

# Higher Order Nonlinear Schrödinger Equation: an exactly solvable nonlinear model for nonlinear optics and biological science

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**Abstract:** A generalized nonlinear Schrödinger equation was recently pointed out as a new exactly solvable model in different context of mathematical sciences. In this paper, we propose a systematic study of a higher order nonlinear Schrödinger equation arising in literature in two different contexts regarding the biological science and the nonlinear optics. The model, in the first context interprets a generalized Davydov model for energy transfer in alpha helical protein and in the second one describes the propagation of femtosecond pulses in nonlinear fibres. Without the restriction of the solitary wave ansatz, but on the contrary, working with the systematic analysis of Lie's theory, we are able to generate exact solutions which carry important physical meanings.

**Keywords:** Partial differential equations, systems, exact solutions.

**MSC2010:** 35J15, 30H35, 42B25

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In the context of biophysics, much attention is devoted to the biological phenomena; one of the well-established problems is the understanding of energy transport along protein molecules. Molecular systems especially those of biological interest are very complicated structures, built from atoms connected by hydrogen bonds.

The energy required for most of the protein activities (such as DNA duplication, active transport of substances through bio-membranes, the neuroelectric pulse transfer on the membranes of neurocyte, etc) is provided by the hydrolysis of the ATP (adenosine triphosphate) molecule.

The mechanism converting this chemical energy into a mechanical motion was for the first time pointed by Davydov who established in [1] that the energy released in the ATP hydrolysis could stay localized in amide-I bond through nonlinear interactions of the vibrational excitation and deformation in the protein structure caused by the excitation [1]-[4].

During the last three decades, the Davydov model has been a subject of intensive studies and has attracted the attention of many researchers. Recently, the Davydov model has been generalized taking into account the interspine coupling, the long-range interaction effects and some additional higher-order molecular excitations and interactions. In a recent contribution, it has been investigated the dynamics of three coupled  $\alpha$ -polypeptide chains of a collagen molecule with the influence of power-law long-range exciton-exciton interactions [5].

The nonlinear dynamics of DNA molecule has been widely studied in the past by Daniel et al. [6]-[8] and several other authors in various contexts (see for example [9]-[11]). For instance, the study of waves propagation, especially solitons through inhomogeneous or disordered one-dimensional model of  $\alpha$ -helical proteins can be found in [12], [13].

In the context of Davydov soliton theory, Todorovic et al. have demonstrated that the soliton velocity is inversely proportional to the soliton amplitude and that two exciton - phonon coupling constants influence separately the soliton behavior [14].

While an interesting study concerning the dynamics of Davydov's model of  $\alpha$ -helical proteins considered by including the influence of inhomogeneities in the monomer units, can be found in [15].

Motivated by all these great number of biophysics applications, our aim in this paper is to make a complete study of a generalized Davydov model arising in literature in two different contexts regarding the biological science and the nonlinear optics; without the restriction of the solitary wave ansatz, but on the contrary, working with the systematic analysis of Lie's theory, we are able to generate exact solutions which carry important physical meanings.

## 1 The Model

In this paper, we focus our attention on the (1+1) dimensional higher order nonlinear Schrödinger equation

$$i \frac{\partial q}{\partial t} + \frac{\partial^2 q}{\partial x^2} + |q|^2 q + i \varepsilon \left( \frac{\partial^3 q}{\partial x^3} + k_1 |q|^2 \frac{\partial q}{\partial x} + k_2 q^2 \frac{\partial q^*}{\partial x} \right) = 0 \quad (1)$$

where  $q(t, x)$  is a complex functions of  $t$  and  $x$ ,  $q^*(t, x)$  is the complex conjugate of  $q(t, x)$  and subscripts denote partial derivatives with respect to space and time coordinates.

In the context of biological sciences, equation (1) was proposed in [6] as a generalized Davydov model. In this interpretation, the dependent variable  $q$  represents the vibrational coordinate of the amide-I vibrations, the coefficient  $k_1$  is a contribution related to self-steepening (also known as Kerr dispersion) and  $k_2$  is linked to stimulated Raman scattering effects, while  $\varepsilon$  represents the lattice parameter.

Moreover in equation (1), the second term is a dispersion term representing the dipole-dipole coupling and arises from the effective mass of the exciton, the third term is a nonlinear term representing coupling to hydrogen bonds, while the last term represents a term related to a global interaction due to molecular excitations along a single hydrogen bonding spine of the helix and the effect of interspine coupling.

Inter alia, the third-order term represent the third-order dispersion and when it loses importance in the model's dynamics then also self-steepening and Raman scattering effects collapse too.

The Davydov model explains lossless energy transfer in alpha helical proteins, in particular Davydov proved that the transfer of metabolic energy and of electrons along the chain describes excitations accompanied by a local deformation of the chain that move uniformly and undamped what is called a soliton. In this context, Davydov showed that the dynamic of alpha helical proteins is governed by the completely integrable nonlinear Schrödinger (NLS) equation which possesses N-soliton solutions [16] and he suggested that solitons in protein molecules are formed as a result of the dynamical balance between the dispersion due to the resonant interaction of intrapeptide dipole vibrations, amide-I and the nonlinearity provided by the interaction of these vibrations with the local displacements of the equilibrium positions of the peptide groups [1].

A generalized Davydov model was proposed in [6] as a model of single spine in order to study the nature of nonlinear molecular excitations and energy transfer along the chain. The generalized Davydov model includes molecular excitations along a single hydrogen bonding spine of the helix and also the effect of interspine coupling and describes the nature of nonlinear molecular excitations and energy transfer along the chain of alpha helical protein molecules [6].

Equation (1) contains some integrable models for certain specific set of parametric values which can be established by carrying out a Painlevé singularity structure analysis [17]. The results of the Painlevé analysis show that equation (1) reduces to completely integrable models and admits N-soliton solutions for different choices of parameters, which are well summarized in the interesting article of Daniel-Latha [6].

When  $\varepsilon = 0$ , equation (1) reduces to the completely integrable cubic nonlinear Schrödinger (NLS) equation; it is interesting to find out that a class of integrable equations belonging to the NLS family are connected to the Heisenberg ferromagnetic spin system via gauge transformation when the Lax pair of operators are known. In this connection, Zakharov and Takhtajan [18] showed that cubic NLS equation is gauge equivalent to the integrable Heisenberg spin equation which describes the dynamics of spins in an isotropic ferromagnet in the classical continuum limit.

The cubic NLS equation is a completely integrable equation admitting N-soliton solutions which can be found using the inverse scattering transform method [19] or by writing the equation in the bilinear form [20] or through Bäcklund transformation [21] or using other methods.

After employing suitable rescaling of  $q$ , equation (1) contains the completely integrable mixed derivative nonlinear Schrödinger (MDNLS) equation [6], which was first studied in the context of soliton and integrability by Wadati et al. [22]-[23] and is of frequent occurrence in various physical systems including nonlinear propagation of Alfvén waves with a small nonvanishing wave number and in explaining the dynamics of the deformed Heisenberg spin chain (see [24] - [25]).

It is worthwhile noticing that, in the framework of nonlinear optics, with a interchange of independent variables ( $t \leftrightarrow x$ ), equation (1), as well as certain version of it, can be written as

$$i \frac{\partial q}{\partial x} + \frac{\partial^2 q}{\partial t^2} + |q|^2 q + i\varepsilon \left( \frac{\partial^3 q}{\partial t^3} + k_1 |q|^2 \frac{\partial q}{\partial t} + k_2 q^2 \frac{\partial q^*}{\partial t} \right) = 0 \quad (2)$$

and describes the propagation of femtosecond pulses in nonlinear fibres. In this context,  $q$  represents the slowly-varying envelope of the electromagnetic field and the coefficients  $\varepsilon, k_1, k_2$  that appear in (2) are real parameters related to group velocity dispersion, self phase modulation, third-order dispersion, self steepening and self-frequency shift due to stimulated Raman scattering respectively.

It is well known that the propagation of picosecond pulses in optical fibres is described by the nonlinear Schrödinger equation [26, 27] to which equation (2) reduces when the last three terms are omitted. However, for ultrashort femtosecond pulses, the last three terms are non-negligible and should be retained [28]-[29].

If  $k_2 = 0$  equation (1) becomes the Hirota equation [20], of which there exist N-soliton solutions, while for  $k_2 \neq 0$  the hyperbolic secant (bright) and hyperbolic tangent (dark) soliton solutions for equation (1) have been obtained in [29]. An interesting set of cusp solitary wave solutions of equation (1), when the cusps are rounded off are obtained in [30].

Finally, it is interesting to observe the meaning of parameter  $\varepsilon$  in two different contexts; in fact in the framework of biological sciences,  $\varepsilon$  represents the lattice parameter and in the context of nonlinear optics can be interpreted as a dispersion parameter.

Our aim in this paper is to investigate, in the framework of the Lie group analysis, the  $(1+1)$  dimensional generalized nonlinear Schrödinger equation (1) in order to obtain exact invariant solutions. The plan of the paper is the following. In the next section we introduce the mathematical method in order to determine the symmetry transformations of the equation (1). In Sec. 3 we investigate the reductions of (1) to ODEs and we formally derived a variety of exact

solutions with distinct structures. In Sec. 4 we make conclusions, the results of our study confirm that the equation can, in general, support periodic wave solutions, soliton solutions and interesting solutions expressed in terms of Bessel functions.

## 2 Mathematical Method

In this section, the basic infinitesimal method for calculating symmetry groups of the model (1) is introduced in order to, first derive the continuous symmetry transformations and then to prove that the model under investigation can, in general, support exact solutions which carry important physical meanings.

For the mathematical analysis, it is convenient to rewrite the model and after introducing  $q = u + i v$ , with  $u(t, x)$  and  $v(t, x)$  real functions, let us first rewrite the complex equation (1) as a system of real equations

$$u_t + v_{xx} + (u^2 + v^2)v + \varepsilon \{u_{xxx} + k_1(u^2 + v^2)u_x + k_2[(u^2 - v^2)u_x + 2uvv_x]\} = 0 \quad (3)$$

$$v_t - u_{xx} - (u^2 + v^2)u + \varepsilon \{v_{xxx} + k_1(u^2 + v^2)v_x + k_2[(v^2 - u^2)v_x + 2uvu_x]\} = 0. \quad (4)$$

So, we search for the symmetry transformations of the equation (1), by applying the classical Lie method to the system (3)-(4) and look for the one-parameter group of infinitesimal transformations in the  $(t, x, u, v)$ -space; following the well known monographs on this argument (see e.g. [31] -[36]), we introduce the third prolongation of the operator  $X$

$$X = \xi^1 \frac{\partial}{\partial t} + \xi^2 \frac{\partial}{\partial x} + \eta^1 \frac{\partial}{\partial u} + \eta^2 \frac{\partial}{\partial v}. \quad (5)$$

in the form

$$X^{(3)} = X + \sum_{i=1}^2 \left( \zeta_t^i \frac{\partial}{\partial y_t^i} + \zeta_x^i \frac{\partial}{\partial y_x^i} + \zeta_{xx}^i \frac{\partial}{\partial y_{xx}^i} + \zeta_{xxx}^i \frac{\partial}{\partial y_{xxx}^i} \right), \quad (6)$$

where we have utilized the local notation  $u = y^1$ ,  $v = y^2$ , and we have set

$$\zeta_t^i = D_t(\eta^i) - y_t^i D_t(\xi^1) - y_x^i D_t(\xi^2), \quad (7)$$

$$\zeta_x^i = D_x(\eta^i) - y_t^i D_x(\xi^1) - y_x^i D_x(\xi^2), \quad (8)$$

$$\zeta_{xx}^i = D_x(\zeta_x^i) - y_{tx}^i D_x(\xi^1) - y_{xx}^i D_x(\xi^2), \quad (9)$$

$$\zeta_{xxx}^i = D_x(\zeta_{xx}^i) - y_{xxt}^i D_x(\xi^1) - y_{xxx}^i D_x(\xi^2), \quad (10)$$

with  $i = 1, 2$  and the operators  $D_t$  and  $D_x$  denote total derivatives with respect to  $t$  and  $x$ , respectively. The invariance conditions of (3)-(4) reads as follow

$$X^{(3)} \left( u_t + v_{xx} + (u^2 + v^2)v + \varepsilon \{u_{xxx} + k_1(u^2 + v^2)u_x + k_2[(u^2 - v^2)u_x + 2uvv_x]\} \right) = 0, \quad (11)$$

$$X^{(3)} \left( v_t - u_{xx} - (u^2 + v^2)u + \varepsilon \{v_{xxx} + k_1(u^2 + v^2)v_x + k_2[(v^2 - u^2)v_x + 2uvu_x]\} \right) = 0, \quad (12)$$

under the constraints that the variables  $u_t$  and  $v_t$  have to satisfy the system equations (3)-(4).

The *determining system* arising from (11)-(12) allows us to obtain:

$$\xi^1 = 9\varepsilon a_2 t + a_1, \quad (13)$$

$$\xi^2 = a_2(2t + 3\varepsilon x) + a_3, \quad (14)$$

$$\eta^1 = -3\varepsilon a_2 u - (a_2 x - a_4)v, \quad (15)$$

$$\eta^2 = (a_2 x - a_4)u - 3\varepsilon a_2 v, \quad (16)$$

$$(k_2 - k_1 + 3)a_2 = 0, \quad (17)$$

where  $a_i$  ( $i = 1, 2, 3, 4$ ), are constants. From (17) arises the following cases:

*Case I:*  $a_2 = 0$ .

In this case the Lie algebra is three-dimensional and is spanned by the operators

$$X_1 = \frac{\partial}{\partial t}, \quad X_2 = \frac{\partial}{\partial x}, \quad X_3 = v \frac{\partial}{\partial u} - u \frac{\partial}{\partial v}, \quad (18)$$

*Case II:*  $k_2 = k_1 - 3$ .

It is worthwhile noticing that the above condition is a *structural condition* of the equation (1). In this case the Lie algebra is four-dimensional and is spanned by the three operators (18) plus the following fourth operator:

$$X_4 = 9\varepsilon t \frac{\partial}{\partial t} + (2t + 3\varepsilon x) \frac{\partial}{\partial x} - (3\varepsilon u + xv) \frac{\partial}{\partial u} + (xu - 3\varepsilon v) \frac{\partial}{\partial v}. \quad (19)$$

### 3 Self-similar solutions of the Higher Order Nonlinear Schrödinger Equation

In this section, the solitary wave ansatz is not used and, working without preliminary assumptions and using the substitution following from the symmetry group obtained in the Cases *I* and *II*, we construct self-similar solutions which carry important physical meanings.

**Case I:**  $a_2 = 0$ .

In this case we consider the operator  $X$  as a linear combination of the operators (18), namely

$$X = \frac{\partial}{\partial t} + c_1 \frac{\partial}{\partial x} + c_2 \left( v \frac{\partial}{\partial u} - u \frac{\partial}{\partial v} \right), \quad (20)$$

where  $c_1$  and  $c_2$  are real constants, which give the following similarity variable

$$z = x - c_1 t \quad (21)$$

and similarity solutions

$$u = \phi(z) \sin(c_2 t) + \psi(z) \cos(c_2 t), \quad (22)$$

$$v = \phi(z) \cos(c_2 t) - \psi(z) \sin(c_2 t), \quad (23)$$

where  $\phi$  and  $\psi$  must satisfy the following system of ODEs to which (3)-(4) are reduced by means of the operator (20):

$$\begin{aligned}
& c_1 \phi' + c_2 \psi + \psi'' + (\phi^2 + \psi^2) \psi \\
& - \varepsilon \{ \phi''' + [(k_1 + k_2) \phi^2 + (k_1 - k_2) \psi^2] \phi' + 2 k_2 \phi \psi \psi' \} = 0,
\end{aligned} \tag{24}$$

$$\begin{aligned}
& c_1 \psi' - c_2 \phi - \phi'' - (\phi^2 + \psi^2) \phi \\
& - \varepsilon \{ \psi''' + [(k_1 - k_2) \phi^2 + (k_1 + k_2) \psi^2] \psi' + 2 k_2 \phi \psi \phi' \} = 0.
\end{aligned} \tag{25}$$

A solution of (24)-(25) is

$$\phi = \cos z, \quad \psi = \sin z, \tag{26}$$

under the condition  $c_2 = c_1 + \varepsilon [(k_2 - k_1) + 1]$ , with the constant of integration normalized to one. Coming back to the original variables, we obtain that the system (2)-(3) of real equation admits a periodic wave solution of the form:

$$u = \cos(x - c_1 t) \sin(c_2 t) + \sin(x - c_1 t), \cos(c_2 t), \tag{27}$$

$$v = \cos(x - c_1 t) \cos(c_2 t) - \sin(x - c_1 t), \sin(c_2 t), \tag{28}$$

If, in particular, in (24)-(25), we have also the validity of the structural condition  $k_2 = k_1 - 3$ , the solution can be expressed in terms of

$$\phi = \operatorname{sech}(z), \quad \psi = \operatorname{sech}(z) \tag{29}$$

When  $c_2 = -1$  and  $c_1 = \varepsilon$ , the model under investigation (2)-(3) admits a soliton solution of the form

$$u = \operatorname{sech}(x - \varepsilon t) \cos(t) - \operatorname{sech}(x - \varepsilon t) \sin(t), \tag{30}$$

$$v = \operatorname{sech}(x - \varepsilon t) \sin(t) + \operatorname{sech}(x - \varepsilon t) \cos(t). \tag{31}$$

We point out that, the soliton solution possesses a remarkable property that it can propagate steadily with two peaks of the same height.

In biological interpretation, as confirmed by Daniel, it turns out that the model (1), as well as certain version of it, describes a protein chain in which the nonlinear coupling, that is responsible for the formation of solitons, comes from slightly different interaction, unlike the Davydov model in which the nonlinear coupling proportional is responsible for the formation of solitons. We can also observe that the energy transfer in alpha helical proteins is in the form of solitons even if the left and right neighbouring interactions are unequal.

On the other hands, looking solutions (30)-(31) from the point of view of nonlinear optics, as predicted by Trippenbach et al. [37], the presence of higher order nonlinearities crucially affects the dynamics (see for example Figure 1).

Upon including self steepening, the trailing edge of the pulse becomes shocked, the peak intensity of the pulse is increased, and the peak of the pulse moves towards the trailing edge of the pulse. Self frequency shifting serves to transfer photons to lower frequency, and the lower frequency photons travel slower in the anomalous dispersion regime. Hence the leading edge of the pulse is suppressed relative to the trailing edge of the pulse because of both self steepening and self frequency shifting. Pulse breakup following self-focusing of the incident pulse is therefore strongly suppressed. However, in this case self steepening, as well as self frequency shift terms are still dominant and should be retained.

**Case II:**  $k_2 = k_1 - 3$ .

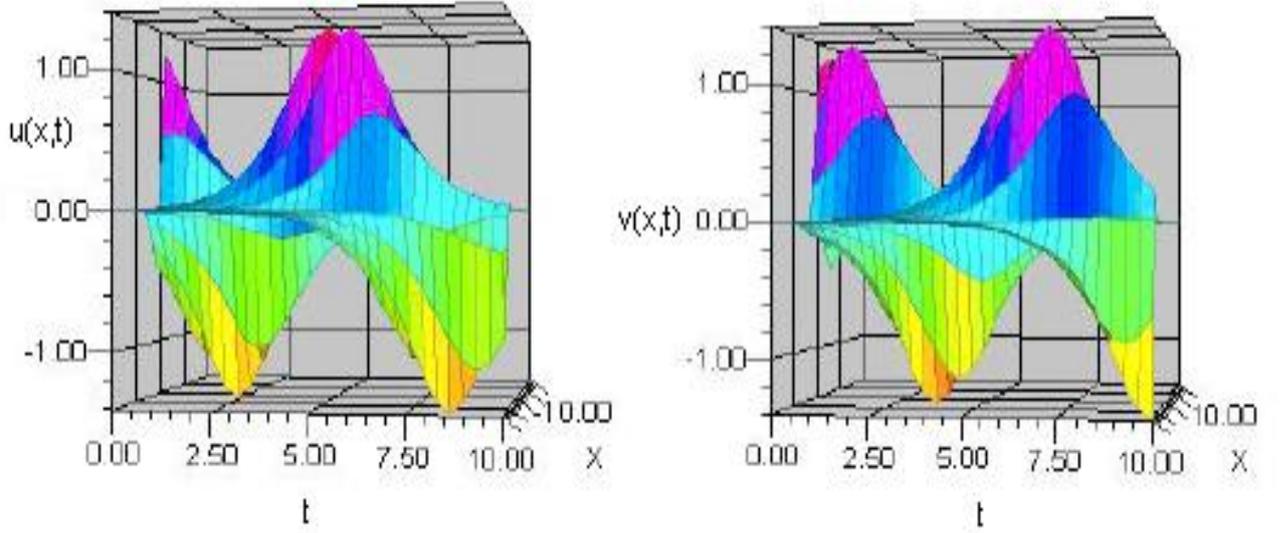


Figure 1: Snapshots of 3D view of the solution (30)-(31) for equation (2), with a interchange of independent variables ( $t \leftrightarrow x$ ), when  $\varepsilon = 1$ .

Proceeding as in the previous case, by applying the invariant surface condition, through the operator (19), namely

$$X_4 = 9\varepsilon t \frac{\partial}{\partial t} + (2t + 3\varepsilon x) \frac{\partial}{\partial x} - (3\varepsilon u + xv) \frac{\partial}{\partial u} + (xu - 3\varepsilon v) \frac{\partial}{\partial v}$$

we obtain the following similarity variable and similarity solutions, respectively:

$$z = \left( x - \frac{1}{3\varepsilon} t \right) t^{-\frac{1}{3}}, \quad (32)$$

$$u = \left[ \phi(z) \cos \left( \frac{x}{3\varepsilon} - \frac{2t}{27\varepsilon^2} \right) - \psi(z) \sin \left( \frac{x}{3\varepsilon} - \frac{2t}{27\varepsilon^2} \right) \right] t^{-\frac{1}{3}}, \quad (33)$$

$$v = \left[ \phi(z) \sin \left( \frac{x}{3\varepsilon} - \frac{2t}{27\varepsilon^2} \right) + \psi(z) \cos \left( \frac{x}{3\varepsilon} - \frac{2t}{27\varepsilon^2} \right) \right] t^{-\frac{1}{3}}. \quad (34)$$

Also here,  $\phi$  and  $\psi$  must satisfy the system of ODEs to which (3)-(4) are reduced by means of the operator (19), i.e.

$$\begin{aligned} 3\varepsilon \{ \phi''' + [(2k_1 - 3)\phi^2 + 3\psi^2] \phi' + 2(k_1 - 3)\phi\psi\psi' \} \\ - z\phi' - \phi = 0, \end{aligned} \quad (35)$$

$$\begin{aligned} 3\varepsilon \{ \psi''' + [(2k_1 - 3)\psi^2 + 3\phi^2] \psi' + 2(k_1 - 3)\phi\psi\phi' \} \\ - z\psi' - \psi = 0. \end{aligned} \quad (36)$$

In this case, we obtain a rational solution of (35)-(36) which reads as

$$\phi = \psi = H z^{-1}, \quad H = \pm \sqrt{\frac{3}{3 - 2k_1}} \quad (37)$$

under the condition  $k_1 \neq \frac{3}{2}$ .

If, on the contrary,  $k_1 = \frac{3}{2}$ , a solution of (35)-(36) can be expressed in terms of Bessel functions

$$\phi = \psi = \sqrt{z} \left\{ h_1 \left[ J_{\frac{1}{3}} \int \frac{\sqrt{z} J_{-\frac{1}{3}}}{i z \sqrt{3 \varepsilon z} \left( J_{-\frac{4}{3}} J_{\frac{1}{3}} - J_{-\frac{2}{3}} J_{-\frac{1}{3}} \right) + 3 \varepsilon J_{-\frac{1}{3}} J_{\frac{1}{3}}} dz \right. \right. \\ \left. \left. - J_{-\frac{1}{3}} \int \frac{\sqrt{z} J_{\frac{1}{3}}}{i z \sqrt{3 \varepsilon z} \left( J_{-\frac{4}{3}} J_{\frac{1}{3}} - J_{-\frac{2}{3}} J_{-\frac{1}{3}} \right) + 3 \varepsilon J_{-\frac{1}{3}} J_{\frac{1}{3}}} dz \right] + h_2 J_{\frac{1}{3}} + h_3 J_{-\frac{1}{3}} \right\} \quad (38)$$

where we have set the Bessel functions as:  $J_\alpha = J_\alpha \left( \frac{2iz^{\frac{3}{2}}}{3\sqrt{3\varepsilon}} \right)$ ,  $(\alpha = \pm\frac{1}{3}, -\frac{2}{3}, -\frac{4}{3})$  and  $h_1, h_2, h_3$  are arbitrary constants.

These class of solutions for (1) is strictly admits for  $\varepsilon \neq 0$  and then it is no longer valid in the limit of cubic nonlinear Schrödinger equation. Under the structural condition for the model  $k_2 = k_1 - 3$ , when  $k_1 \neq \frac{3}{2}$ , its traveling wave front is detailed in Figure 2.

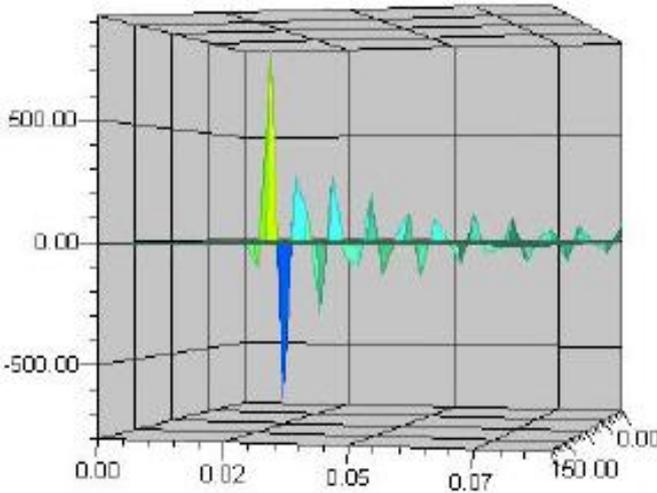


Figure 2: Snapshot of 3D view of the solution (33)-(34), when  $\phi = \psi = H z^{-1}$ ,  $H = \sqrt{\frac{3}{3-2k_1}}$  with  $k_1 = 1$ .

## 4 Conclusions

Usually, the nonlinear Schrödinger equation describes physical processes in which nonlinearity and dispersion cancel giving birth to solitons. The literature shows that the higher order nonlinear Schrödinger equation can, in general, support both soliton and periodic wave solutions. We studied the higher order nonlinear Schrödinger equation and we showed that, using the systematic methods of group analysis, it admits some beautiful and most interesting reductions to ordinary differential equations. Moreover, our results complement and generalize the well-known results in literature.

The hyperbolic secant and hyperbolic tangent soliton solutions for equation (1) have been obtained [29]. In [28], it is also shown that a higher-order nonlinear Schrödinger equation is solvable by means of the inverse scattering transform.

In our study, the solitary wave ansatz is not used and, working without preliminary assumptions, our results confirm that the model can, in general, support periodic wave solutions, soliton solutions and interesting solutions expressed in terms of Bessel functions and then the results are consistent with literature.

Moreover, the literature shows that some solutions of cubic nonlinear Schrödinger equations (i.e.  $\varepsilon = 0$ ) can be found in term of Bessel function under the assumption of cylindrical symmetries.

In this paper, we have also recover solutions in term of Bessel functions when we incorporate in the model the propagation of ultrashort femtosecond pulses and working without the hypothesis of separation of variables in polar coordinates.

## Acknowledgements

The author acknowledges the support of the Research Project 2015/2017 of the Kore University of Enna: "Methods for finding exact and numerical solutions for Partial Differential equations and systems of Mathematical Physics", coord. Prof. Antonino Valenti.

The author also acknowledges the support by G.N.F.M. of I.N.d.A.M.

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