Discrete energy transport in collagen molecules

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The modulational instability in the three coupled α-polypeptide chains of a collagen molecule is investigated. Choosing symmetric and asymmetric solutions, and applying the so-called rotating-wave approximation, we describe the dynamics of the system by the discrete nonlinear Schrödinger (DNLS) equation. The linear stability analysis of the continuous wave solution is performed. The numerical simulations show the generation of trains of solitonic structures in the lattice with increasing amplitude as time progresses. The effect of damping and noise forces of the physiological temperature ($T = 300$ K) introduces an erratic behavior to the formed patterns, reinforcing the idea that the energy used in metabolic processes is confined to specific regions for efficiency.

Keywords: modulational instability, collagen molecules, damping, noise force

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1. Introduction

A long-standing problem that remains of great interest is the way in which energy is localized and transported in molecular systems. One of the molecular systems which attracts much attention in biology is a collagen molecule.[1–4] The collagen molecules are the main constituents of animals' frameworks, tendons, bones, ligaments, blood vessels, skin, and supporting membraneous tissues. There are twenty-eight different types of collagen molecules categorized in eight subfamilies on the basis of their function, assembly, and domain homology.[5–7] Fibrillar collagens for example form the major component of the complex extracellular matrix in connective tissues. Collagen I is abundant in skin, tendon, bone, and ligament, and collagen II is predominantly expressed in cartilage. In the reticular (deeper) dermis, well ordered thick collagen fibrils predominate, whereas in the papillary (upper) dermis underlying the epidermis and basement membrane. Collagen III is associated with thinner collagen I fibrils in tendons,[8] and collagen XI has been reported to inhibit the lateral growth of collagen II fibrils in cartilage.[9]

A collagen molecule consists of three coupled α-polypeptide chains of equal length,[1] and each contains a regular helical structure which forms a left-handed helix. The right-handed major helix is formed by the three chains coiled around the central axis, which are stabilized by the interchain hydrogen bonds and the Van der Wall force. The fundamental aspect that attracts much attention is that the collagen molecules, as the material basis of acupuncture branches and channels,[10] can support the long-distance transport of energy, electron, and information. A long time ago, Davydov and Kislukha[11–13] suggested that the energy of hydrolysis of adenosine triphosphate, which is about 0.42 eV, can be transferred without loss along the protein molecules as special collectively excited states. To explain the mechanism of the muscle contraction, they showed that in the α-helical protein molecules, the energy could be transported in the form of solitary waves. Since then, the Davydov soliton model has been a subject of intensive experimental and theoretical works in various contexts.

Following Davydov's original suggestion, a three-chain model of a collagen molecule was presented by Xiao and Lin.[14] In that model, as in the Davydov model, the amide-I vibrations can also be transported along the backbones of the protein molecules by coupling with the torsion of the peptide planes since the dipole–dipole interaction is affected by the torsion of the peptide planes formed by the four atoms O, C, N, H of each amino acid. In order to describe the dynamics of the three coupled chains in one collagen molecule, we consider the following Hamiltonian:[14]

$$\begin{aligned} H = \sum_n \sum_{j=1}^{3} \Big\{ & \frac{1}{2}[M\dot{u}_{n,j}^2 + Ku_{n,j}^2] + Ju_{n,j}u_{n-1,j} - Tu_{n,j}u_{n,j-1} \\ & + \frac{1}{2}[I\dot{\phi}_{n,j}^2 + L(\phi_{n,j} - \phi_{n-1,j})^2] \\ & + \chi(\phi_{n,j} - \phi_{n-1,j})u_{n,j}u_{n-1,j} \Big\}, \end{aligned} \tag{1}$$

where the subscript n counts unit cells (H–N–C=O) along the chains, while j specifies one of the three chains. The variable $u_{n,j}$ characterizes the displacement of the high frequency amide I oscillator with mass M in the j-th chain. The parameter K is the spring constant or elasticity coefficient, J is the

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resonance interaction between neighboring amide I oscillators in the same chain, and T is the resonance interaction between amide I oscillators in the neighboring chains. The variable $\phi_{n,j}$ characterizes the torsion angle of the peptide plane of the n-th amino acid in the j-th chain with the moment of inertia I. The parameter L is the resonance interaction between the neighboring peptide planes in the same chain, while χ is the coupling constant between the amide I vibrations and the plane torsion.

It has been shown that the three-chain model for the collagen molecule has symmetric and asymmetric soliton solutions.[14] For symmetric solutions, i.e., $u_{n,1} = u_{n,2} = u_{n,3}$, three solitons move with the same velocity along the three chains, respectively. While two solitons move only in two of the three chains for asymmetric solutions, i.e., $u_{n,j} = -u_{n,j-1} = u_n$ and $u_{n,j+1} = 0$. However, to the best of our knowledge, no work on the modulational instability (MI) of this model has been reported in the literature. So, the main objective in the present paper is to study the energy transport in the three-chain model of the collagen molecule through the MI. It has been shown that the MI is a direct way through which solitonic structures emerge in a nonlinear system as a consequence of the interplay between dispersion and nonlinearity.[15–20] Recently, taking into account the three-strand model of an α helix and the long-range dipole–dipole interactions, we showed the possibility of energy transport trough the MI.[20] Motivated by the obtained results, we extend the study in the above described model and investigate the effect of thermal fluctuations in pattern formation. The rest of this paper is organized as follows. In Section 2, we first reduce the model to a more simple system and take into account its symmetric and asymmetric solutions, and we perform the linear stability analysis of the MI. The instability zone as well as the growth rate of the MI are obtained numerically and discussed. In Section 3, numerical simulations of the analytical predictions are reported, and we show the effect of temperature on the MI. In Section 4, we conclude the work.

2. Equations of motion and linear stability analysis

2.1. Equations of motion

From Hamilton's equations, the following equations for the displacement $u_{n,j}$ and the torsion angle of the peptide plane $\phi_{n,j}$ are derived:

$$\begin{aligned}\ddot{u}_{n,j} &= -u_{n,j} - J(u_{n+1,j} + u_{n-1,j}) + T(u_{n,j+1} + u_{n,j-1}) \\ &\quad - \chi[u_{n+1,j}(\phi_{n+1,j} - \phi_{n,j}) + u_{n-1,j}(\phi_{n,j} - \phi_{n-1,j})],\end{aligned} \tag{2a}$$

$$\begin{aligned}\ddot{\phi}_{n,j} &= L(\phi_{n+1,j} - 2\phi_{n,j} + \phi_{n-1,j}) \\ &\quad + \chi(u_{n+1,j} - u_{n-1,j})u_{n,j},\end{aligned} \tag{2b}$$

where the following dimensionless variables and parameters have been introduced:

$$\begin{aligned}&u_n \to \sqrt{\chi/L}u_n,\ \ t \to \sqrt{K/M}t, \\ &J \to \frac{J}{K},\ \ T \to \frac{T}{K},\ \ \chi \to \frac{\chi}{K},\ \ L \to \frac{M}{KI}L.\end{aligned}$$

With the adiabatic approximation,[21] i.e., $\dot{\phi}_{n,j} = 0$, equation (2b) gives

$$\phi_{n+1,j} - \phi_{n,j} = -\frac{\chi}{L}u_{n+1,j}u_{n,j}. \tag{3}$$

Introducing Eq. (3) into Eq. (2a) and using new dimensionless parameters $U_n = u_n/\mu$, $\alpha = J/\mu$, and $\beta = -\chi^2/\mu$, we obtain

$$\ddot{U}_n = -U_n - \alpha(U_{n+1} + U_{n-1}) - \beta(U_{n+1}^2 + U_{n-1}^2)U_n, \tag{4}$$

where $\mu = 1 - 2T$ for symmetric solutions and $\mu = 1 + T$ for asymmetric solutions.

Linear oscillations of frequency ω and wave number q are described by the following dispersion relation:

$$\omega = 1 + 2\alpha\cos(q), \tag{5}$$

where the lattice spacing has been taken as equal to unity.

2.2. Linear stability analysis

For a finite amplitude wave, nonlinearities of the system give rise to the generation of higher harmonics. It is therefore convenient to reduce Eq. (4) to a more simple system under some approximations. We use the so-called rotating-wave approximation which essentially neglects the high harmonics. For this, we substitute into Eq. (4) the trial solution[22]

$$U_n(t) = \psi_n(t)\,\mathrm{e}^{-\mathrm{i}t} + \text{c.c.}, \tag{6}$$

where the terms proportional to $\mathrm{e}^{\pm \mathrm{i}t}$ lead to the derivative nonlinear Schrödinger (DNLS) equation

$$\begin{aligned}&-2\mathrm{i}\dot{\psi}_n + \psi_n + \alpha(\psi_{n+1} + \psi_{n-1}) \\ &+ 2\beta(|\psi_{n+1}|^2 + |\psi_{n-1}|^2)\psi_n = 0.\end{aligned} \tag{7}$$

As the function ψ_n is slowly changing with n, we can assume $|\psi_{n+1}|^2 + |\psi_{n-1}|^2 \approx 2|\psi_n|$. Then, equation (7) can be rewritten as

$$-2\mathrm{i}\dot{\psi}_n + \psi_n + \alpha(\psi_{n+1} + \psi_{n-1}) + 4\beta|\psi_n|^2\psi_n = 0. \tag{8}$$

The modulation instability in the lattice can be easily analyzed using Eq. (8), which has an exact plane-wave solution

$$\psi_n(t) = \psi_0\,\mathrm{e}^{\mathrm{i}(qn - \omega_1 t)}, \tag{9}$$

where the frequency ω_1 is characterized by the nonlinear dispersion

$$\omega_1 = \frac{1}{2} + \alpha\cos(q) + 4\beta|\psi_0|^2. \tag{10}$$

To examine the linear stability of the initial plane wave, we look for a solution of the form

$$\psi_n(t) = \psi_0[1 + B_n(t)]\,\mathrm{e}^{\mathrm{i}(qn-\omega_1 t)}, \tag{11}$$

where the perturbation amplitude $B_n(t)$ is assumed to be small in comparison with the carrier wave amplitude ψ_0. The equation which describes the evolution of the perturbation is given by

$$\begin{aligned} &-2\mathrm{i}\dot{B}_n + \alpha[(B_{n+1} - 2B_n + B_{n-1})\cos(q) \\ &+ \mathrm{i}(B_{n+1} - B_{n-1})\sin(q)] + 4\beta(B_n + B_n^*)|\psi_0|^2 = 0. \end{aligned} \tag{12}$$

We further assume the perturbation to be of the form

$$B_n(t) = B_1\,\mathrm{e}^{\mathrm{i}(Qn-\Omega t)} + B_2^*\,\mathrm{e}^{-\mathrm{i}(Qn-\Omega^* t)}, \tag{13}$$

where the asterisk denotes the complex conjugation, Q and Ω represent the wave number and the angular frequency of the perturbation, respectively, and B_1 and B_2^* are complex constant amplitudes. The condition for the existence of nontrivial solutions of the linear homogeneous system for B_1 and B_2^* leads to a second order equation for the frequency Ω, that is

$$\begin{aligned} &\Omega^2 + [2\alpha\sin(q)\sin(Q)]\Omega - 4\alpha^2\cos^2(q)\sin^4\left(\frac{Q}{2}\right) \\ &+ 8\alpha\beta\cos(q)\sin^2\left(\frac{Q}{2}\right) + \alpha^2\sin^2(q)\sin^2(Q)|\psi_0|^2 = 0, \end{aligned} \tag{14}$$

which can also be written as

$$\begin{aligned} &[\Omega + \alpha\sin(q)\sin(Q)]^2 \\ &= 4\alpha\cos(q)\sin^2\left(\frac{Q}{2}\right)\left[\alpha\cos(q)\sin^2\left(\frac{Q}{2}\right) - 2\beta|\psi_0|^2\right]. \end{aligned} \tag{15}$$

The system under our study will, therefore, display an MI if the right-hand side of Eq. (15) is negative; this gives the following instability criterion:

$$4\alpha\cos(q)\sin^2\left(\frac{Q}{2}\right)\left[\alpha\cos(q)\sin^2\left(\frac{Q}{2}\right) - 2\beta|\psi_0|^2\right] < 0. \tag{16}$$

It will be satisfied if the initial amplitude $|\psi_0|$ exceeds the threshold amplitude $\psi_{0,\mathrm{cr}}$ defined by

$$|\psi_0|^2 \geq |\psi_{0,\mathrm{cr}}|^2 = \frac{\alpha}{2\beta}\cos(q)\sin^2\left(\frac{Q}{2}\right). \tag{17}$$

In the long-wavelength limit, when $Q \ll 1$ and $q \ll 1$, equation (15) reduces to

$$[\Omega + \alpha q Q]^2 = \frac{1}{4}\alpha Q^2[\alpha Q^2 - 8\beta|\psi_0|^2]. \tag{18}$$

We have represented the MI in Fig. 1, where the stability/instability diagram and the growth rate of instability are plotted. In the stability/instability diagram (Fig. 1(a)), the black region is the region where the MI is expected, while the white region is the region where the plane wave solution is supposed to be stable under modulation. In Fig. 1(b), a soliton train is generated through the modulational instability spectrum in which the plane wave is unstable for all Q. The main observation is that the choice of q leads to the decision of the instability domain and, therefore, increases our chances of choosing appropriate parameters that could give rise to the solitonic structures in the model.

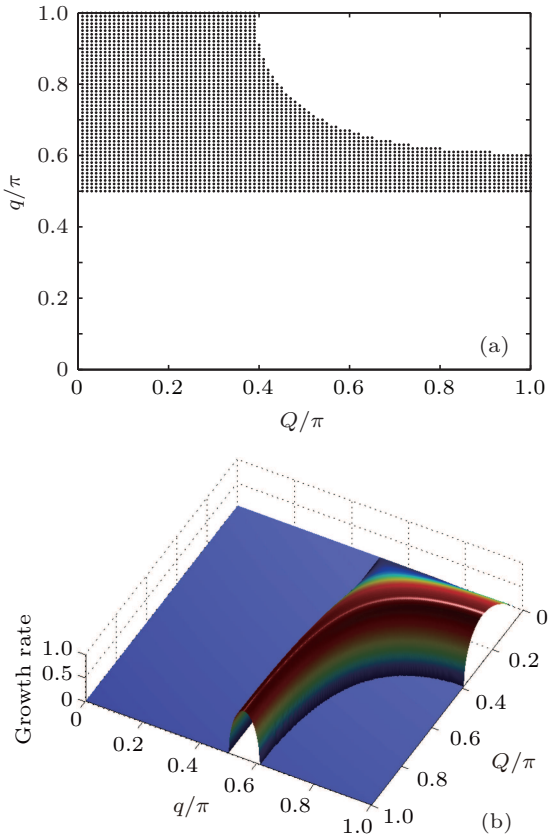


Fig. 1. (color online) (a) The stability/instability diagram and (b) the growth rate of instability for $\psi_0 = 1$, $\alpha = 3$, and $\beta = -0.5$.

3. Numerical simulations

As it is well known, the linear stability analysis is limited because it can only detect the onset of instability, and therefore does not tell us anything about what kind of dynamical patterns one might obtain in the system when the instability grows for a long time. In order to verify the analytical predictions, we carry out numerical simulations of discrete Eqs. (2a) and (2b) using the fourth-order Runge–Kutta computational scheme with periodic boundary conditions. We use initial conditions in the form

$$\begin{aligned} &u_n(t=0) = u_0[1 + 0.01\cos(Qn)]\cos(qn), \\ &\phi_n(t=0) = 0, \end{aligned} \tag{19}$$

where $u_0 = 1$. The wavenumbers q and Q have been chosen to be $q = 0.95\pi$ and $Q = 0.3\pi$ as belonging to the region of instability. The referred point is expected to give rise to patterns of energy. To make sure that the collagen molecular system really supports the MI, we first study the case of non-damped and non-thermal lattice. In so doing, as shown in Fig. 2, the generation of a periodic array of patterns of energy like pulses confirms not only our analytical predictions but also the fact shown in numerous papers that energy is better transported in biological molecules through the MI.[15–20] In this figure, as also found by Ondoa *et al.*[15] and Mimshe *et al.*,[19] we observe that the patterns do not saturate, and their amplitudes continuously increase. The formation of these localized structures confirms the efficiency of energy transport in the collagen molecules; this once more proves that the MI is an excellent and direct mechanism with which energy can be transferred and localized in biological molecules. For the symmetric case, wave patterns with the same amplitude and energy are generated along the three chains, respectively, while for the asymmetric case, the wave patterns are generated only in two of the three chains. However, in the physiological environment, in particular at the biological temperature of 300 K in the living system, the biological molecules are always subjected to thermal fluctuations and dissipation. It is therefore needed to further study the bearing of the patterns when the above-noticed environmental factors are taken into account. Then, we add dissipation and fluctuations in the Langevin sense to Eq. (2a)

$$\begin{aligned} \ddot{u}_n = & -\mu u_n - J(u_{n+1} + u_{n-1}) - \chi[u_{n+1}(\phi_{n+1} - \phi_n) \\ & + u_{n-1}(\phi_n - \phi_{n-1})] - \gamma \dot{u}_n + \sqrt{2D_b}\xi(t), \end{aligned} \tag{20}$$

where γ is the damping constant. The stochastic term $\xi(t)$ is the Gaussian white noise with zero mean and delta correlation, i.e., $\langle \xi(t) \rangle = 0$ and $\langle \xi(t)\xi(t') \rangle = \delta(t - t')$. The strength of the damping, γ, on the right-hand side of Eq. (20) is related to the amplitude of the stochastic force via the fluctuation dissipation theorem $D_b = k_B T\gamma/M$, with k_B being the Boltzmann constant and $T = 300$ K the temperature. The thermal effects on the nonlinear dynamics of the solitonic structures have been a subject of intensive works in many models of protein molecules. Just to cite a few, Ekobena *et al.*[16] showed a gradual increase of energy patterns due to the presence of thermal noise in a complex bi-exciton molecular chain through an MI analysis. Simo and Caputo[23] found that the thermal fluctuations are not sufficient to destroy the soliton localization in protein molecules. Pang[24] showed that the additional nonlinear coupling interaction between the lattice and the vibrational quanta with the one proposed by Davydov is able to stabilize the Davydov soliton and therefore the soliton is very robust against the thermal fluctuations of the environment.

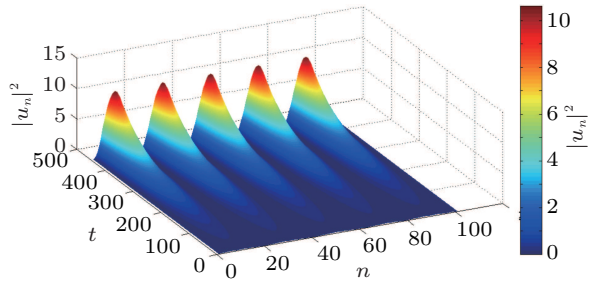


Fig. 2. (color online) The initial plane wave solution breaks into localized structures in the absence of thermal fluctuations. The wavenumbers have been chosen as $q = 0.95\pi$ and $Q = 0.3\pi$. The parameters are $u_0 = 1$, $J = 0.9$, $\chi = 0.2$, $L = 0.001$, and $\mu = 0.05$.

The above mentioned results are confirmed as displayed in Fig. 3, where we have investigated the impact of thermal perturbations on the pattern propagation with two values of the damping constant, $\gamma = 0.075$ and $\gamma = 1$. In Fig. 3(a), choosing $\gamma = 0.075$, we observe that the thermal effects bring an erratic behavior into the formed patterns. This is further confirmed by the features in Fig. 3(b) for $\gamma = 1$, where the formed patterns are shown to become more erratic with the increase of the damping constant γ. These erratic structures tend to form peaks that seem to enhance the energy localization and transport in the collagen molecule as demonstrated in Ref. [19]. As their amplitudes continuously grow, obviously it leads to a gradual increase of the energy patterns in the lattice, thus confirming the recent results by Ekobena *et al.*[16] It has also been shown recently that these erratic structures are highly localized, which reinforces the idea that the energy to be used in the metabolic processes is rather confined to specific regions

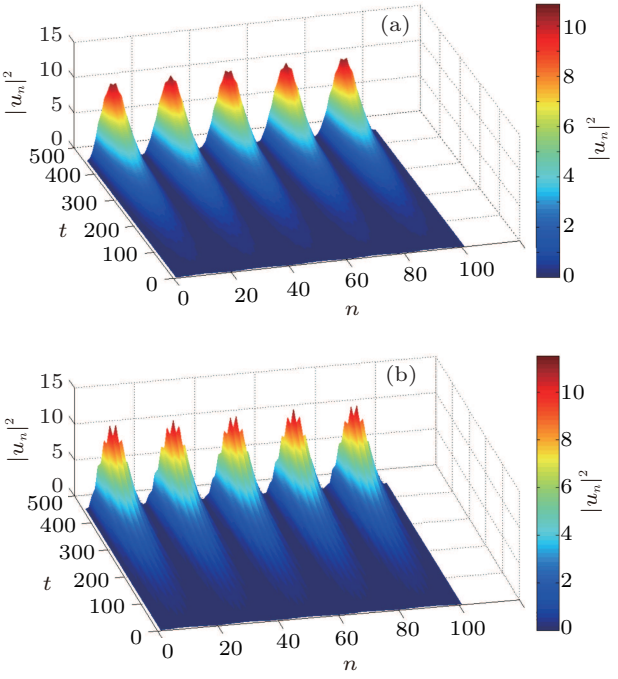


Fig. 3. (color online) The effect of thermal fluctuations on modulational instability with $T = 300$ K, $\gamma = 0.075$ (panel (a)), and $\gamma = 1$ (panel (b)). The setup is the same as that in Fig. 2.

for efficiency.[19] This is probably why the collagen can support the long-distance transport of energy and information. This also can explain the way in which energy is provided in the fibrillar collagen that may contribute mainly in the vicinity of anchoring plaques to stabilizing the cohesion between the upper dermis and the basement membrane zone.[7]

4. Conclusion

In this work, using the MI, we have investigated the generation of localized structures in the three coupled α-polypeptide chains of a collagen molecule taking into account symmetric and asymmetric cases. We have used the rotating-wave approximation to reduce the dynamics of the system to the DNLS equation. Through the linear stability analysis, we have established the instability criterion, and we have revealed that the model could be subjected to the MI. In order to confirm the analytical predictions, we have used numerical simulations showing the generation of a periodic array of localized structures with increasing amplitude as time progresses. Finally, we have investigated the influence of thermal perturbations on the pattern formation. The lattice is brought in contact with a heat bath mimicked by a stochastic force acting upon the lattice and a corresponding damping related to the temperature via the fluctuation-dissipation theorem.[25] In agreement with some recent studies, the formation of patterns of energy have been found to be in favor with the thermal fluctuations of the environment. The present work may be considered as a good improvement study for energy localization in collagen molecules.

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