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**DNA Nonlinear Dynamics With Non-classic Solitary Waves****Ma. de Lourdes Najera\***,  
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The nonlinear Schrödinger equation was obtained by using the method of generalized coherent states (GCS) applied to the quasi spin configuration of the DNA lattice model. In this model the DNA macromolecule is subjected to the influence of thermal phonons. By analyzing the nonlinear saturated Schrödinger equation, several non classical soliton-like solutions describing the hydrogen bonds are obtained. Among them there is a couple of compact-anticompact soliton that evolves as a healing mechanism for repairing the eventual open states of the hydrogen bonds.

**Key words and phrases:** nonclassical solutions, generalized coherent states, DNA, compactons.

## 1. Introduction

The existence of regimes where nonlinear optical propagation and DNA (or BEC) evolution models obeys the same type of equations are well known [1]. Among them the resulting for intense light pulses or spatial beams, the most fascinating is certainly the formation of solitons, which can also be considered in DNA dynamics.

The theoretical studies of DNA macromolecule dynamics in many aspects show the appearance of nonlinear traveling structures along the chain. That studies have led to many interesting types of solutions like the cnoidal, compact, peak solutions, etc.

Different approaches for variety of models of the DNA molecule have been applied. After the first proposal made by Englander [2], the model that is being deal with rotational degrees of freedom, and the first one was proposed by Yomosa [3, 4]. In his pioneering work Yomosa S. presented an important DNA model which include the rotation of pair bases along the spiral model proposed by Watson and Crick. This approach takes into consideration a dynamic of a plane base rotation perpendicular to the helical axis  $z$  around the backbone structure. Further improvements were done in the papers [5–8]. Along the other type of model, the principal one in the sense of dynamics of the hydrogen bonds, is due to the Peyrard - Bishop model [9]. These two version of modeling DNA received a great improvements by many important contributions that one can find for example in the papers [5, 6, 10, 11] and citation therein.

It is assumed that open states of the DNA is a principal requirement for arising other important features of this molecule, specifically for transcription and replication processes. Therefore, it is obvious that the opposite type of states the anti - open sates are suggested to appear inside the DNA molecule. In case of existence of these waves, this inverse process dual to the open ones, will repair the disruption or elongation of hydrogen bonds.

On the other order of things, the study of many body problems whose Hamiltonian has been explicitly written in terms of spin or quasi-spin operators, can be reduced by appropriated approximations to a quasi-classical treatment. For doing this, certain reduction procedure from the quasi - spin operator description to a classical one is

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needed. This procedure consists in choosing trial functions which can be used for averaging the Hamiltonian. Then it is natural to choose for this aim, coherent states since these states are the most classical and minimized the uncertainty relation [12–14].

In this contribution we study a dynamical model related to the emergence of traveling waves in the DNA molecule by using the quasi - classical approximation due to the generalized coherent states approach. This treatment was possible to implement because of the quasi spin character of the Hamiltonian of the DNA that is written in terms of the Spin operators  $\mathbf{S}$  proposed by Takeno-Homma (TH) in [5, 6]. The approach to derive analytical solutions was implemented explicitly for the case of traveling waves. In the next section we briefly expose the main features of the Takeno-Homma model and the generalized coherent state approach applied to the nonlinear lattice equation of DNA. The equation of motion derived from the application of GCS method is reported in section 3. The nonlinear soliton-like patterns are obtained by analyzing the equations in the continuum limit of the nonlinear lattice equation, that is reported in the fourth section. In the 5-th section we analyze the analytical solutions for hydrogen bond displacements. Comments and conclusion are done in the last section.

## 2. The Coherent States and Quasi-Spin Model of DNA

The model of the DNA can be done by constructing a Hamiltonian for description the nonlinear dynamics of the isotropically homogeneous coupled quasi-spin chain model in the nearest neighboring interactions. Additionally, since the functions of DNA are switched on under the biological temperature, it should be convenient to include thermal surrounding phonons. Thus, the total Hamiltonian that will be analyzed is written as [7, 8]

$$H = \sum_n \left[ -J(\mathbf{S}_n \cdot \mathbf{S}_{n+1} + \mathbf{S}'_n \cdot \mathbf{S}'_{n+1}) - (\mu - \alpha_1(X_{n+1} - X_{n-1}))(\mathbf{S}_n \cdot \mathbf{S}'_n) + \frac{p_n^2}{2m_1} + k_1(X_n - X_{n+1})^2 \right]. \quad (1)$$

The quasi-spin operators  $\mathbf{S}_n = (S_x, S_y, S_z)$  are related to the rotational angles  $\vartheta_n$  and  $\varphi_n$  as

$$\mathbf{S}_n = (S_x, S_y, S_z) = (\sin \vartheta_n \cos \varphi_n, \sin \vartheta_n \sin \varphi_n, \cos \vartheta_n). \quad (2)$$

This representation is given for the two strands that compose the DNA. The angles  $\vartheta_n(\vartheta'_n)$  and  $\varphi_n(\varphi'_n)$  represent the angles of rotation of the bases in the  $n^{\text{th}}$  base pair in the  $xz$  and  $xy$  plane respectively. The notation for the second strand will differ to the first one by the apostrophe in the mathematical expressions for its corresponding magnitudes. We will analyze the symmetric case when  $z_n = z'_n$ . We denote by  $X_n$  as the displacement of the bases along the hydrogen bond at the  $n^{\text{th}}$  site and by  $p_n = m_1 \dot{X}_n$  their corresponding momentuma. Details on how to construct the hamiltonian model for the DNA with torsion can be found in the works [5–8, 15, 16]. In some sense here the double strand DNA model is mapped onto a two coupled spin chain model or a spin ladder system with ferromagnetic legs.

On the other hand, there is a powerful method of the generalized coherent state. that allows to obtain a quasi-classical version of the model by averaging the quantum or quasi-quantum Hamiltonian over some states that minimizes uncertainties [17]. Here as mentioned above, we investigate the particle-like localized nonlinear excitation in the quasi quantum Hamiltonian for DNA obtained by Takeno-Homma [5, 6] by making use the reduction procedure, based on the generalized coherent states (GCS) on the group  $SU(2)/U(1)$ . We consider the homogeneous system that means all exchange integrals in the Hamiltonian (1) are constants and do not differ from point point to point. The quasi-spin piece of the Hamiltonian (1) is formally written in terms of spin

operators with spin value  $j = 1/2$ . Since, the spin Hamiltonian and the  $SU(2)$  coherent states are constructed on the operators of the same group, here is not necessary to carry out the bozonization procedure of the Hamiltonian. The exchange integrals in the  $x, y, z$  direction are the same so we have a quasi spin system with zero anisotropy. This type of system according to Makhankov [18] has the  $SU(2)$  symmetry. Also we can consider the easy axis of the model the axis  $z$  that is the direction of helical axis of anisotropy. All these qualities permit us to use the approach of generalized coherent states based on  $SU(2)$  group.

It is known that the system of spin coherent states (GCS constructed on the  $SU(2)/U(1)$  space; which is the classical Hopf fibration  $S^1 \rightarrow S^3 \rightarrow S^2$ ) may be written as [12]:

$$|\psi\rangle = T(g)|\psi_0\rangle = e^{\alpha S^+ - \hat{\alpha} S^-} |0\rangle = (1 + |\psi|^2)^{-j} e^{\psi S^+} |0\rangle \quad (3)$$

with  $\hat{S}^\pm = \hat{S}^x \pm i\hat{S}^y$ ,  $\psi = \frac{\alpha}{|\alpha|} \text{Tan}|\alpha|$ ,  $\alpha, \psi$  are complex numbers,  $|0\rangle = |j, -j\rangle$  and  $j$  defines the unitary representation of the group  $SU(2)$ . Formally we have the triplet:  $\langle G, \pi, G/P \rangle$ , where  $\pi$  is the continuum projector.

After averaging the Hamiltonian (1) with the aid of  $SU(2)$  GCS it is obtained

$$H = \sum_n \left\{ -\frac{J}{2} \left( \frac{(\bar{\psi}_n \psi_{n+1} + \bar{\psi}_{n+1} \psi_n) + (1 - |\psi_n|^2)(1 - |\psi_{n+1}|^2)}{(1 + |\psi_n|^2)(1 + |\psi_{n+1}|^2)} + \right. \right. \\ \left. \left. + \frac{(\bar{\xi}_n \xi_{n+1} + \bar{\xi}_{n+1} \xi_n) + (1 - |\xi_n|^2)(1 - |\xi_{n+1}|^2)}{(1 + |\xi_n|^2)(1 + |\xi_{n+1}|^2)} \right) - \right. \\ \left. - \frac{1}{4} (\mu - \alpha_1 (X_{n+1} - X_{n-1})) \frac{2\bar{\psi}_n \xi_n + 2\bar{\xi}_n \psi_n + (1 - |\xi_n|^2)(1 - |\psi_n|^2)}{(1 + |\xi_n|^2)(1 + |\psi_n|^2)} + \right. \\ \left. + \frac{p_n^2}{2m_1} + k_1 (X_n - X_{n+1})^2 \right\}. \quad (4)$$

### 3. Equations of Motion

let us study the continuum version of the Hamiltonian model (4). Therefore, we consider the inter-site distance between nucleotides are quite small in comparison with the DNA length. Introducing the new variable fields  $X_n \rightarrow X(z, t)$  with  $z = na$  and as usual making the standard procedures we have

$$\psi_{n\pm 1} = \psi(z, t) \pm a\psi_z + \frac{a^2}{2!}\psi_{zz} + \dots,$$

also

$$|\psi_{n\pm 1}|^2 = |\psi|^2 \pm a(|\psi|)_z + \frac{a^2}{2!}(|\psi|)_{zz} + \dots,$$

and

$$\sum_n - > \int \frac{dz}{a}.$$

The similar expansion can be straightly done for  $\xi_{n\pm 1}$  and  $|\xi_{n\pm 1}|^2$ . These last variables correspond to the complementary strand (apostrophe variables) of the double ladder of DNA. Also similar approximation is done for  $X_{n\pm 1}$ . After some algebra we obtain the quasi-classical Hamiltonian

$$H = \int \left\{ \frac{aJ}{2} \left( \frac{|\psi_z|^2}{1+|\psi|^2} + \frac{|\xi_z|^2}{1+|\xi|^2} \right) - \frac{(\mu - 2\alpha_1 a X_z)}{4a} \left( \frac{2(\psi\bar{\xi} + \bar{\psi}\xi) + (1-|\xi|^2)(1-|\psi|^2)}{(1+|\xi|^2)(1+|\psi|^2)} \right) + \frac{p^2}{2am_1} + k_1 a (X_z)^2 \right\} dz + \text{const.} \quad (5)$$

The equation of motion for the unknown variables can be obtained using the standard Hamiltonian method. Thus, for finding the unknown displacements  $X(z, t)$  from the Eq.(5) we can use the standard Hamiltonian equations of motion  $\dot{X} = \frac{\partial H}{\partial p}$  and its canonical conjugate counterpart. The equation of motion for the unknown field functions  $\psi(z, t)$  and  $\xi(z, t)$  can be written using the variational derivative as [19]

$$i\psi_t = -(1+|\psi|^2)^2 \frac{\delta H}{\delta \bar{\psi}}.$$

The similar equation of motion is directly built also for the field variable  $\xi$ . Considering these two nonlinear equations after some algebra we can find the next nonlinear Nonlinear Schrödinger equation with saturation equation

$$i\psi = -\frac{Ja}{2}\psi_{zz} + aJ\frac{\psi_z^2\bar{\psi}}{1+|\psi|^2} + \left(\frac{2\mu}{a} - 4\alpha_1 X_z\right)\frac{1-|\psi|^2}{1+|\psi|^2}\psi. \quad (6)$$

For description the hydrogen bond displacements  $X(z, t)$  one can obtain the next also nonlinear equation that depend on the torsions ( $\psi$ ) of the previous nonlinear equation

$$m_1 X_{tt} = 2ak_1 X_{zz} + \frac{\alpha_1}{2} \left( \frac{1+|\psi|^4 - 6|\psi|^2}{(1+|\psi|^2)^2} \right)_z. \quad (7)$$

#### 4. Nonclassical Traveling Waves

We will look forward for traveling wave solutions. For doing this we change the variables  $\sigma = z - vt$ . Applying the procedure due to Vasumathi and Daniel [7, 8] i.e. making  $X_z = W(z, t)$ , after some algebra it yields

$$X_z = \frac{\alpha_1}{2(m_1 v^2 - 2ak_1)} \frac{1+|\psi|^4 - 6|\psi|^2}{(1+|\psi|^2)^2}. \quad (8)$$

Replacing the equation (8) in to the nonlinear Schrödinger equation (6) and by considering restriction on the exchange integrals and the change of variables  $z = s\sqrt{\frac{Ja}{2}}$  the equation (6) can be reduced to the well known Cubic-Quintic Nonlinear Schrödinger Equation (CQNSE):

$$i\psi_t + \psi_{ss} + \kappa_1\psi + \kappa_3|\psi|^2\psi - \kappa_5|\psi|^4\psi = 0 \quad (9)$$

with the following parameter relations

$$\kappa_1 = -2\mu + \beta, \quad \kappa_3 = 4\mu - 10\beta, \quad \kappa_5 = 4\mu - 34\beta \quad (10)$$

with

$$\beta = \frac{2\alpha_1}{m_1v^2 - 2ak_1}. \tag{11}$$

Let us analyze some particular interesting cases of the obtained equation (9)

**I. Case:**  $\kappa_5 = 0$ . In this particular case, the equation (9) reduces to the well known nonlinear Schrödinger equation

$$i\varphi_t + \varphi_{ss} + \gamma|\varphi|^2\varphi = 0 \tag{12}$$

with the following redefined functions and parameters  $\psi = \varphi e^{i\kappa_1 t}$  and  $\kappa_1 = -\frac{9}{8}\gamma$ ,  $\kappa_3 = \gamma = 24\beta$ . The previous nonlinear equation is the famous nonlinear Schrödinger equation that is completely integrable. Thus there does exist a method for instance an inverse scattering or Hirota methods for finding its N-soliton solutions [20].

For obtaining some information on for the hydrogen bond displacement of the DNA macromolecule let us take some solution of the Schrodinger nonlinear equation (12). First we consider the sign of the parameter  $\gamma$  to be positive. For this case as is well known [21] when  $\gamma > 1$  the solution of the NSE (12) with the trivial boundary condition that means when the field tends to zero as  $|x| \rightarrow \infty$  is

$$\varphi(s, t) = \left(-\frac{2\nu}{\gamma}\right)^{1/2} \text{Sech} [\sqrt{-\nu}s] \exp\{-i\nu t\} \tag{13}$$

being  $\nu$  an arbitrary constant. Since we are interested in obtaining traveling wave solution, we will use the well established fact that NSE is invariant under the Galilean transformations

$$\zeta = s - Vt, \quad \tau = t, \quad \varphi' = \varphi \exp\left\{-\frac{iV}{2}\left(s - \frac{1}{2}V\tau\right)\right\}, \tag{14}$$

where  $\zeta = \sigma/\sqrt{\frac{Ja}{2}}$ ,  $V = v/\sqrt{\frac{Ja}{2}}$  that finally gives us the traveling soliton

$$\varphi(s, t) = \left(-\frac{2\nu}{\gamma}\right)^{i/2} \text{Sech} [\sqrt{-\nu} \zeta] \exp\left[\frac{iV}{2} - \frac{i}{2}\left\{\left(\frac{V}{2}\right)^2 + 2\nu\right\}t\right].$$

This solution applied to DNA molecular dynamics should imply that a collective wave of bell type forming a certain open state for the angle deviation defined by  $|\psi|^2 = |\varphi|^2 = (\tan(\vartheta/2))^2$  should be propagated along the chain due to the interaction of the DNA molecule with thermal phonons surrounding molecule. This because the collective wave is constructed by the two types of bell solutions for  $\psi$  and for  $\xi$  field variables correspondingly.

**II. Case.**  $\alpha_3 = 0$  In this case we have the Quintic Schrödinger equation.

$$i\varphi_t + \varphi_{ss} + \gamma_2|\varphi|^4\varphi = 0. \tag{15}$$

This nonlinear equation supports soliton solution in the attractive case when the coefficient  $\gamma_2$  is positive. The solution that divides the scenario of the evolution equation in two sectors is possible to exist [22]

$$\varphi(s, t) = \frac{3^{1/4}(-w)^{1/4}}{\sqrt{\text{Cosh}(2\sqrt{-ws})}} e^{-iwt}.$$

The first sector as is well known is the sector of collapse when the amplitude of the solution infinitely grows in a finite time. The second scenario correspond to the dispersion solution when the amplitude decays and the area of its localization grows. The collapse is not physical well solution. Then, in this case it is convenient to introduce other effects perhaps dissipative ones for compensate the blow up of solutions. These can be numerous nonlinear dissipation mechanisms such as inelastic collisions of the pair of base of DNA with surrounding proteins molecules which results in loss of energy by emitting heat. This interesting issue could be studied further.

## 5. Hydrogen bond displacements

The mixture of both solutions  $\psi$  and  $-\psi$  will maintain a certain configuration state along the chain for angle rotations  $\vartheta$  and  $\varphi$ . For instance, we can see a configuration made by  $\text{Sech}^2(\zeta)$  and by  $-\text{Sech}^2(\zeta)$  in such a manner that along the DNA chain should be created a wooden spinning top state, for the angle  $\vartheta$  deviation. In this case, one can observe the envelope of the edges of quasi-spin arrows. The angle that forms the arrows of quasi spins with respect to the axes  $\zeta$  represents the angle deviation from equilibrium position. Far from the central part the excitation zone, the angle deviations  $\vartheta$  in the middle site acquires the maximum value while outside of the center the angles vanish.

For calculating the traveling waves for displacements  $X$  along the hydrogen bonds we can use the analytical solution (13). We replace this solution into the equation (8) and integrate once with respect to the variable  $\zeta$ . After integration we have obtained a traveling solution for the displacements  $X(\zeta)$  with an arbitrary constant of integration  $X_0$ . This constant of integration can be considered by some initial condition imposed to the nonlinear equation (8). Further, the integration has been done numerically and we found the pair compacton structure represented in the Fig. (1), by virtue of satisfying the trivial boundary condition at infinity and initial conditions. Resuming, we found a solutions for the hydrogen bond displacements that can be represented by

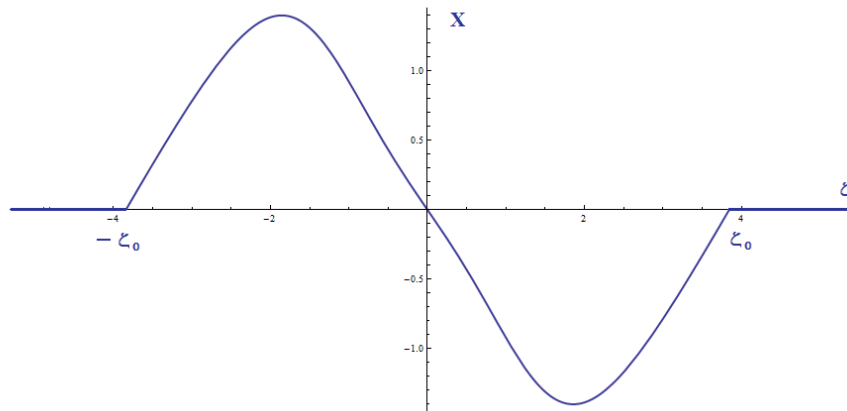
$$\begin{aligned} X(\zeta) &= X(s - Vt) = \delta \int F(|\varphi|^2) d\zeta, \quad \text{for } -\zeta_0 \leq \zeta \leq \zeta_0 \\ X(\zeta) &= 0, \quad \text{elsewhere} \end{aligned} \quad (16)$$

$$\text{with } F(|\varphi|^2) = \frac{1 + |\varphi|^4 - 6|\varphi|^2}{(1 + |\varphi|^2)^2} \quad \text{and} \quad \delta = \frac{\beta}{4} \sqrt{\frac{Ja}{2}}. \quad (17)$$

This solution represents a couple of compact and anti-compact fused structures. Specifically, the sector for negative values of independent variable  $-\zeta_0 \leq \zeta \leq 0$  corresponds to the compact piece of the solution and in the region of  $0 \leq \zeta \leq \zeta_0$  lives the anticompaton branch of the solution. Thus, this solution is made of two different contributions of the waves. As it is well common for similar compact structures [23] we observe the discontinuity on its first derivative at points  $\pm\zeta_0$ . Thus, the compacton sector ensure the formation of open states due to positive values of displacement of hydrogen bonds, while the anti-compacton sector represents the reconstruction of hydrogen bonds, see Fig.(1). The compacton and the anti-compacton parts collaborate each other in such a manner that the DNA molecule preserves its identity. We observe here a natural mechanism of healing the open states that profusely can be created along the different sector of DNA molecule.

For the second case or the quintic Schrödinger equation, the hydrogen bond displacements can be obtained analytically and we have the particular solution for example when  $w = -1$

$$X(\zeta) = \frac{1}{2} \delta \left( 2\zeta + 4\sqrt{6} \text{ArcTanh} \left[ \frac{(-1 + \sqrt{3}) \text{Tanh}(\zeta)}{\sqrt{2}} \right] - \frac{12 \text{Sinh}(2\zeta)}{\sqrt{3} + \text{Cosh}(2\zeta)} \right) \quad (18)$$



**Figure 1. A couple compacton anti-compacton solution for hydrogen bond displacements along the DNA. The positive values of displacements elongate the separation of the two strands while the negative ones stretch this separation. The values of  $\beta = 1$  was used for numerical integration of the corresponding equations**

for  $-\zeta_0 \leq \zeta \leq \zeta_0$ .

The profile of this solution has the similar fashion of the previous solution found for the case of cubic Schrödinger equation with the Fig. (1). Again this solution represents a typical couple of compacton and anti-compacton pair solution. Although the angle deviations undergo collapse effects, the corresponding hydrogen displacement shows a regular behavior.

The energy of the compacton pair can be easily calculated by virtue of equation (5). The integration with respect to the variable  $\zeta$  in the interval  $[-\zeta_0, \zeta_0]$  of first pair compacton anticompacton can be evaluated directly using the energy density

$$E = g(X_\zeta^2) + hX_\zeta F(|\varphi|^2) \quad (19)$$

with  $g = \frac{mv^2 + 3k_1a}{Ja}$ ,  $h = \frac{\alpha_1}{\sqrt{2}Ja}$  and  $F(|\varphi|^2)$  is defined by the relation (17). The compacton solution can emerge only when the velocities do not satisfy the relation  $mv^2 - 2ak_1 = 0$ . Otherwise, we could encounter nonphysical solutions with infinity values of energy.

## 6. Conclusions

We have discussed in this contribution the appearance of non classical soliton-like excitations along the DNA molecular model based on the pioneering work of [5, 6]. These solutions could eventually be responsible for various fundamental processes inside the DNA macromolecule. As is well known the relation of the quasi-classical field variable of the GCS approach  $\psi$  and the angle  $\vartheta$  being the deviation of the angle of the classical spin  $\mathbf{S}$  see Eq. (2) from the  $OZ$  axis is the following  $|\psi|^2 = \tan^2(\vartheta/2)$  [12]. Thus the using of generalized coherent state approach provides us directly with the possibility to calculate the angle deviation of the “classical” spin with respect the chosen direction  $z$ . This approach allows us to derive a familiar NSE, that for very specific parameter values represents the well known completely integrable model. The angle deviation from the axis  $z$  will completely determined by the solutions of integrable NSE. These exact solutions that could serve as a good first approximation in a complex and deep theoretical and experimental analysis of the DNA molecule.

The hydrogen bond displacements, shows unexpected behavior represented by the couple of compacton anti-compacton solution. The velocities of these solutions are determined from the parameters  $\kappa$  (10) that are restricted by the relation  $\beta > 0$  from equation (11).

The evaluation of displacements of the hydrogen bonds along the DNA can be carried out straightforwardly by integrating their corresponding nonlinear equations (8). We considered that for displacements that occur sufficiently far from the excitation zone, vanish. Therefore, in both direction of the axis  $\zeta$  we will observe the physical interesting case of vanished values of hydrogen bond displacements at long distances from the active zone. By taking in mind this physical reason and integration of the equation (8) we obtain for specific parameter values the compacton anti-compacton couple while the angle  $\vartheta$  deviation evolves like a bell soliton along the DNA macromolecule.

As is well known the open states of DNA chain is considered the precursors of denaturation of this macromolecule. As soon as the nonlinear excitations in whichever segment of the DNA molecule is being activated by external factors for example phonons in our case, nonlinear waves of coupled compacton and anti-compacton pieces could appear, describing the evolution of hydrogen bonds. The anti-compacton piece one could be interpreted as a healing wave part e that cures the bubble or open states on the DNA segments.

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### Нелинейная динамика неклассических уединённых волн

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Методом обобщённых когерентных состояний (ОКС) в применении к решеточной модели ДНК получено нелинейное уравнение Шрёдингера. В этой модели макромолекула ДНК подвержена влиянию тепловых фононов. Путем анализа уравнения Шрёдингера с насыщением получено несколько солитонно-подобных решений, описывающих водородные связи. Среди них имеется пара «компактный и антикомпактный солитоны», которая эволюционирует в соответствии с механизмом восстановления открытых состояний с водородными связями.

**Ключевые слова:** неклассические решения, обобщённые когерентные состояния, ДНК, компактоны.