of the soliton center will change over time. It is found that the propagation direction of solitons is mainly related to the imaginary part of k ($\mathrm{Im}(k)$). When $\mathrm{Im}(k) > 0$, the center of the solitons shifts toward the negative x axis as time goes on. When the $\mathrm{Im}(k) < 0$, the center of the solitons shifts toward the positive x axis over time. Moreover, the larger the absolute value of the imaginary part ($|\mathrm{Im}(k)|$), the more the x coordinate of the soliton center deviates from $x = 0$.

Figure 3 shows the effect of the parameter λ on the width of the soliton and the central position of the soliton. It is found that the soliton width decreases and narrows with the increase of λ, and the central position of the soliton moves towards the positive direction of the x axis, as shown in Figs. 3(a)–3(e). Figure 3(f) clearly shows that x coordinate of the soliton center moves in the positive direction of the x axis as λ increases, When $k = 1$, the x coordinate of the soliton center is always negative and moves toward $x = 0$ as λ increases. However, the amount of soliton center movement becomes smaller and smaller as λ increases.

Figure 4 shows the effect of parameters k_1 and k_2 on the evolution of the two solitons. It shows that the two solitons also have the periodic oscillation behavior and move towards each other. After the collision, they are separated again. The sum of the amplitudes of two solitons remains the same as shown in Fig. 4. It indicates there is no energy loss occurs during the collision. What is more, the influence of the parameters k_1 and k_2 on the propagation direction of the two solitons is the same as that of one soliton, that is, the larger the absolute value of the imaginary part ($\mathrm{Im}(k_1)$ and $\mathrm{Im}(k_2)$), the more the x coordinate of the soliton center deviates from $x = 0$.

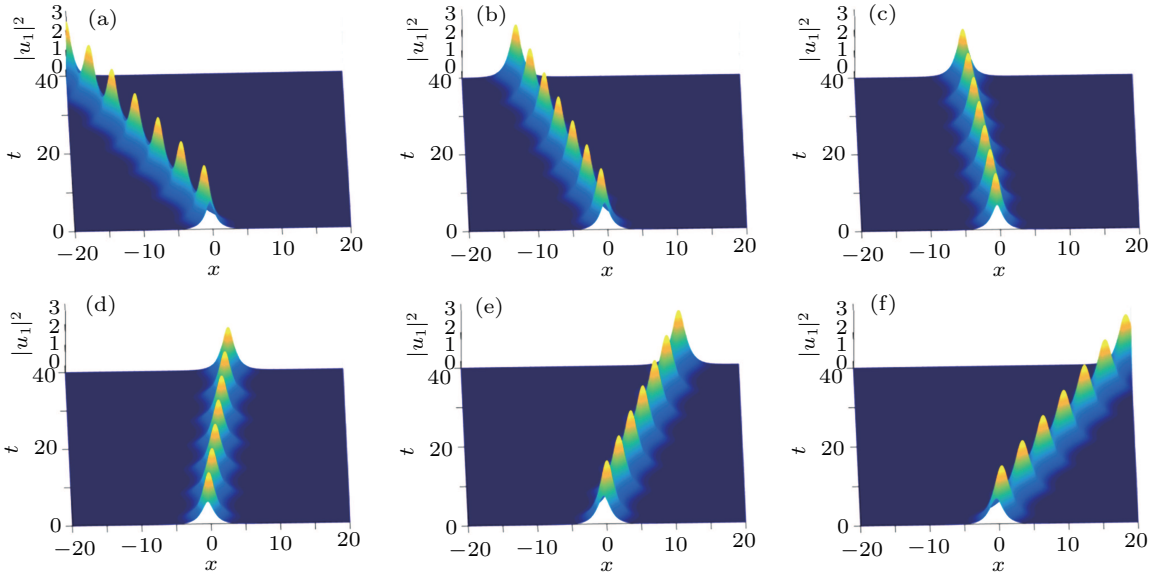


Fig. 2. The influence of k on the propagation direction of solitons: $\lambda = 0.2$, $\zeta_1 = \zeta_2 = \zeta_3 = 1$. The values of k are (a) $1+0.5\mathrm{i}$, (b) $1+0.3\mathrm{i}$, (c) $1+0.1\mathrm{i}$, (d) $1-0.1\mathrm{i}$, (e) $1-0.3\mathrm{i}$, (f) $1-0.5\mathrm{i}$, respectively.

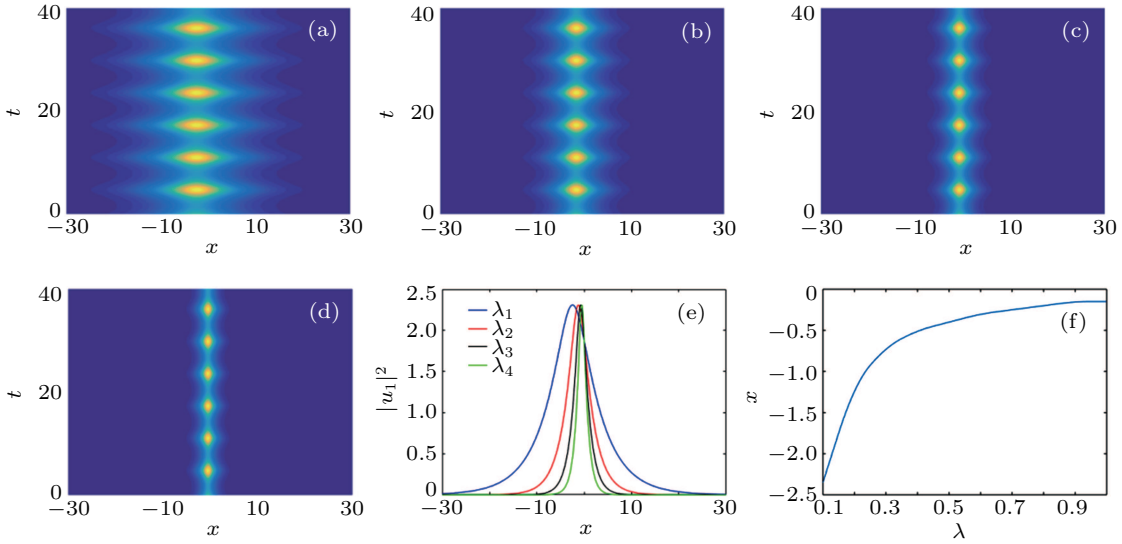


Fig. 3. (a)–(d) The influence of λ on the width of the soliton and the center position of the soliton; the values of λ respectively are (a) 1/10, (b) 1/5, (c) 1/3, (d) 1/2. Other parameters are $\zeta_1 = \zeta_2 = \zeta_3 = 1$, $k = 1$. (e) The soliton amplitude $|u_1|^2$ varies with x for different λ at $t = 11.25$. Panel (f) is the central position of soliton changing with λ.

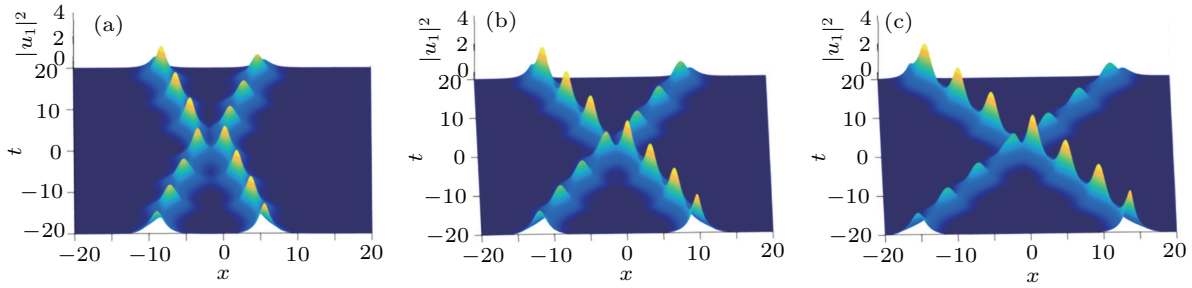


Fig. 4. The evolution figures of the two solitons for different k_1, k_2: (a) $k_1 = 1+0.3\mathrm{i}$, $k_2 = 1-0.3\mathrm{i}$; (b) $k_1 = 1+0.5\mathrm{i}$, $k_2 = 1-0.5\mathrm{i}$; (c) $k_1 = 1+0.7\mathrm{i}$, $k_2 = 1-0.7\mathrm{i}$, and other parameters are given as $\lambda = 0.5$, $\zeta_1^{(1)} = \zeta_2^{(1)} = \zeta_3^{(1)} = \zeta_1^{(2)} = \zeta_2^{(2)} = \zeta_3^{(2)} = 1$.

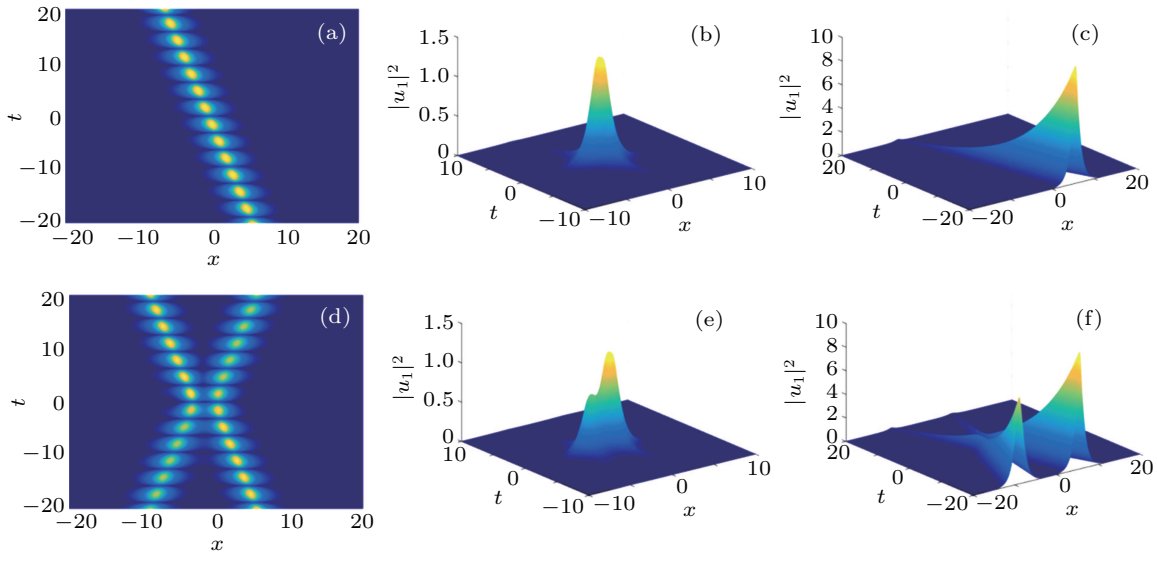


Fig. 5. The evolution figures of one-soliton and two-soliton for different m_1: (a) and (b) $m_1 = \sin(t)^2$; (c) and (d) $m_1 = 1/(4t^2+1)$; (e) and (f) $m_1 = \mathrm{e}^{-0.2t}$. Other parameters are given as $\lambda = 0.5$, $\zeta_1 = \zeta_2 = \zeta_3 = 1$, $k = 1+0.3\mathrm{i}$ in panels (a), (c), (e), and $\lambda = 0.5$, $\zeta_1^{(1)} = \zeta_2^{(1)} = \zeta_3^{(1)} = \zeta_1^{(2)} = \zeta_2^{(2)} = \zeta_3^{(2)} = 1$, $k_1 = 1+0.3\mathrm{i}$, $k_2 = 1-0.3\mathrm{i}$ in panels (d), (e), and (f).

In Fig. 5, different types of one-soliton and two-soliton are obtained by choosing different forms of m_1. Figures 5(a)–5(b) show the single breather soliton and two breather solitons, whose amplitude vary periodicity. Figures 5(c)–5(d) show a lump single soliton and two lump solitons, which are localized and do not move with time. The dissipative single soliton and two solitons are obtained whose amplitude decay as time goes on, as shown in Figs. 5(e)–5(f).

4. Conclusion

The one-soliton and two-soliton solutions of three-coupling MNLS equation with variable-coefficients are obtained by similarity transformation to describe the dynamics of soliton in alpha helical protein. The effects of different parameters on soliton solutions are discussed in detail. It is found that the composition of the three chains ζ_j will affect the amplitude of soliton and soliton center, k determines the direction of soliton propagation, λ affects the width of soliton and the position of soliton center along the x axis. By adjusting the parameter m_1, different types of solitons including breather soliton, lump soliton, and dissipative soliton have been obtained. Our results will be helpful in understanding of biological energy transport in alpha helical protein and it provides theoretical support for the experimental study of soliton excitation and control.

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