Proceedings of *RAGtime 20–22, 15–19 Oct., 16–20 Sept., 19–23 Oct., 2018/2019/2020, Opava, Czech Republic*
Z. Stuchlík, G. Török and V. Karas, editors, Silesian University in Opava, 2020, pp. 55–71

Quantum information in biomolecules: Transcription and replication of DNA using a soliton model

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ABSTRACT
By performing a Majorana transformation on the total molecular Hamiltonian operator for electrons adiabatically following nuclear motion, the electrons in a hydrogen bond in DNA can be treated as a chain of quasiparticles resulting in a Kitaev chain with a delocalized fermion state. Delocalized fermions define Majorana qubits which can give rise to entanglement and form the foundation of molecular quantum information processes. During transcription and replication of DNA hydrogen bonds are severed. This process can be investigated by employing the soliton model for DNA proposed by Peyrard and Bishop. The effects of solitons in the DNA double helix are studied and, in particular, their effects on decoherence.

Keywords: Quantum information – Majorana fermions – hydrogen bonds – solitons – DNA – transcription and replication of DNA

1 INTRODUCTION

The nature of the life and what distinguishes it from the inanimate is notoriously difficult to identify with any precision (Schrödinger, 1944; Cleland and Chyba, 2002; Tirard et al., 2010; Benner, 2010; Prossr, 2012). In his famous lectures delivered in Dublin in

1943, Schrödinger (Schrödinger, 1944) put the problem succinctly with the question "How can the events in space and time which take place within the spatial boundary of a living organism be accounted for by physics and chemistry?"

Today, whilst the relationship between the mathematical and physical sciences, on the one hand, and the life and mind sciences, on the other, has elucidated much of the complexity of living processes and the dynamical chemical reactions underpinning them, as Nurse (Nurse, 2008) has observed, a "comprehensive understanding of many higher-level biological phenomena remains elusive". There is, however, an emerging consensus that information is a key property of the life phenomenon (Szathmáry, 1989; Küppers, 1990; Yockey, 2002; Davies, 2005; Hazen et al., 2007; Walker and Davies, 2013; Walker et al., 2017; Davies and Walker, 2016; Davies, 2019). There has also been renewal of interest in quantum biology (see, for example Marais et al. (2018); Jim Al-Khalili (2016)) a field of research begun in 1965 by Löwdin (Löwdin, 1963) as a "field of research which describes the life processes and the functioning of the cell on a molecular and submolecular level" (Löwdin, 1963). Here we continue to develop our suggestion (Hubač et al., 2017) on the role of quantum information in biomolecules.

In this paper, we suggest the potential exploitation of *quantum* information in living processes and, in particular, the role of emergent quasiparticles called Majorana fermions associated with the hydrogen bonds in the DNA molecule. This paper builds on our previous study Hubač et al. (2017) of quantum information in biomolecules by investigating transcription and replication of DNA using a soliton model.

In section 2, Majorana fermions are associated with the hydrogen bonds in DNA and associated with the possibility of quantum information being exploited in biomolecules. In section 3, the transcription and replication of DNA is considered using a soliton model. Specifically, we use the Peyrard-Bishop model (Peyrard and Bishop, 1989) and make a small amplitude expansion.

2 MAJORANA FERMIONS AND QUANTUM INFORMATION IN DNA

Recent years have witnessed renewed interest in Majorana fermions and their realization in condensed matter systems has been intensively studied (Wilczek, 2009; Franz, 2013; Leijnse and Flensberg, 2012; Elliott and Franz, 2014; Alicea, 2012). Although initially introduced over 80 years ago by Etore Majorana (Majorana, 1937) as solutions of the Dirac equation (Dirac and Fowler, 1928) describing a neutral spin $\frac{1}{2}$ particle which is its own antiparticle and distinct from the Dirac solutions, for a long time Majorana fermions were regarded as rather abstract entities. (A review of the original work of Majorana is given in the recent volume by Esposito (Esposito, 2014).) Majorana fermion has been extensively investigated in nuclear and particle physics. Over the past decade, Majorana fermions have been realized as emergent quasiparticles (Wilczek, 2009; Franz, 2013; Leijnse and Flensberg, 2012; Elliott and Franz, 2014) in certain condensed matter systems. Specifically, they were studied in p-wave superconductivity by Leijense and Flensberg (Leijnse and Flensberg, 2012), using the Kitaev chain (Kitaev, 2007). The Kitaev chain is a one–dimensional model of a topological superconductor developed by Kitaev in 2001 and illustrated in Figure 2.

As can be seen from this Figure, the Kitaev chain is chain of fermions, which are strongly delocalized. This delocalization is an important property which makes the study of Majorana fermions very interesting. The Kitaev chain or delocalized Majorana fermions is very stable system. However, the delocalization can be lost by decoherence. The stability of the Kitaev chain makes it interesting for quantum information. If we are able to construct a qubit from these delocalized Majorana fermions, the system is very stable and has the potential play an important role in quantum information. The delocalization property of Majorana fermions were studied in connection with non-adiabatic processes by Scheurer and Shnirman (Scheurer and Shnirman, 2013).

In this paper, we use the delocalization property of the hydrogen bonds in the DNA (Deoxyribonucleic acid) molecule and try to use Majorana fermions as a source of quantum information in biomolecules. DNA is the information storage medium for most organisms. Genetic information is encoded in a sequence of pairs of nitrogenous bases which are held together via hedrogen bonds: adenine - thymine (A-T) and guanine - cytosine (G-C). Each base is attached to a five-carbon sugar forming a nucleoside which in turn is attached to a phosphate group creating a nucleotide. Nucleotides are arranged in two antiparallel strands of polynucleotides in a right-handed double-helix structure. In a given DNA molecule each polynucleotide strand is held in place by interactions between complementary base pairs. Genetic information is copied when the strands separate during DNA replication and in transcription, which is the first step in protein synthesis. DNA opens locally allowing only a segment of the sequence to be copied by a ribonucleic acid (RNA), messenger RNA (mRNA). The sense strand of the DNA molecule has the same sequence as the mRNA (mRNA) whilst the antisense strand provides its template. The sequence of nucleotides in mRNA is identical to that in the sense strand of the corresponding DNA except that uracil is used instead of thymine. In both replication and transcription processes the hydrogen bonds between the bases are severed. The area of partially separated DNA strands is known as the denaturation bubble.

The study of replication or transcription of DNA at a quantum mechanical level is a difficult problem because of the complexity of DNA molecule. Progress can be made by constructing low-resolution model descriptions of DNA, which facilitate computationally tractable schemes for investigating these phenomena. One popular choice is a mechanical model of DNA in which the nucleotides are represented by point masses.

The key advantage of such simplified models is that the dynamics of DNA are rendered solvable numerically and can be used to investigate non-linear phenomena, which might gain us some insight into how the denaturation bubble (a precursor for RNA transcription) might form. a staple of non-linear phenomena is the presence of solitons, which are particle-like non-linear waves representing a moving pattern of highly concentrated energy.

In our recent paper Hubač et al. (2017) (see also Hubač and Svrček (1988, 1992b,a); Hubač and Wilson (2008)), we introduced the non-adiabatic Hamiltonian for molecular systems. The relation between this molecular Hamiltonian and the solid state non-adiabatic Hamiltonian was also explored. Our derivation is based on a supersymmetric transformation. We began with a 'crude' adiabatic Hamiltonian, then we introduced new creation and annihilation operators which were functions of the normal coordinates B. Furthermore, we made these new operators functions of the corresponding momentum $\tilde{B}$.

$$\bar{a}_p = \sum_q C_{pq}\left(B, \tilde{B}\right) a_q \tag{1}$$

$$\bar{a}_p^\dagger = \sum_q C_{pq}\left(B, \tilde{B}\right) a_q^\dagger. \tag{2}$$

$$\bar{a}_p = \frac{1}{2}\left(\gamma_{p,1} + \mathrm{i}\gamma_{r,2}\right) \tag{3}$$

$$\bar{a}_p^\dagger = \frac{1}{2}\left(\gamma_{p,1} - \mathrm{i}\gamma_{r,2}\right), \tag{4}$$

We see that the creation and annihilation operators correspond to delocalized fermions; delocalization being realized through B and $\tilde{B}$. We identify these delocalized operators with Majorana fermions. A similar approach was followed by Scheurer and Shnirman (Scheurer and Shnirman, 2013) in their study of non-adiabatic processes in condensed matter systems. We focus our attention on the hydrogen bonds in the DNA molecule. There are several studies which describe the hydrogen bonds in DNA as a non-adiabatic system, with the hydrogen bonds being strongly delocalized (McKenzie, 2014). We therefore found it interesting to apply the quasiparticle concept of Majorana fermions to the hydrogen bond. We investigate Majorana fermions which have been discussed widely in the condensed matter and solid state literature (Wilczek, 2009; Leijnse and Flensberg, 2012; Franz, 2013; Elliott and Franz, 2014; Zuo and Mourik, 2016; Kitaev, 2007; Finck et al., 2012; Nadj-Perge et al., 2014; Bunkov and Gazizulin, 2015; Williams et al., 2012; Rokhinson et al., 2012; Deng et al., 2012; Das et al., 2012; Knez et al., 2012), as emergent quasi–particles in quantum molecular systems and, in particular, associated with the hydrogen bonds in the DNA biomolecule.

The hydrogen bond in DNA is characterized by double-well potential such as that shown in Figure 1. In early work in the field of quantum biology, Löwdin (Löwdin, 1963) constructed double-well potentials for the hydrogen bonds in DNA by a superposition of two Morse potentials. Delocalization occurs between the two minima and we, therefore, place the Majorana fermions, γ_1 and γ_N, into these minima. In some respect this is Kitaev chain between γ_1 and γ_N. By this concept we were able to define qubits and entangled states (Hubač et al., 2017).

There is extensive discussion in literature about proton tunnelling between two double-well minima (see, for example Löwdin (1963); Godbeer et al. (2015)). It is assumed that proton tunnelling can play a role in both mutation and replication of DNA. But even recent sophisticated calculations (Godbeer et al., 2015) using density functional theory (DFT) to model the double-well potential, did not support the role of proton tunnelling. The lack of evidence for proton tunneling supports our assumption that it is not, in fact, a proton but a highly delocalized fermionic quasiparticle which constitutes each of the hydrogen bonds between the DNA strands.

In this paper, we study the effect of solitons on the Majorana fermions associated with the hydrogen bonds in DNA and their possible role in mutation and replication. As described in our previous work Hubač et al. (2017), two hydrogen bonds in DNA represent one qubit and three hydrogen bonds give rise to entangled states. We were therefore able to introduce

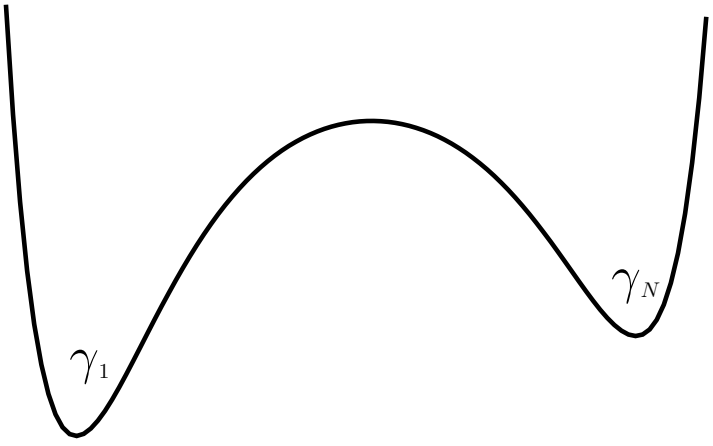

Figure 1. Double-well potential representation of the hydrogen bond. Asymmetric double-well potential obtained by superposition of two Morse potentials. Majorana fermions γ_1 and γ_N are associated with the two minima.

quantum entropy and quantum information. In the present work, we show that solitons can push the delocalized Majorana fermions close to each other leading to decoherence and to a decoupling of the strong electron-phonon interaction. We note that decoherence on a double well potential was demonstrated in the recent work of Marais *et al.* (Marais et al., 2018) (see their Figure 2 on the photosystem II reaction centre in higher plants).
In this way the quantum information associated with the Majorana fermions can be changed. We note that the question of the role of information flow in the cell and and how information is communicated was recently addressed by Nurse (Nurse, 2008).

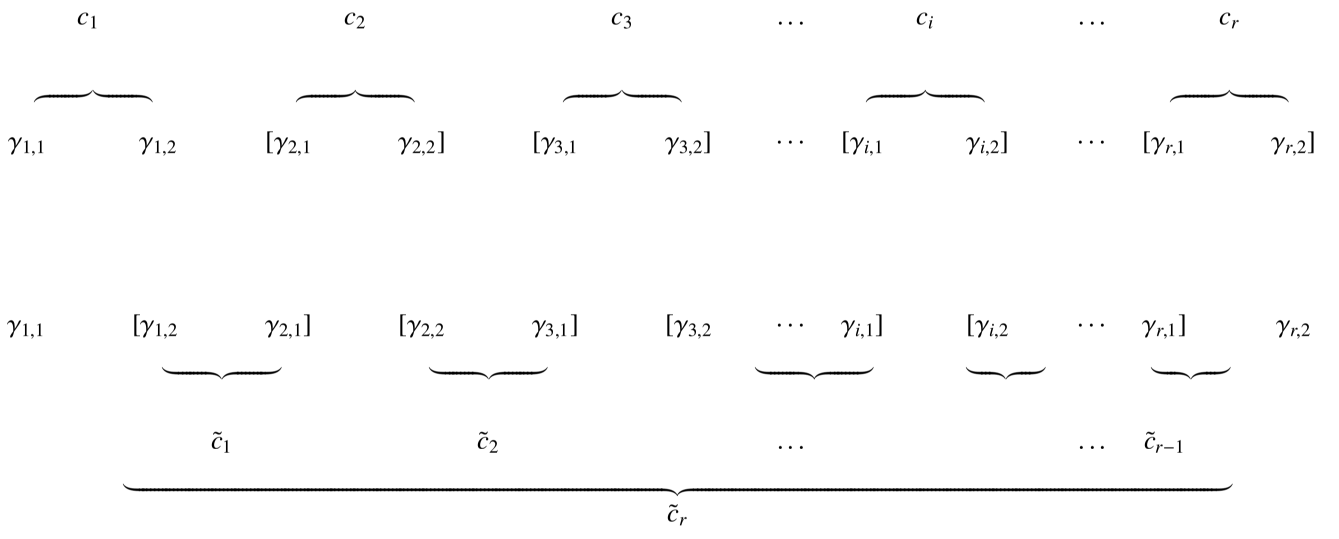

Figure 2. A Kitaev chain. In a product of fermion operators $c_1 c_2 \dots c_i \dots c_r$ each operator is written as a sum of two Majorana operators $\gamma_{i,1}$ and $\gamma_{i,2}$. The Majorana operators are then recoupled so as to leave the isolated γ operators $\gamma_{1,1}$ and $\gamma_{r,2}$ at either end of the chain.

3 SOLITONS ON DNA

An advantage of the drastic simplification adopted in this work is that the dynamics of DNA becomes (at least numerically) solvable and we can look for non-linear phenomena, which might gain us some insight into how the denaturation bubble (a precursor for RNA transcription) might form. A staple of non-linear phenomena is the presence of solitons, which are particle-like non-linear waves representing a moving pattern of highly concentrated energy. Furthermore, solitons are ubiquitous in all media where dispersion can be compensated by non-linear effects. As such, DNA can be also regarded as non-linear medium and both existence and utility of solitons has been anticipated a long time ago (Englander et al., 1980). In particular, the role of solitons in emergence of denaturation bubbles has been studied extensively (Tabi, 2016) (for fuller description see the report by Manghi and Destainville (Manghi and Destainville, 2015a) and references therein).

Many approximate models of DNA were proposed over the years in order to illuminate the role and importance of non-linear excitations (solitons) on DNA processes.
Yakushevich (Yakushevich, 2006) presented a hierarchy of important models. In these models, the focus is on torsion modes. In the continuous limit, the equations governing these models transform into either the famous sine-Gordon (sG) equation or equations related to it. As is well known, sG equation has analytic solitonic solutions. A complementary model, the so-called Peyrard-Bishop model (Peyrard and Bishop, 1989) has also attracted considerable attention and many studies have been devoted to its properties (see Zdravkovic (2011) and references therein).

In this paper, we propose that solitons may be also critical for quantum information specifically regarding braiding of qubits on the hydrogen bonds. As we mentioned, solitons in DNA has been studied for their capacity of promoting local openings, *i.e.* denaturation bubbles. However, they can also serve in the opposite way of creating small depressions where the strands of DNA are squeezed together. In particular, here we focus on collisions of solitons with regard to this issue. A squeezing of DNA strands may result in braiding of the qubits on hydrogen bonds, giving us a basic form of quantum computing. Quantum computing based on Majorana fermions is discussed in recent paper by Robinson *et al.* (Robinson et al., 2019). Our Majorana model of DNA is very similar to quantum computation model presented in Figure 2 of that paper (Robinson et al., 2019). Left vertical bubbles correspond to a A-T base pair (*i.e.* two hydrogen bonds). Horizontal bubbles correspond to a C-G base pair (*i.e.* entangled states) and right bubbles correspond to a T-A base pair (*i.e.* two hydrogen bonds).

As this is all highly speculative, in the following subsection we will work in the simplest setting possible to make our presentation concise. To that end, we will work within the Peyrard-Bishop model in the continuous limit. We first demonstrate the existence of solitons using Renormalization Group (RG) perturbation expansion technique developed by Chen, Goldenfeld and Oono (Chen et al., 1994). Then we discuss their properties and in the last subsection we show our numerical results regarding their collisions.

3.1 Peyrard-Bishop model

In the Peyrard-Bishop (PB) model, DNA strands are represented as two parallel chains of point masses. Along each chain the points are coupled together via harmonic force representing covalent bonds between nucleotides, while the hydrogen bonds between the strands is modelled via the Morse potential. Since the masses of the different nucleotides (*i.e.* with different bases A, T, C and G) do not differ from each other dramatically (about 4% (Zdravkovic, 2011)), it is convenient to adopt only the mean mass for every nucleotide. Moreover, since the covalent bonds are far stronger than the hydrogen bonds, the PB model assumes only transversal motion disregarding longitudinal and torsion movements which effectively reduces the problem to a single dimension.

Indeed, if we denote the deviation form the equilibrium distance of the two strands at the n-th site as y_n the PB model can be written as

$$H = \sum_n \left\{ \frac{m}{2}\dot{y}_n^2 + \frac{k}{2}(y_n - y_{n-1})^2 + D\left(\mathrm{e}^{-a\sqrt{2}y_n} - 1\right)^2 \right\} . \tag{5}$$

From here on we adopt the following values for the parameters of PB model (taken from Zdravkovic (2011))

$$k = 12\frac{\mathrm{N}}{\mathrm{m}} \approx 0.74892\frac{\mathrm{eV}}{\mathrm{\AA}^2}\,, \quad m = 307.2 \text{ a.m.u.}\,, \tag{6}$$

$$a = 1.2\,\mathrm{\AA}^{-1}\,, \quad D = 0.07\mathrm{eV}\,, \quad l = 3.4\,\mathrm{\AA}\,. \tag{7}$$

Here, k is the spring constant for harmonic potential, m is the average mass of the nucleotides, a and D are the inverse length and depth of the Morse potential, respectively. Lastly, l is the distance between adjacent sites along the strands.

The equation of motion reads

$$m\ddot{y}_n = k\,(y_{n+1} + y_{n-1} - 2y_n) + 2\sqrt{2}aD\left(\mathrm{e}^{-\sqrt{2}ay_n} - 1\right)\mathrm{e}^{-\sqrt{2}ay_n}\,. \tag{8}$$

Being both discrete and non-linear this equation is very difficult to solve. However, since we only want to illustrate how solitons could lead to decoherence of qubits we will take a continuous limit to simplify matters as much as possible. Hence, we take the distance between sites l to zero, while we keep $\tilde{k} \equiv kl^2$ finite (and numerically equal to $\tilde{k} = 8.6575$ eV). Further, let us denote the continuous variable tracing the distance along strands as $nl \to x$ and the field variable which replaces transversal motion at the n-th side as $y_n(t) \sim y(nl, t) \to y(x, t)$. In this way, the equations of motion becomes

$$m\partial_t^2 y - \tilde{k}\partial_x^2 y = 2\sqrt{2}a\,D\left(\mathrm{e}^{-a\sqrt{2}y} - 1\right)\mathrm{e}^{-a\sqrt{2}y}\,. \tag{9}$$

In the dimensionless units defined as

$$t \equiv \frac{\sqrt{m}}{2a\sqrt{D}}\tilde{t} \approx 28\,\tilde{t}\,[\mathrm{ps}]\,, \qquad x \equiv \frac{\sqrt{\tilde{k}}}{2a\sqrt{D}}\tilde{x} \approx 4.63\,\tilde{x}\,[\mathrm{\AA}]\,, \tag{10}$$

$$y = \frac{\tilde{y}}{a\sqrt{2}} \approx 0.59\,\tilde{y}\,[\mathrm{\AA}]\,, \tag{11}$$

the equation takes especially simple form

$$\partial^2 y = (\mathrm{e}^{-y} - 1)\,\mathrm{e}^{-y}\,, \tag{12}$$

where we dropped all˜ signs for brevity and where we used relativistic notation $\partial^2 \equiv \partial_\mu \partial^\mu = \partial_t^2 - \partial_x^2$. For future purposes it is advantageous to use substitution $y = \log(1+u)$, which transforms (12) into

$$(1+u)\,\partial^2 u - \partial_\mu u \partial^\mu u + u = 0\,. \tag{13}$$

3.2 Small amplitude expansion

Let us study small amplitude perturbations of Eq. (13). Inserting a series expansion

$$u = \varepsilon\left(u_0 + \varepsilon u_1 + \varepsilon^2 u_2 + \ldots\right), \tag{14}$$

where ε is a bookkeeping parameter which we assume to be small $|\varepsilon| \ll 1$, we obtain a hierarchy of equations

$$H_0 u_{n+1} = \sum_{k=0}^{n} \left(\partial_\mu u_{n-k} \partial^\mu u_k - u_{n-k} \partial^2 u_k\right), \tag{15}$$

where $H_0 = \partial^2 + 1$.

For the zero order, let us start with a monochromatic wave, *i.e.*

$$u_0 = A_0 \mathrm{e}^{\mathrm{i}\theta} + \text{c.c.}\,, \quad \theta \equiv qx - \omega t\,, \tag{16}$$

with $\omega = \sqrt{q^2+1}$.

Solving the hierarchy up to the second order we get

$$u_1 = 4\,|A_0|^2\,, \tag{17}$$

$$u_2 = -2A_0\,|A_0|^2\,\mathrm{e}^{\mathrm{i}\theta}\left(\xi\bar{\theta}^2 + \mathrm{i}\,(1-\xi)\,\theta\right) + \text{c.c.} \tag{18}$$

Here, ξ is an arbitrary constant and we have introduced an auxiliary variable $\bar{\theta} \equiv \omega x - qt$, which appears in u_2 as a part of the so-called secular term. This term is a sign of resonance phenomena and arise due to the identity

$$\frac{1}{\partial^2+1}\mathrm{e}^{\mathrm{i}\theta} = -\frac{1}{2}\mathrm{e}^{\mathrm{i}\theta}\left(\xi\bar{\theta}^2 + \mathrm{i}\,(1-\xi)\,\theta + c\right), \tag{19}$$

where c is an arbitrary constant.

The presence of secular term is a bad news for our perturbation series since – as the name indicates – secular term quickly outgrow any other terms with increasing t (or x) casting a doubt on the convergence of our series.

In order to eliminate terms like u_2 we employ Renormalization Group (RG) method developed by Chen, Goldenfeld and Oono (Chen et al., 1994). This method calls for introduction of artificial renormalization scales θ_0 and $\bar{\theta}_0$ via innocuous shifts in the secular term:

$$\bar{\theta}^2 \to \bar{\theta}^2 - \bar{\theta}_0^2 + \bar{\theta}_0^2\,, \qquad \theta \to \theta - \theta_0 + \theta_0\,. \tag{20}$$

Now we redefine the so-called 'bare' amplitude A_0 in terms of 'dressed' amplitude A in such a way that the dependence on the second instances of θ_0 and $\bar{\theta}_0$ disappears:

$$A_0 = \left(1 + 2\varepsilon^2 |A|^2 \left(\xi\bar{\theta}_0^2 + \mathrm{i}\,(1-\xi)\,\theta_0\right) + O\left(\varepsilon^4\right)\right) A\,, \tag{21}$$

In other words, the renormalization scales only shows up in the combinations $\theta - \theta_0$ and $\bar{\theta}^2 - \bar{\theta}_0^2$. This is important, since, as we will see, we want to ultimately set $\theta_0 = \theta$ and $\bar{\theta}_0 = \bar{\theta}$. Because the renormalization scales are completely artificial, meaning that the solution does not depend on them, we can make this identification. However, since $A \equiv A(\theta_0, \bar{\theta}_0)$ can be in principle an arbitrary function of renormalization scales we must enforce the independence of the solution by ensuring that

$$\frac{\partial u}{\partial \theta_0} = \frac{\partial u}{\partial \bar{\theta}_0} = 0\,, \quad \forall x, t\,, \tag{22}$$

holds. These conditions gives us the Renormalization Group Equations (RGE's):

$$\frac{\partial A}{\partial \theta_0} = -2\mathrm{i}\varepsilon^2 a\ |A|^2\,(1-\xi) + O(\varepsilon^4)\,, \tag{23}$$

$$\frac{\partial A}{\partial \bar{\theta}_0} = -2\varepsilon^2 a\ |A|^2\,\xi\bar{\theta}_0 + O(\varepsilon^4)\,. \tag{24}$$

However, solving these equations would give us wrong global behaviour since these are not *slow motion* equations, meaning that the derivatives can get arbitrary large. A proper RGE is therefore a differential consequence of these equations, which is the famous non-linear Schrödinger (NLS) equation:

$$\mathrm{i}\frac{\partial A}{\partial \theta_0} - \frac{1}{2}\frac{\partial^2 A}{\partial \bar{\theta}_0^2} = 2\varepsilon^2 a\ |A|^2 + O(\varepsilon^4)\,. \tag{25}$$

Solving NLS equation and plugging it into the expansion we arrive at a single soliton solution in the form

$$u_R = \frac{u_0}{\cosh\left(\frac{u_0}{\sqrt{2}}\frac{x - V_E t}{\sqrt{1-V_E^2}}\right)} \cos\left(\left(1 - \frac{u_0^2}{4}\right)\frac{t - V_E x}{\sqrt{1-V_E^2}}\right) + \frac{u_0^2}{\cosh^2\left(\frac{u_0}{\sqrt{2}}\frac{x - V_E t}{\sqrt{1-V_E^2}}\right)}\,. \tag{26}$$

Several comments are in order:
i) This solution is independent on ε due to the fact that it can be rescaled away via scale invariance of NLS; however, the solution is still only valid for small u_0 – the core amplitude of the soliton. This is as it should be since ε was only a bookkeeping parameter and not a true parameter of the equation of motion.
ii) The parameter q has been replaced in favor of the envelope velocity via $q = V_E/\sqrt{1-V_E^2}$.
iii) This solution has a manifestly Lorentz symmetry structure, *i.e.* it is a boost of a standing wave solution with modulated amplitude. This is due to the underlying Lorentz symmetry of the equation of motion even though NLS is not Lorentz invariant.

iv) The width of the soliton is roughly $\sim 10\sqrt{2\left(1-V_E^2\right)}/u_0$, while its core height is $u_0+u_0^2$. Of course, not all values of u_0 is physically acceptable. In Zdravkovic (2011) it is argued that a typical length of a DNA segment participating in a transcription bubble is between 8 to 17 nucleotides. This translates into a typical width of the soliton between 27 to 58 Å. This means that the width of the soliton (in dimensionless units) is in the range $6-12$.
v) The energy of a single soliton (at leading order) is given as (in dimensionful units)

$$E = 2D\sqrt{\frac{2}{1-V_E^2}}u_0 + O\left(u_0^2\right), \tag{27}$$

which is again fully consistent with special relativity, making the solitons rest mass to be $\sqrt{2}Du_0$.

3.3 Scattering of solitons in the continuous PB model

In this subsection, we broadly outline key features of soliton scattering in continuous PB model. At least qualitatively, findings presented here should be the same to that of discrete PB model for reasons which we outline below.

In the continuous PB model the interesting thing about scattering of solitons is its mundaneness. We have performed numerous numerical simulations where initially well-separated solitons of various sizes (parametrized by u_0) are sent against each other with various speeds (controlled by V_E). From these studies it became clear that solitons interact with each other only minimally and after they pass through each other they rapidly regain their original shapes. The only impact of the interaction is a slight phase shift and delay compared with completely noninteracting solitons, as can be seen on Figure 3. Furthermore, these differences are less and less pronounced as the velocity increases due to the fact that for larger velocities the effective interaction time between the solitons becomes smaller.

This behaviour is paramount to scattering of solitons in integrable theories. As it is well known, NLS equation can be solved via the inverse scattering method (Zakharov and Shabat, 1972). The implication is that NLS equation is an integrable theory and soliton scattering has the features which makes solitons solitons, *i.e.* rapid shape recovery with only a phase shift gained through the interaction. On the other hand, in a generic, non-integrable model with solitons, we typically observe a wealth of interesting associated phenomena, such as soliton bouncing, formation of bound states and others (for details see a recent paper on collisions solitons in the Montonen-Sarker-Trullinger-Bishop (MSTB) model (Izquierdo, 2017) and references therein).

Our observations in the continuous PB model can be therefore explained as a result of an *approximate integrability* for small amplitudes, which is inherited from NLS. Since the solitons in discrete PB model are also governed by NLS equation we can thus claim that the same should be (and indeed is) observed in the discrete PB model.

Here, we are interested in assessing whether collision of solitons can lead to a substantial squeezing of DNA strands. To this end we will focus only on the case where the colliding solitons are of the same size and starts with the same phase, so that their internal oscillations positively interfere at the point of collision. Further, we explore the collisions for various

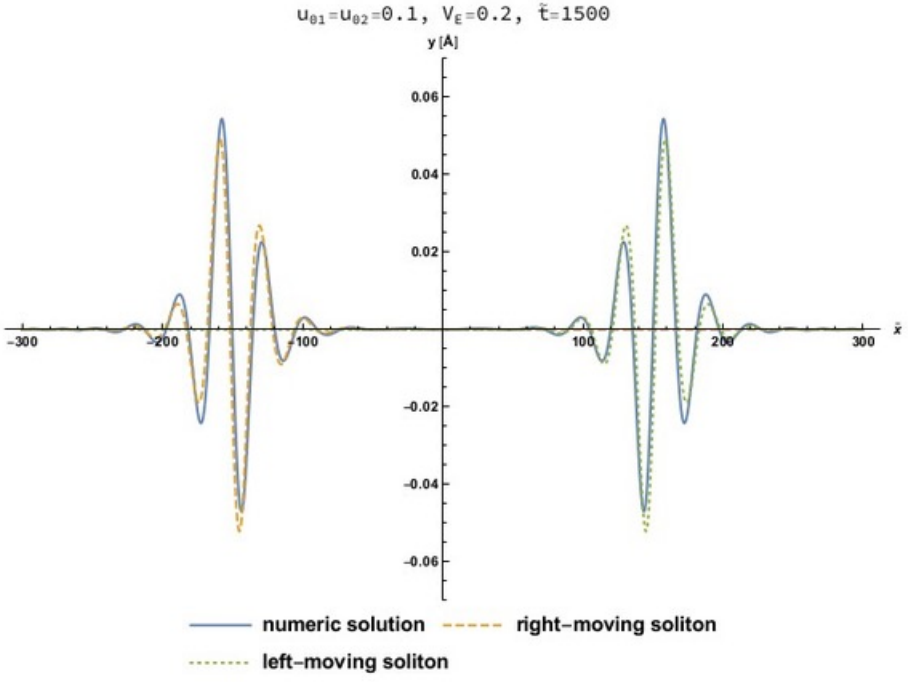

Figure 3. A typical outcome of soliton scattering where two well-separated but otherwise identical solitons are sent against each other with velocity V_E. Compared with noninteracting solitons (yellow dashed line and green dotted line) we see that the only marks of interaction are slight time delay.

sizes u_0 and envelope velocities V_E in order to pinpoint the best circumstances for the most negative values of y.

The results are sumarized in Figure 4. There, we show minimal values $y_{\min} \equiv \mathrm{Min}[y(0,t)]$ which the field reaches when the solitons collides. We show the results for initial sizes $u_0 = \{0, 1, 0.2, 0.3, 0.4\}$ and for various velocities V_E.

A minimal value of y for a single soliton is $\frac{1}{\sqrt{2}a} \log(1 - u_0 + u_0^2) + O(u_0^3)$. Therefore we expect that for two roughly non-interacting overlapping solitons the *theoretical* minimum is twice as low. Indeed, if $u_0 = 0.1$ this theoretical minimum is ≈ -0.11 Å which is almost reached for $V_E = 0.75$ and above. This is due to the fact that for larger velocities, the time for non-linear effects of PB model to kick in is smaller and solitons behaviour is more in accordance with the above expectations. As we increase the size, however, two effects grow in importance. First, the approximate initial solitonic solution becomes more unreliable and deformations start to develop even before the collision. Typically, the solitonic wave tend to settle into more accurate shape (described by higher-order corrections to the approximate solution) and, in the process, emit small waves. Second, as the field probes the negative half of the Morse potential it feels more of the exponential suppression to the negative

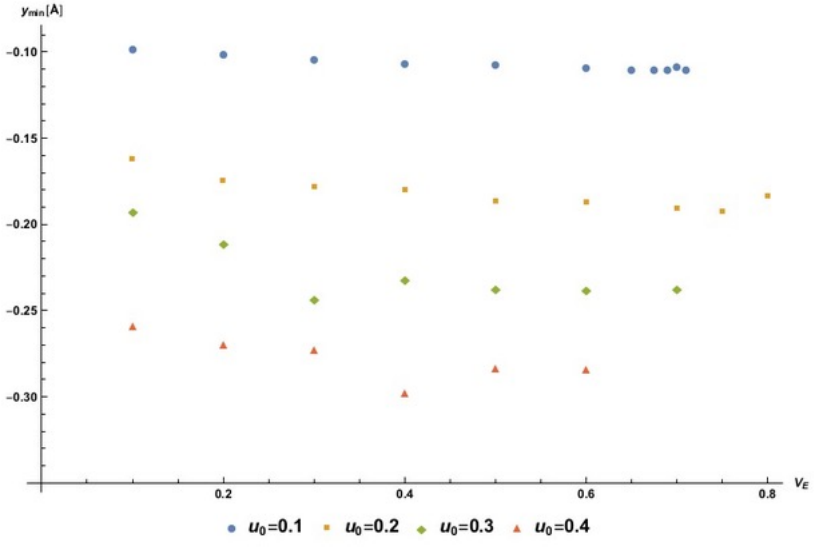

Figure 4. Minimal values of the field $y_{\min} \equiv \mathrm{Min}[y(0,t)]$ attained at the time of collision between equal solitons for various sizes u_0 and velocities V_E.

deviations compared with only polynomial suppression for positive deviations. Therefore, for higher u_0 solitons cannot attain even their theoretical minima. These expectations are fully manifested in Figure 4 as, for example, for $u_0 = 0.4$ the observed minimum $y_{\min}$ never approaches theoretical one ≈ -0.323 Å even at high velocities.

Our findings suggest that local squeezing of DNA strands is propagated by solitons and can be enhanced via soliton collisions. However, let us stress that we are talking about very small depressions, *e.g.* $|y| \leq 0.3$Å. We were not able to find larger depressions within the limitations of our approach. Nevertheless, it is quite possible that even a mild squeezing of DNA strands can influence the distance of minima of the double-well potential for hydrogen bonds sufficient to cause decoherence of associated Majorana fermions or to trigger braiding. To quantify this precisely is, however, far outside the scope of this work.

Furthermore, there are additional reasons to mistrust the picture of events we are painting here when deformations get larger. For instance, we have completely neglected rotational degrees of freedom. It is easy to imagine, that trying to squeeze DNA strands would at some point just result in rotation of the bases or slight twisting/untwisting of the double helix and would not manifest in reducing their distance. Another matter, which we completely neglect here, and which can heavily impact the dynamics of solitons is viscosity. It is clear, that viscosity would play a major role in the motion and lifetime of solitons, perhaps rendering soliton collisions untenable. Again, this is outside the scope of our study and we recommend the paper by Manghi and Destainville (Manghi and Destainville, 2015b), where the impact of viscosity on mechanical models of DNA are summarized. Let us, however,

say that for the small amplitudes to which our study is confined, it is quite plausible that the damped motion of sugar-phosphate backbone of DNA would not play as a significant role on small deformations of hydrogen bonds we are interested in.

4 CONCLUDING REMARKS

In this article, we have developed further our ideas about quantum information in biomolecules. These ideas are based on the observation that the hydrogen bonds in the DNA molecule are strongly delocalized systems characterized by double well potential. If this double well potential is described by the non-adiabatic Hamiltonian, fermion quasiparticles are obtained which we can identified with Majorana fermions. This result then allows us to introduce qubits. We found similarities between this fermion quasiparticles and Majorana quasiparticles. Both are emergent quasiparticles and are delocalized. Our idea is also supported by the fact that proton tunelling was not found. This is due to the effect of delocalization and coupling of electrons and vibrations (phonons). The two hydrogen bonds associated with the base pairs A-T or T-A represent one qubit and the three hydrogen bonds associated with C-G or G-C represent entangled states. In this way, we can introduce quantum information and quantum entropy.

It is expected that solitons play a role in the transcription and replication of DNA. We have, therefore, studied the effects of solitons on our model. Specifically, we have used the Peyrard and Bishop model of DNA. Solitons may be critical for quantum information, in particular, with regard to the braiding of qubits on the hydrogen bonds. Solitons can play a role in decoherence of delocalized Majorana fermions. We note that decoherence on a double well potential was demonstrated in the recent work of Marais *et al.* (Marais et al., 2018) (see their Figure 2). These effects may be important for quantum computation. We also studied solitons in DNA for their capacity of promoting local openings, *i.e.* denaturation bubbles. Our results are presented in Figures 3 and 4.

The solitons in the PB model are natural candidates for agents of quantum computation on DNA molecule because they are coherent, extended and stable wave patterns where energy is concentrated. Here, we have shown that during their collisions the strands of DNA do become closer compared with the isolated soliton if only for a brief time. If sufficiently large solitons participate in collision, the negative deviation can reach values such that braiding or decoherence of qubits on the hydrogen bonds may take place. As we have already mentioned, we have kept our analysis in the present work at the most basic level as a proof-of-concept.

Building on the emerging consensus that information is a key property of the life phenomenon, we have continued to develop our suggestion that quantum information has a role in biomolecules and, in particular, in DNA.

ACKNOWLEDGEMENTS

This work was supported by the Albert Einstein Centre for Gravitation and Astrophysics financed by the Czech Science Agency Grant No. 14-37086G (F.B.) and by the program

of Czech Ministry of Education Youth and Sports INTER-EXCELLENCE Grant number LTT17018 (F.B.).

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