Modulation instability gain and modulated wave shape incited by the acoustic longitudinal vibrations in molecular chain model

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Abstract

The propagation of the modulated wave (MW) pattern and its instability in the nonlinear medium is an important study from where experimental results are obtained. In this work, we use the nonlinear Schrödinger equation (NLSE) with saturation nonlinearity (SN) which describes the solitonic waves in the molecular chain (MC) model. We set our study on the effectiveness of the acoustic longitudinal velocity (ALV) which is related to the acoustic longitudinal vibration to investigate the behavior of the MW patterns as well as the modulation instability (MI) gain. Its results are that the ALV creates instability zones, increases MI bands, and shortens the transition regime of the MW pattern. For a long time of simulation and a great enough value of the ALV, the MWs feature chaos-like motion. Alongside these results the ALV obvious itself as a tool control of MWs as well as an energy source for the propagation of diverse MW-shaped in the MC.

1. Introduction

Nowadays, investigations of MW patterns in nonlinear media have grown in nonlinear fiber optics, ion-acoustic, plasma, alpha-protein and so on [1–23]. It has been more emphasized on solitary waves which propagate as a single ensemble with the identical velocity called ‘solitons’ [24]. Solitons are waves that can propagate over long distances without any twist and can preserve their shapes [25]. More precisely solitons are usually resulting from the confrontation between nonlinear and dispersions terms However, solitons propagation is described by nonlinear evolution equations such as NLSE, nonlinear modified Zakharov–Kuznetsov equation of ion-acoustic waves, the dissipative Kuramoto-Sivashinsky equation, the perturbed Chen–Lee–Liu equation, the fractional second and third-order nonlinear Schrödinger equation, the complex Swift-Hohenberg equation, the space-time fractional nonlinear Schrödinger equation, the high-order nonlinear Schrödinger equation, the specific coupled nonlinear Schrödinger equations, just to name a few [1–19]. Owing to the nonlinear term of the NLSE, diverse forms are known in literature such as Kerr law, Cubic-Quintic Nonlinearity (CQN), parabolic law including saturable nonlinearity [7, 12–14, 22].

Nonlinear terms are thus involved in the structuring of the MW patterns and act with dispersions coefficients for a perfect accomplishment of the propagation of solitonic waves (SWs). For example, it has been studied the behavior of solitons in MCs where nonlinear interaction between molecules is considered [24]. More recently, it has been studied in MCs, the propagation of the bell soliton and kinks-like soliton where SN is used
[26, 27]. Alongside, it has been shown that dromion-like soliton can be obtained in the alpha-protein array when CQN acts together with the ALV. In this way, in the MC array, diverse other studies have been successfully done by implying the SN. In [28, 29], it has been shown how the saturation terms can deeply affect the MW and modulation bands in bi-exciton alpha-helical protein chains. MI is the powerful method where the confrontation between dispersion and nonlinearity terms is exhibited by using the small perturbations of the continuous waves (CWs) [3, 7].

Besides, in optical fibers (OFs), Alves et al [30] use the SN and higher-order dispersions to exhibit the MI growth rate. More recently, the effects of both anti-cubic nonlinearity and cross-phase modulation on MI bands have been stressed [31]. MI is the paramount tool used to establish the stable/unstable zones of the perturbed CWs in nonlinear media [32, 33].

The nonlinear effects in the MC have been proposed in the literature, but few of them have included the effects of the acoustic sound waves. Since the works of [27], where ALV has been used to control solitons velocity in the presence of CQN, we have set our interest on both SN and ALV to study the modulated solitary waves and MI growth rate in the MC. The goal of this work is to point out the effectiveness of ALV on both MI growth rate and MW patterns in the MC with SN.

The paper is organized as follows: In section 2, we overview the model of NLSE with SN which describes the propagation of SWs in the MC. The effects of the ALV on MI bands and MI growth rate was highlighted in section 3. In section 4, by using the numerical simulation (NS), we have shown the MW pattern by varying the ALV and fixed value of the SN term during a long time of the simulation. Some relevant results have been obtained to confirm the effectiveness of the ALV. We provided the summary in the last section.

### 2. Nonlinear Schrödinger equation with saturable nonlinearity

Recently NLSE with SN which describes the propagation of the solitary waves in MC has been derived [26–28]. These relevant works are based on the pipe given by Davydov’s model where interactions of neighbors are included [28]. However, to achieve the goal of this work, we consider here a one-dimensional chain where interactions are considered between neighbor molecules.

Following the processes used in [28] and after some calculation in the continuum limit, the CQN with SN gives

$$i\hbar \frac{\partial b}{\partial t} + \frac{\partial^2 b}{\partial x^2} - \lambda b + \frac{k_1|b|^2b}{G - k_3|b|^2} + \frac{k_2|b|^4b}{(G - k_3|b|^2)^2} = 0. \tag{1}$$

with $b$ the density of the wave pattern which is related to the probability of finding the quantum system. Meanwhile, $\hbar$ is a shortened Planck’s constant, and $k_1$, $k_2$, and $k_3$ are respectively the attractive and repulsive nonlinearity terms and the NS term. They are connected to the exciton-phonon coupling coefficient as $k_1 = \frac{\partial^2 D}{\partial \varepsilon^2}$, $k_2 = \frac{\partial D}{\partial \varepsilon}$, and $k_3 = \frac{\partial D}{\partial \varepsilon^2}$. The coefficient $\lambda = \varepsilon + T + U - D - J$, while $G = v_s^2 - v^2$. Here, $v_s$ represents the ALV or longitudinal vibrations of molecules and $v$ the soliton velocity. The dipole-dipole interaction is given by $J = \frac{2\mu^2}{\mu r}$. The variable $M$ represents the mass of the infinite chain of weakly bound molecules (or groups), $\varepsilon$, $T$, and $U$ are respectively the energy of the intramolecular excitation, the kinetic and potential energies of the longitudinal movement. Furthermore, $R$ denotes the intramolecular distances and the exciton-phonon coupling is given by $\chi = \frac{\partial D}{\partial \varepsilon}$. The details of these parameters are given in [28]. We remind that equation (1) can be singular when $G = k_3|b|^2$. In this present study, we conjecture that $G \neq k_3|b|^2$.

Recently, Muniyappan and co-workers [27] have displayed the effects of the ALV on dromion structures in alpha-helical proteins by using the CQNLSE without SN. They have pointed out the robustness of the obtained analytical results. Besides, M Aguero et al [26], have established the effectiveness of different excitations in a one-dimensionless array model of the MC. They have exhibited that the soliton velocity can be controlled by ALV which is known as longitudinal vibrations of molecules. We aim in what will be followed to examine the effects of the acoustic longitudinal vibrations on MWs. We use the NS which is well-known for its complexity during integration to point out the behavior of the MWs for a long time of propagation under the effects of the ALV. Comparing our results with [26, 27], new behaviors of the MW patterns have been obtained. To our knowledge, these results are new and could be useful for many applications such as communication systems, and strong technologies for penetrating protein behest-function relationships.

### 3. Linear stability and modulation instability

In this section, we point up the efficiency of the ALV on both MI [34–36] bands and the MI growth rate of the CWs by using the linearizing scheme.
3.1. Linear stability
We assume the plane wave solution of equation (1) in the form
\[ b(\xi, t) = u_0 e^{i(k_0 \xi - \omega_0 t)}, \]
where \( u_0, k_0, \) and \( \omega_0 \) are respectively the complex amplitude, the wave vector, and angular frequency. Inserting equation (2) into equation (1) gives the dispersion relation as
\[ \omega_0 = \frac{k_0^2}{\hbar} + \frac{\lambda}{\hbar} - \frac{k_1 |u_0|^2}{\hbar (G - k_3 |u_0|^2)} + \frac{k_3 |u_0|^4}{G (G - k_3 |u_0|^2)^2}. \]

The obtained dispersion relation depends on the wave vector, attractive and repulsive terms. To linearize equation (1), we assume its solution in the form of the CWs given by
\[ b(\xi, t) = u_0 (1 + \psi(\xi, t)) e^{i(k_0 \xi - \omega_0 t)}. \]

Inserting equation (4) into equation (1), we get the linearizing expression as follows:
\[ i\hbar \frac{\partial \psi(\xi, t)}{\partial t} + \frac{\partial^2 \psi(\xi, t)}{\partial \xi^2} + 2i k_0 \frac{\partial \psi(\xi, t)}{\partial \xi} + \frac{k_1 G |u_0|^2 (\psi(\xi, t) + \psi^*(\xi, t))}{(G - k_3 |u_0|^2)^2} + \frac{2k_3 G |u_0|^4 (\psi(\xi, t) + \psi^*(\xi, t))}{(G - k_3 |u_0|^2)^3} = 0. \]

We aim in the forthcoming section to inspect the effects of the \( v_a(\text{ALV}) \) on such MI growth rates and MI bands.

3.2. Modulation instability
The MI \([34–36]\) is the event from which nonlinear and dispersion terms are used to exhibit the stable or unstable zones of the CWs in sundry media such as nonlinear OFs, plasma, and ion-acoustic just to mention these \([1–23]\). Let’s set the following with perturbed terms as the solution of the given equation (5) above
\[ \psi(\xi, t) = \delta_1 e^{i(K_1 - \Omega t)} + \delta_2 e^{-i(K_1 - \Omega t)}. \]

Here, \( \delta_j, (j = 1, 2) \), \( K \), and \( \Omega \) are respectively the complex amplitude, perturbed wave number, and angular frequency. Using equation (6) into equation (5) we get the 2 × 2 matrix form where the dispersion relation can be obtained
\[ \left( \begin{array}{c} \Omega \hbar - JK^2 - 2k_0 K + N \\ -\Omega \hbar - JK^2 + 2k_0 K + N \end{array} \right) \left( \begin{array}{c} \delta_1 \\ \delta_2 \end{array} \right) = \left( \begin{array}{c} 0 \\ 0 \end{array} \right), \]
with
\[ N = \frac{G k_1 |u_0|^2}{(G - k_3 |u_0|^2)^2} + \frac{2Gk_3 |u_0|^4}{(G - k_3 |u_0|^2)^3}. \]

The obtained matrix vanishes when the following constraint relation is satisfied
\[ \lambda_3 \Omega^2 + \lambda_4 \Omega + \lambda_5 = 0. \]

and
\[ \lambda_3 = 6G(1) + 3G^2(1)^2 k_3^2 - 3G^3(1)^3 k_3^3, \]
\[ \lambda_4 = -4G^4(1)^4 k_3^4 + 12G^5(1)^5 k_3^5 - 12G^6(1)^6 k_3^6, \]
\[ \lambda_5 = -2G^7(1)^7 k_3^7 + 3G^8(1)^8 k_3^8 + 4G^9(1)^9 k_3^9 - 3G^{10}(1)^{10} k_3^{10} - 3G^{11}(1)^{11} k_3^{11} - 3G^{12}(1)^{12} k_3^{12} - 12G^{13}(1)^{13} k_3^{13} - 12G^{14}(1)^{14} k_3^{14} - 12G^{15}(1)^{15} k_3^{15} - 12G^{16}(1)^{16} k_3^{16}, \]
\[ \lambda_6 = 2G^{17}(1)^{17} k_3^{17} + 12G^{18}(1)^{18} k_3^{18} + 12G^{19}(1)^{19} k_3^{19} - 4G^{20}(1)^{20} k_3^{20} - 2G^{21}(1)^{21} k_3^{21} - 4G^{22}(1)^{22} k_3^{22} - 4G^{23}(1)^{23} k_3^{23} - 2G^{24}(1)^{24} k_3^{24} - 2G^{25}(1)^{25} k_3^{25}, \]

In figures 1(a)–(d), we display the behavior of the MI gain with the effects of the \( v_a(\text{ALV}) \) and fixed value of soliton velocity. In figure 1(a), we assume \( v_a > v(\text{velocity of the bright soliton}) \) and fixed values of attractive and
repulsive nonlinearity. We have shown how the MI band increases both in amplitude and wavenumber range, for $v_a = 4.8$ (blue line) and $v_a = 6.8$ (red line) respectively. From figure 1(b), we have increased strong enough the ALV. One observes how the amplitude of the MI gain increases for $v_a = 9.8$ (green line) and $v_a = 10.8$ (black solid line) respectively. Alongside figures 1(a), and 1(b), we have used the reverse situation in figures 1(c)–(d) (i.e. $v_a < v$). It is observed to decrease MI growth rate both in amplitude and wavenumber range compared to figures 1(a), (b). More precisely for $v = 10.3$ and a fixed value of $v_a = 4.8$ (green), we have observed in figure 1(c) the MI growth rate with decreasing amplitude and wavenumber range between $(0, 1)$. Further, we have increased the soliton velocity to $v = 20.3$ and fixed the value of the ALV, we have pointed out that the MI growth rate decreases and vanishes for $v = 25.3$. It could be predicted that the ALV can provoke unstable CW during the formation of MWs in the MC. However, the situation could be supposedly controlled by increasing the soliton velocity. In the next section, after some assumptions, we use the transformation hypothesis to obtain bright soliton as the initial condition for NS. In the end, we examine numerical behavior like MW patterns under the effects of the longitudinal acoustic vibration.

4. Numerical analysis of modulated wave pattern

In what follows, our goal is to examine the effectiveness of the NS on MW patterns in MCs. It is worth highlighting that equation (1) is now assumed without saturation term, as we goal to underline only the effects of the ALV. So in this case, equation (1) can obey some analytical solutions where the nonlinearity is less than $O(k_3|b|)$ and $k_3 < k_1 k_2$ (i.e. $k_3|b|^2 \ll G$). Therefore, equation (1) becomes a NLSE with CQ-term, and owing to this assumption, we apply the transformation in the form of

$$b(\xi, t) = f(\xi - vt)e^{i(\kappa t + \omega t)},$$

where $\xi = \xi - vt$. The parameters $f(\xi - vt)$, $\kappa$, and $\omega$ are respectively the complex function of the MW, the vector wave, and the angular frequency respectively. Owing to the assumption of $k_3 < k_1 k_2$, we insert equation (11) into equation (1) and the soliton velocity is obtained as

$$v = \frac{2f\kappa}{h}.$$  

Subsequently, the ordinary equation related to equation (1) is set in the form of

$$f''(\zeta) + \alpha_0 f(\zeta) + \alpha_1 f^{\sigma+1}(\zeta) + \alpha_2 f^{2\sigma+1}(\zeta) = 0,$$
where $\sigma = 2$, along with the constant coefficients

$$
\alpha_0 = - \frac{Jk^2 - \hbar \omega + \lambda}{J}, \\
\alpha_1 = \frac{k_1}{GJ}, \\
\alpha_2 = \frac{k_2}{JG^2}.
$$

(14)

Following [37, 38], equation (13) satisfy the bright-like soliton and a pair of kink-profile as solutions by using the undermined coefficients method. In [31], four exact solutions to equation (13) have also been highlighted. We aim here to show only the effects of the ALV on MW patterns, we only consider one of the solutions of equation (13). For this fact, we have $\sigma = 2$ and then we assume the following constraint relation:

$$
\alpha_0 < 0, \\
\alpha_1 = 0, \\
\alpha_2 > 0.
$$

(15)

Hence, the following solution is obtained as:

$$
b(\xi, t) = \sqrt{\frac{3 (k_1^2 - \hbar \omega + \lambda)}{Jk_2}} \text{sech} \left( \frac{\sqrt{3Jk^2 - \hbar \omega + \lambda}}{J} (\xi - vt) \right) e^{i(k_1 + \omega)t}.
$$

(16)

It is obvious that the obtained bright soliton-like solution depends on the coefficient of the dipole-dipole interaction, the ALV as well as the repulsive nonlinearity, and the reduced Planck’s constant. Let’s now focus on the numerical investigation of equation (1) with the initial condition equation (16) to point out the efficiency of the velocity of sound waves corresponding to longitudinal vibrations of molecules on the MW patterns. We assume for this $\chi_0 = n/2$. To carry out the effects of ALV on the MW patterns, we have fixed the other parameters related to the alpha-helical proteins. For this purpose, we set the vector wave $\kappa = 0$, and therefore the soliton velocity is $v = 0$. In figures 2(a)–(f), we examine the behavior of the MW under the effects of the ALV. For $\nu_a = 0.5[\hbar]$, we observe the formation of breather-like soliton with concentrated energy at $n/2$ in figure 2(a), while the breathing behavior is pointed out in figure 2(d) for $T \in [0, 500[\hbar]$. In order to fully appreciate the behavior of the MW, we increase the ALV to $\nu_a = 0.6[\hbar]$, the breathing behavior has extended in time propagation in figure 2(e) and a high concentration of energy is obtained at $n/2$ in figure 2(b). In addition, it also appears a less disorderly behavior for $T \rightarrow 1500[\hbar]$ in figure 2(e). Once more, we increase $\nu_a = 0.7[\hbar]$ and we

Figure 2. Effects of ALV ($\nu_a$) on soliton. (a, b, c) are the temporal soliton in terms of the cell index and (d, e, f) are the behavior of the temporal soliton evolution in terms of time at different cell index (d, e, f). (a) $\nu_a = 0.5[\hbar]$, (b) $\nu_a = 0.6[\hbar]$, (c) $\nu_a = 0.7[\hbar]$, (d) $n = 20$, (e) $n = 50$, (f) $n = 100$. The other parameters are $J = 0.08[\hbar]$, $\lambda = 0.1[\hbar]$, $k_2 = -1.2[\hbar]$, $k_3 = 0.4[\hbar]$, $\nu = 0$, $\omega = 0.8[\hbar]$, and $\kappa = 0$. 


observe the nonlinear propagation of the MW in figure 2(c). For $n = 100$, we have pointed out in figure 2(f) the chaotic behavior in the MC. In figure 3, we maintain a long time of propagation and fixed value of the ALV and of course with zero soliton velocity. We portray the soliton-like MW in terms of cell index. In figure 3(a)–(c) for $T = 10[\mu s]$, $T = 250[\mu s]$, and $T = 750[\mu s]$, the chaotic propagation of the MW is fulfilled. We portray the soliton-like MW in terms of cell index. On the bottom panel of figure 3, we have shown the propagation of the MW pattern such as bell-shaped in figure 3(d) for $n = 120$, dipole soliton in figure 3(e) where $n = 150$ and W-shaped profile in figure 3(f) for cell index $n = 200$. We have observed MW patterns with decreasing amplitude during the propagation in the MC. The decrease in amplitude observed as a function of cell index could also reflect a loss of energy during the propagation of the MWs in the MC. To better appreciate the different shapes of the MW we display the propagation of the intensity of the MW at different times in figures 4(a)–(f). We set $T = 150[\mu s]$ in figure 4(a), and the W-shaped profile is obtained at the center of the cell index. We increase the propagation time to $T = 450[\mu s]$ the M-shaped is observed with increasing amplitude. To better appreciate different shapes of the MWs patterns with a time of propagation, we have increased the propagation time such as $T = 550[\mu s]$, $T = 750[\mu s]$, $T = 900[\mu s]$, and $T = 950[\mu s]$ respectively in figures 4(d)–(f). We have shown W-shaped with one peak of concentrated energy and with a reduced width in figure 4(d). More particularly, for $T = 950[\mu s]$, it appears a MW pattern with high amplitude and small width. After increasing deeply the propagation time to $T = 950[\mu s]$, it is shown how the amplitude of the obtained new shape in figure 4(f) increases. To highlight the vector wave effects on the MW patterns, we set $\kappa = \frac{2}{6}$ and $\kappa = -\frac{2}{6}$ respectively. For this event, we have fixed the ALV value. From figures 5(a)–(c), we set $\kappa = \frac{2}{6}$ and the velocity of the soliton is $v = 1.13[\mu m/s] > v_{\text{th}}$. It is observed the propagation of the modulated forward wave in figure 5(a) while in figure 5(b) the bright-like soliton is fulfilled. At the same time, we have shown the breathing behavior of the MW pattern in figure 5(c). From the bottom panel figures 5(d)–(f), we reverse the sign of the vector wave $\kappa = -\frac{2}{6}$ and the $v = -1.13[\mu m/s] < v_{\text{th}}$, we have shown the propagation of the modulated backward wave (i.e. group velocity and phase velocity have conversed). This is one of the promising results in a MC that may open up a view of the propagation of backward waves which have been demonstrated in media with a negative refractive index.

We can predict that during propagation of the MW pattern the ALV has a lot of effects on the soliton-like solution and for a long time of propagation in the MC there is energy transfer between neighbors and the MW can change shape. Otherwise, despite the soliton velocity being sometimes zero we have observed how the MW pattern is affected in time and can also preserve high energy.

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![Figure 3](image-url)
5. Conclusion

In this study, we have shown the effects of the ALV on the MI growth rate and modulated wave patterns in the MCs where SN is considered. We have shown on MI bands and MW patterns the effectiveness of ALV. For this purpose, we use NS to show for a long time of simulation the chaos-like motion. We have established for the strong value of ALV the propagation of dipole soliton, W-shaped profile as well as dark soliton. These results

Figure 4. Dynamics of bright solitons in terms of cell index at different times of propagation with a fixed value of the velocity of sound waves. a, b, c, d and f correspond respectively to $T = 150[h], T = 450[h], T = 550[h], T = 750[h], T = 900[h]$ and $T = 950[h]$. The other parameters are $v_s = 0.6[h], J = 0.08[h], \lambda = 0.1, k_2 = -1.2[h], k_3 = 0.4[h], \nu = 0, \omega = 0.8[h]$, and $\kappa = 0$.

Figure 5. Soliton propagation with the variation of wave number ($\kappa$). For (a, b, c) $\kappa = +\frac{\pi}{6}$ and (d, e, f) we set $\kappa = -\frac{\pi}{6}$. (b, e) are obtained where the cell index value is respectively $n = 150$ and $n = 1$ while (c, f) is displayed for $T = 10[h]$. The other parameters are $v_s = 0.9[h], J = 1.08[h], \lambda = 0.1, k_2 = 1.8[h], k_3 = 1.1[h]$, and $\omega = 0.8[h]$.

5. Conclusion

In this study, we have shown the effects of the ALV on the MI growth rate and modulated wave patterns in the MCs where SN is considered. We have shown on MI bands and MW patterns the effectiveness of ALV. For this purpose, we use NS to show for a long time of simulation the chaos-like motion. We have established for the strong value of ALV the propagation of dipole soliton, W-shaped profile as well as dark soliton. These results
have also shown the feature of the backward wave for a negative value of the soliton velocity and the acoustic sound waves behave as being an energy source for the MW patterns for a long time during the simulation. This study opens the gate to the new behavior of the MW-like reverse wave in the MCs.

Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

Competing interests

The authors declare no competing interests.

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