Coupled Schrödinger equations as a model of interchain torsional excitation transport in the DNA model

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Abstract
In this report we consider two weakly coupled Schrödinger equations as a reduced model of interchain energy transport in the DNA double-helix torsional model. We employ a reduction of the Yakushevich-type model that considers the torsional dynamics of the DNA as effective chains of pendula. In previous works, only small amplitude excitations and stationary dynamics were investigated, whereas we focus on the nonstationary dynamics of the double helix. We consider the system to be a model of two weakly interacting DNA strands. Assuming that initially only one of the chains is excited in the form of a breather, we demonstrate the existence of an invariant that allows us to reduce the order of the problem and examine the system of the phase plane. The analysis demonstrates the utility of an analytical tool for predicting the periodic interchain excitation transitions of its localisation on one of the chains. The technique also takes into account the spreading of the excitations over time.

1. Introduction

The dynamic properties of DNA have attracted the attention of researchers from different fields of science for decades [1]. The DNA molecule is an extraordinarily complex system containing numerous degrees of freedom and a hierarchy of structural properties. However, some of its features can be investigated at a fundamental level. The structural transformations of the macromolecule are known to define its dynamic properties. Several dynamic aspects of DNA functioning, which are related only to the weak electrostatic bonds, can be conventionally analysed within a framework of dynamical modelling. The dynamics of DNA molecule are important for a range of biological processes, such as replication, conformation transitions, transcription, and formation of higher-order structures [2]. Some of the processes are also important for applications [3].

Given its importance, several different models have been developed to describe the dynamics of DNA. For molecular dynamical modelling, full models are used that take into account all the potentials for interaction; several also consider the actions of solvents and ions [4, 5]. Such techniques permit a deeper understanding of the mechanisms underlying these processes; however, they are extremely time-consuming and cannot be used to analyze long fragments of DNA for lengthy periods of time. To study dynamics across greater time scales, it is necessary to use reduced models that only take into consideration certain structural elements and dynamic features to produce more general results [5–7]. Several attempts have been made to reduce the DNA model through the use of coarse graining. Some have generated a reasonable description of different processes in the double helix [8], including transitions between the A-form and B-form [9]. However, to make semi-analytical predictions of the dynamics of the DNA double-helix, further reductions are necessary.

Different dynamic processes in the DNA are associated with different models of its motion. Replication and denaturation processes imply separation between the two DNA strands. Therefore, they are better considered in the context of models with radial evolution. The pioneering model of the type developed by Bishop and Peirard [10] which can be solved analytically in the strong (intra-strand) coupling regime using continuum approximation. However, approximation of the strong intra-strand coupling breaks down for DNA [11]. The
model was later extended by Dauxois et al. [12] and Barbi et al. [13]. Another type of model is associated with the transcription process, which is defined mostly by torsional (rotational) excitations. Regarding the latter, one of the first models to be developed was proposed by Yakushevich [14]. This model examines only the torsional dynamics of the double helix together with the bases connecting the strands. This model was later modified into a ‘composite’ model by Cadoni et al. [15]. All the theoretical models are, of course, a compromise between the accuracy of the description and ease of the study. Simple mechanical models can yield a qualitative picture of the processes in the real DNA [16, 17]. However, they can also help to define some mechanisms of the pre-melting and replication in the DNA dynamics [18]. In the mentioned processes as well as for the functioning of the nanodevices, the nonstationary dynamics of DNA can be significant. However, the study of nonstationary processes in non-linear and complex systems is not a simple task. Therefore, simplified models can be used to sketch the dynamical mechanisms of the energy localization and transition in the processes of DNA transformations.

The focus of this paper is on the dynamics of the DNA molecule connected with the local opening process. Our aim is to study regimes with locally excited DNA in the low-amplitude case. Therefore, we consider the thoroughly validated Yakushevich-type model [17]. Our primary interest is in the study of inter-chain breather transport. Such work was first initiated by Kovaletza et al. [19, 20]; however, it was only examined phenomenologically, the spreading of the excitations was not taken into account, and the phase evolution of the reduced system was not cleared. In our paper we present a regular multiple-scales procedure that we employ to reduce the Yakushevich-type model [21] to a system of two coupled Schrödinger equations.

The non-linear Schrödinger equation is a universal tool used for the description of multiple non-linear systems and objects in different fields of science such as optics, physics of plasmas, and solid-state physics. Because it is classical, this equation has been studied in detail [22–27]. Our principal focus is on the exchange of interchain excitations. The variational approach to the solitons in the coupled non-linear Schrödinger equations was earlier reported in connection with the system of twin-core optical fibers [28, 29]. In this system, the bifurcation analysis of the stationary solutions was provided for the symmetric and asymmetric coupler and the role of different types of dispersion was considered. The dynamics of the ensembles of the interacting non-linear chains was also examined by [30]. In this study, the dynamics of the weakly non-linear coupled chains was also reduced to the coupled non-linear Schrödinger equations. Inter-chain energy transport was considered for plane waves and for localised solutions. However, the dispersion of the localised solutions was not taken into account. We therefore present a detailed study of the exchange of interchain breathers using a simplified model of the DNA.

We consider the breather that corresponds to localised excitation of one of the strands of DNA. Applying the collective coordinates technique, we assume that the form of excitation is not altered via inter-chain interactions. We reveal the new invariant of the reduced-order system, which enables us to represent the evolution of the system on the phase plane. The analysis provides the value of the system parameters for the dynamic threshold, which is the point when the transition from interchain excitation exchange to excitation localisation occurs. We verify our analysis using the results of the numerical modelling of the initial model.

2. Model formulation

We first examine the B form of a DNA molecule in which the double helix is considered to be two coupled chains of equivalent pendula. The Hamilton function of the double strand is described by the angular displacements of the n-th base at the corresponding first and second chains [17, 19–21]

\[
H = \sum_n \left\{ \frac{1}{2} I_n, \dot{\psi}_{n,1}^2 + \frac{1}{2} I_n, \dot{\psi}_{n,2}^2 + \varepsilon_{n,1} \sin^2 \frac{\psi_{n+1,1} - \psi_{n,1}}{2} + \varepsilon_{n,2} \sin^2 \frac{\psi_{n+1,2} - \psi_{n,2}}{2} + V_{n,\beta}(\psi_{n,1}, \psi_{n,2}) \right\}
\]

\[
V_{n,\beta}(\psi_{n,1}, \psi_{n,2}) = C_1(1 - \cos \psi_{n,1}) + C_2(1 - \cos \psi_{n,2}) - C_4(1 - \cos (\psi_{n,1} - \psi_{n,2}))
\]

where the parameters are defined as follows:

\[
C_1 = K_{n,\beta} r_0 (r_0 + r_\beta), \quad C_2 = K_{n,\beta} r_\beta (r_0 + r_\beta), \quad C_4 = \frac{1}{4} K_{n,\beta} \left( 1 - \frac{\omega_{n,1,2}}{\omega_{n,1,2}^2} \right) (r_0 + r_\beta)^2
\]

\[
\omega_{n,1,2}, \omega_{n,1,2}^2
\]

are the frequencies of the rotational vibrations of the same and opposite directions, respectively, while \(K_{n,\beta}\) denotes the stiffness of the base-pair interaction. The interaction along the chains is accounted for in the nearest-neighbour approximation. The two first terms of the Hamiltonian represent the kinetic energy of the n-th base pair, while \(I_n,\dot{\psi}_{n,1}^2\) and \(I_n,\dot{\psi}_{n,2}^2\) are the inertia moments of the n-th base of the first and second chains, respectively. The third and the fourth terms describe the interaction between the neighbouring base pairs along each of the macromolecule chains. Parameter \(\varepsilon_{n,1} = \varepsilon_{n,2} = \varepsilon_{n,1,2}\) characterises the energy of interaction of the n-th base with
the \((n+1)\)-th base of the \(i\)-th \((I = 1, 2)\) chain. The final term of the Hamiltonian represents the energy of interaction between the coupled bases of different chains. The parameters of the model were thoroughly verified with the experimental data and with the molecular dynamical simulations. The model itself, its spectra, and possible solutions have been discussed in previous works \cite{19, 20}. However, the localised excitations wandering between the chains have not been studied in detail.

3. Breathers and their inter-chain transport

The model (1) permits different types of localised solutions, including solitons and breathers \cite{20, 21}. Their properties and form were reported earlier \cite{20, 21}. We would like to underline, that the solutions discussed were smooth enough to be considered in the continuum limit. The possible connection of such excitations with the opened states of the real DNA double-helix are discussed in the review by Shigaev at al.\cite{18}. In numerical studies of the coupled system (1), we have observed the breathers wandering between the two chains or the localisation of breathers on one chain depending on the value of the coupling parameter between the two chains. To proceed with further observations of the phenomenon, we make several assumptions concerning the properties of the excitation. Within the limits of small amplitudes and the long-wave approximation, the equations of motion can be transformed into a quasi-continuum to obtain two coupled non-linear Schrödinger equations (see Appendix for details). These can be transformed into a simple form as follows:

\[ \frac{d^2\tilde{\varphi}_1}{dt^2} = \frac{d^2\tilde{\varphi}_1}{dx^2} + |\tilde{\varphi}_1|^2\tilde{\varphi}_1 + \mu (\tilde{\varphi}_1 - \tilde{\varphi}_2), \]

\[ \frac{d^2\tilde{\varphi}_2}{dt^2} = \frac{d^2\tilde{\varphi}_2}{dx^2} + |\tilde{\varphi}_2|^2\tilde{\varphi}_2 + \mu (\tilde{\varphi}_2 - \tilde{\varphi}_1) \]

where \(\mu\) is the effective coupling parameter. In the uncoupled system, when \(\mu = 0\) the breather solution can be found as follows:

\[ \tilde{\varphi}_1 = A_1 \text{sech}(a_1(x - V_1\tau)) \exp(i(x - V_1\tau)\xi_1 + i\eta_1); \]

\[ \tilde{\varphi}_2 = A_2 \text{sech}(a_2(x - V_2\tau)) \exp(i(x - V_2\tau)\xi_2 + i\eta_2); \]

(3)

To study the possibility of the breather wandering between the chains or localisation on one chain we employ the collective coordinates technique, which is a type of variational approach \cite{35}. We assume that the breather wandering between the chains is slow due to weak coupling between the chains. This enables us to consider the solution in the form (3) but with all the parameters being super-slow time-dependent (the new time scale is defined as \(\tau\)). The Lagrange function of the system can be formulated as follows:

\[ L = \sum_n \left\{ \frac{1}{2} \left( \frac{\partial^2\tilde{\varphi}_n}{\partial \xi_n^2} + \frac{\partial^2\tilde{\varphi}_n}{\partial \eta_n^2} \right) - \left| \frac{\partial^2\tilde{\varphi}_n}{\partial x^2} \right|^2 + |\tilde{\varphi}_n|^4 \right\} + \mu |\tilde{\varphi}_1 - \tilde{\varphi}_2|^2, \quad n = 1, 2 \]

(4)

All the parameters of the solution (4) serve as collective coordinates of the system. Performing the effective Lagrangian with respect to the collective coordinates, we demonstrate that the solution (3) can exist in the coupled system in case \(V_1 = V_2\), and it admits an invariant:

\[ N = \frac{\xi}{a}(A_1^2 + A_2^2) \]

(5)

where \(\xi = \xi_1 = \xi_2\), \(a_1 = a_2 = a\).

Thus, we can assume that \(\xi = \text{const}\), based on which we obtain the integral in the following form:

\[ N_0 = \frac{1}{a}(A_1^2 + A_2^2) \]

(6)

Such an invariant allows consideration of the weak spreading of the excitation and a description of the dynamics with dispersion. When the amplitude of the excitation is decreased, the width of the solution increases. An analogous form of integral was obtained in \cite{28}, but with slightly different definitions of the parameters.

If we assume that the dispersion is weak enough to permit the exchange of interchain breathers, then we can assume spreading with time, namely neglect the \(\frac{d^2}{dt^2}\) in the leading approximation. The integral of motion then takes the form of the norm:

\[ N_i = A_1^2 + A_2^2 \]

(7)

Such an integral enables us to introduce angular representation:

\[ \tilde{\varphi}_1 = N_i \cos(\theta(\tau)) e^{i\psi_1(x, \tau)} \]

\[ \tilde{\varphi}_2 = N_i \sin(\theta(\tau)) e^{i\psi_2(x, \tau)} \]
where $\varphi(x, \tau)$—is the soliton solution of the isolated chain with amplitude equal to unity.

The equations of motion can now be transformed into the following form:

$$\frac{d\theta}{d\tau_1} = \sin(\Delta);$$

$$\frac{d\Delta}{d\tau_1} \sin(2\theta) = k \sin(2\theta) + \cos(\Delta) \cos(2\theta),$$

where $k = \frac{N_1}{2\mu}$. The evolution of the system can be represented on the phase plane.

We begin the analysis of (9) by seeking the fixed points of the system, which are crucial for a proper understanding of the entire mechanism triggering the inter-chain energy transfer. The first fixed point $(\Delta_1, \theta_1)$, which corresponds to the in-phase periodic motion of the full system with an equal energy distribution between the coupled chains, is derived from (9):

$$\Delta_1 = 0, \theta_1 = \frac{\pi}{4}$$

There are three additional fixed points that correspond to the out-of-phase periodic motion of the full model $(\Delta_2, \theta_2)$. The evolution of the stationary solutions for symmetric and asymmetric cases is discussed in detail in [27]. The stationary solution for the modulated system, corresponding to the out-of-phase motion of the two oscillators between which energy is equally distributed, is as follows:

$$\Delta_2 = \pi, \theta_2 = \frac{\pi}{4}$$

For simplicity, we only consider coordinates in the range $0 \leq \theta_k \leq \frac{\pi}{2}, -\pi < \Delta_k \leq \pi$ due to the periodicity of the angular coordinates $(\theta, \Delta)$.

In the super–slow flow model, the regime of complete energy exchanges between the chains corresponds to a special orbit that passes through $\theta = 0$ and reaches a value of $\theta = \pi/2$. This special type of trajectory is referred to in the literature as a Limiting Phase Trajectory (LPT). The concept of LPTs was first introduced in [31] and appears to be an extremely useful methodology for generating an adequate description and understanding of nonstationary resonant processes emerging in the various oscillatory models (see also [32]). The LPT is a nonstationary oscillatory regime that exhibits a complete energy exchange between the coupled systems. The initial conditions corresponding to the LPT are $\theta = \Delta = 0$, which can also be interpreted as the complete initial energy localisation on the first chain while the second is at the rest.

If the coupling parameter $k$ is low, there are only two stationary points on the phase plane (see figure 1). When starting from one of these points, the LPT passes both the $\theta = 0$ and $\theta = \pi/2$ points. If the coupling increases, the anti-phase stationary point loses stability, and two new stationary points are born, separated by a separatrix passing through the saddle point. However, below the critical value $k_{cr} = 0.5$, the form of the LPT does not change. When the coupling parameter increases, a new bifurcation occurs, the topological transformation of the phase space takes place, and the LPT collides with the separatrix and becomes localised around one of the new-born stationary points. The LPT transformation corresponds to localisation of excitation on one of the chains when the initial conditions correspond to excitation of one of the chains in the system.

4. Numerical verification of the results

To verify the results obtained in the asymptotic analysis, we examine the evolution of the system (1) where initial conditions correspond to excitation in the form of a breather placed only on one chain. The parameters of the model as well as the form of the initial excitation correspond to the excitation obtained in [20]. According to the results discussed previously, we should observe localisation of the breather on one of the chains or wandering of the breathers between the chains on a super-slow time scale. We demonstrate in figures 2 and 3 that prediction generally works well for the defined parameter range, corresponding to weak coupling and the small amplitude excitations limit. As expected, the localised excitations spread and the width of the signal increases, while the amplitude of excitation decreases. This type of evolution is clearly supported by the invariant (7). We can also represent the evolution as a time space diagram (see figure 4). This depicts the realisation of the interchain transport of the excitation. The profiles at different time-steps show the spread of the energy in the oscillating background, which moves from the breather towards the ends of each chain. However, until the amplitude of the background excitation is considerably lower than the amplitude of the breather solution, the results of our analysis remain relevant to the evolution of the breathers in the full system (1). The effective coupling parameter plays the role of controlling parameter of our system. We should note that in the real DNA dynamics the effective
coupling is defined both by the type of the coupled bases and by the environment. The interchain wandering of the excitation or its localisation should be affected by both factors.

5. Conclusions

In the current work we analysed the process of breather excitation wandering between the chains of the double helix of DNA within the low-amplitudes limit. This is the first study in which the nonstationary regimes of the...
torsional localised solutions wandering between the two coupled chains have been addressed in detail. We reduced the system to weakly coupled non-linear Schrödinger equations. The effective Lagrangian and collective coordinates technique revealed the invariant of the system in the regime of breather exchange between the two chains. All the simulations are provided for the initial model (1).

**Figure 3.** Breather profile and time evolution of the middle element corresponding to the controlling parameter $k = 0.2$, excitation exchange between the two chains: (a) and (b) profile snapshots at different moments in time; (c) and (d) time-evolution of the middle-element of the chain. All the simulations are provided for the initial model (1).

**Figure 4.** Breather time-space evolution corresponding to the different controlling parameter values: (a) $k = 0.2$, (b) $k = 0.5$. Left panes show the evolution of the breather at the first chain; right panes show the evolution of the breather at the second chain. All the simulations are provided for the initial model (1).
chains. We verified our analysis through a numerical simulation of the initial system. Although evolution of anti-phase and in-phase breathers has been reported in previous studies, interchain transport was not considered in detail and was only reported phenomenologically. Through our analysis we demonstrated the existence of a regime of intensive excitation exchange and its transition to localisation. We believe that the type of excitations taking place in inter-chain transport are relevant for other weakly non-linear systems described by the coupled Schrödinger equations.

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Data availability statement

The data generated and/or analysed during the current study are not publicly available for legal/ethical reasons but are available from the corresponding author on reasonable request.

Appendix

In the model considered in our paper, two different types of non-linear excitations can be found: high-energy kink solutions \[33\] and low-energy breather waves. The latter was considered in detail and compared with the results of the molecular-dynamics simulations in earlier work \[20\]. It was reported \[20, 21\] that the low-amplitude breathers are quite ‘wide’ localized excitations and demonstrate a smooth profile along the chain. All possible cases where such excitations can appear are considered in detail in the review paper \[18\], and we will not discuss this aspect of the model’s applicability. As the typical space scale of the breather is much higher than the distance between the two neighboring elements of the model, we proceed to the analysis with the continuum model. We should note that the assumption of the strong coupling is not necessary to reduce the model.

Starting the analysis with the Hamiltonian (1), we assume that the amplitudes are small and proceed to the long-wave approximation:

\[
\sin (\psi_{n+1,i} - \psi_{n,i}) - \sin (\psi_{n,i} - \psi_{n-1,i}) \approx \\
\approx \psi_{n+1,i} - \psi_{n,i} - (\psi_{n,i} - \psi_{n-1,i}) \approx \hbar^2 \frac{\partial^2 \psi_{n,i}}{\partial z^2} \quad (1A)
\]

Where \(h\) is a typical distance between the bases, space variable \(\chi = \sqrt{\varepsilon} z = \sqrt{\varepsilon} nh, \) \(\varepsilon\) is a small parameter characterising the relation between the distance \(h\) and the wavelength of the excitation. Introducing the dimensionless time variable \(\tau = \omega_0 t, \) where \(\omega_0 = \sqrt{K_{\alpha \beta} r_{\alpha}(r_{\alpha} + r_{\beta})} \) \(12,\) we obtain a system of non-linear PDEs:

\[
\dot{\psi}_1 - \sqrt{\varepsilon} c_1^2 \frac{\partial^2 \psi_1}{\partial \chi^2} + \gamma_1 \sin \psi_1 - \varepsilon \eta_1 \sin(\psi_1 - \psi_2) = 0 \]

\[
\dot{\psi}_2 - \sqrt{\varepsilon} c_2^2 \frac{\partial^2 \psi_2}{\partial \chi^2} + \gamma_2 \sin \psi_2 - \varepsilon \eta_2 \sin(\psi_2 - \psi_1) = 0 \quad (2A)
\]

where \(c_1^2 = \frac{\varepsilon_{n,i}}{2I_1 \omega_0^2}, \gamma_1 = \frac{C_i}{I_1 \omega_0^2}, \varepsilon \eta_1 = \frac{C_{i2}}{I_1 \omega_0^2}.\) The values of coefficients in both equations are assumed to be close to each other: \(\gamma_2 = \gamma_1(1 + a_2 \varepsilon), \eta_2 = \eta_1(1 + a_2 \varepsilon), c_2^2 = c_1^2(1 + a_2 \varepsilon).\) Taking into account the smallness of the amplitudes of excitations we proceed with the variable transformation \(u = \sqrt{\varepsilon} \psi_1, \nu = \sqrt{\varepsilon} \psi_2\) and the expansion of the trigonometric functions in the small-amplitude limit:

\[
u_{\tau\tau} - \varepsilon c_1^2 u_{x\chi} + \gamma_1 u - \frac{1}{6} \gamma_1 u^3 - \varepsilon \eta_1 (u - \nu)
+ \varepsilon^3 \frac{1}{6} \eta_1 (u - \nu)^3 = 0,
\]

\[
u_{\tau\tau} - \varepsilon c_2^2 \nu_{x\chi} + \gamma_2 \nu - \frac{1}{6} \gamma_2 \nu^3 + \varepsilon \eta_2 (u - \nu)
- \varepsilon^3 \frac{1}{6} \eta_2 (u - \nu)^3 = 0. \quad (3A)
\]
Let us rescale the time-variable to simplify the representation: \( t = \sqrt{\tau_0} \). To perform an asymptotic analysis, we apply complexification of the variables:

\[
\dot{u} = \frac{1}{2} (\psi_1 + \psi_1^*); \quad u = -\frac{1}{2i} (\psi_1 - \psi_1^*);
\]

\[
\dot{\psi} = \frac{1}{2} (\psi_2 + \psi_2^*); \quad v = -\frac{1}{2i} (\psi_2 - \psi_2^*)
\]

Separating ‘fast’ \( \tau_0 = \tau \) and ‘slow’ \( \tau_1 = \varepsilon \tau_0 \) time-scales, we employ the two-scale procedure:

\[
\psi_j(\tau_0, \tau_1) = \psi_j^0(\tau_0) + \varepsilon \psi_j^1(\tau_0, \tau_1), \quad j = 1, 2;
\]

\[
\dot{\psi}_j^0 = \frac{d}{d\tau_0} \psi_j^0 + \frac{\varepsilon}{d\tau_1} \dot{\psi}_j^0 = 0, \quad j = 1, 2.
\]

For more information on the multiple-scales procedure, see [36, 34].

The solution gives the following form for the variables:

\[
\psi_j^0(\tau_0) = \varphi_j(\tau_0) \exp(i\tau_0), \quad j = 1, 2.
\]

In the next order of the expansion \( (\varepsilon^2) \) excluding the secular terms we obtain the system of PDEs:

\[
\frac{d}{d\tau_1} \varphi_1 = \frac{c_1^2}{\gamma_1} \frac{d^2 \varphi_1}{dx^2} + \frac{1}{16} \left| \varphi_1 \right|^2 \varphi_1 + \frac{\eta_2}{2\gamma_1} (\varphi_1 - \varphi_2);
\]

\[
\frac{d}{d\tau_2} \varphi_2 = \frac{c_2^2}{\gamma_1} \frac{d^2 \varphi_2}{dx^2} + \frac{1}{16} \left| \varphi_2 \right|^2 \varphi_2 + \frac{\eta_2}{2\gamma_1} (\varphi_2 - \varphi_1).
\]

Additional change of variables \( \tau_2 = \frac{\tau_1}{16} \), \( \chi_2 = \frac{\gamma_1}{\sqrt{16c_2^2}} \chi \) yields:

\[
\frac{d}{d\tau_2} \varphi_1 = \frac{d^2 \varphi_1}{d\chi_2^2} + \left| \varphi_2 \right|^2 \varphi_1 + \mu (\varphi_1 - \varphi_2);
\]

\[
\frac{d}{d\tau_2} \varphi_2 = \frac{d^2 \varphi_2}{d\chi_2^2} + \left| \varphi_2 \right|^2 \varphi_2 + \mu (\varphi_2 - \varphi_1).
\]

where \( \mu = \frac{8\eta_2}{\gamma_1} \)

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