https://dx.doi.org/10.22161/ijaers.4.5.33 ISSN: 2349-6495(P) | 2456-1908(O)

Charge Discreteness as Model in Charge Migration in a Chain of DNA Molecules under Radiation

Hector Torres-Silva , Erik Santos

Universidad de Tarapacá, EIEE, Arica, Chile

Abstract*— *Charge migration through DNA is a problem to be solved. A numerical wavefront solution for quantum transmission lines with charge discreteness is obtained as model for the charge migration of a chain DNA molecules induced by electromagnetic radiation. The nonlinearity of the system becomes deeply related to charge discreteness. The wavefront velocity depends on the normalized (pseudo) flux variable. Finding the dispersion relation for the normalized flux ϕ / ϕ_0 we show that the condition $v^2 \geq 0$ on the wave-front velocity gives the band-gap conditions for the charge propagation on the system..

***Keywords*— Charge migration, DNA, wavefront, quantum transmission line, discreteness.**

I. INTRODUCTION

Currently nanostructures are embedded in countless devices and systems [1-5] . Naturally, at this scale and for low temperature, quantum mechanics plays a key role. Lately, much effort has been dedicated to study nanostructures, using as model of quantum circuits with charge discreteness [6-12]. On the other hand, the discovery of charge migration in deoxyribonucleic acid (DNA) stimulated intensive investigations of the electronic properties of DNA due to their significance in biosynthesis and radiation-induced damage and repair processes [1-3]. Furthermore, considerable interest in nanodimensional structures of DNA possessing unique self-assembling and self-recognition properties has increased the last decade in connection with the possibility of the development of molecular nanoelectronic devices which are expected to provide high storage of information and high-speed signal processing within a wide temperature range [4-6]. In fact, DNA molecules can be well combined with silicon technology transcending the potential of the present quantum wires and are supposed to be used in modern computer technology as a binary data structure by applying a programmable linear self assembly of the sequence of complementary nucleic base pairs of DNA. It is in this context that we are interested in spatially transmission lines with charge discreteness [13]. In this work we will consider a wavefront solution for a quantum circuit (transmission line) simulating the DNA molecule in a cell sample. A numerical solution is founded and characterized for this specific system with charge discreteness, which can extended for the description of more complex extended systems a. In section 2 we will introduce a generalization of classical transmission line with charge discreteness and we present the quantum transmission lines with charge discreteness, the Hamiltonian for coupled circuits, and the equations of motion for the spatially continuous system. In Sec. 3, the wavefront solution is considered. Finally, we give our conclusions.

II. GENERALIZATION OF TRANSMISSION LINE AND QUANTUM DISCRETENESS

For a chain of molecules of DNA, we consider a homogeneous classical transmission line, assumed infinite, where the every cell is constituted of a LC circuit with inductance L and capacitance C per unit length. Assume that the interaction between neighbor cells is trough the capacitors (direct line), the classical evolution equations for the electrical current and charge, become in this case

$$L\frac{d}{dt}i_m = \frac{1}{C}(2q_m - q_{m+1} - q_{m-1}) \tag{1}$$

Where the integer m designates the cell at position in the chain and, as usual, $i_m = \frac{d}{dt}q_m$ is the electrical current. The above linear equation of evolution becomes directly from the classical Lagrangian L_{ag} given by

$$L_{ag} = \sum_m (\frac{L}{2}i_m^2 - \frac{1}{2C}(q_m - q_{m-1})^2) \tag{2}$$

Using the Lagrange equations one obtains (1).

Supporting solutions like a plane wave. Explicitly we have,

https://dx.doi.org/10.22161/ijaers.4.5.33 *ISSN: 2349-6495(P) | 2456-1908(O)*

$$q_m = q_0 \exp(i\omega t - ikm) \qquad (3)$$

Where, as usual in this case, the frequency ω and the wavenumber k become related through the dispersion relation. The variable q_0 is a constant parameter describing the amplitude of the wave. Note that we have considered by sake of simplicity the lattice-size a as one, ($a = 1$). That is the adimensional number k in the equation (6) is really ka.

After some algebra, one obtains from (3) the dispersion relation. The infrared limit ($ka \to 0$) related to the continous –space structure becomes direct and corresponds to the dispersion relation $\omega = k/\sqrt{LC}$, namely a non dispersive medium.

From $\omega = k/\sqrt{LC}$, we get the phase velocity and group velocity

$$v_p = \frac{\omega}{k} = 1/\sqrt{LC}, \; v_g = \frac{\partial \omega}{\partial k} = 1/\sqrt{LC} \qquad (4)$$

From a general point of view, for arbitrary composition of a cell in the line, the Hamiltonian of this generalized electrical transmission line becomes quadratic, namely,

$$H = \sum_{m,s} \left(\frac{1}{2}\left(\frac{1}{L}\right)_{m,s} \phi_m \phi_s + \frac{1}{2}\left(\frac{1}{C}\right)_{m,s} q_m q_s\right) \qquad (5)$$

.

As illustration and following [6-12, 14], and from the Hamiltonian (5), the usual quantization procedure for flux and charge, and the prescription (2) for charge discreteness, we could construct the quantum Hamiltonian for the direct transmission line with charge discreteness (q_e), which may be written as:

$$H = \sum_{m=-\infty}^{\infty} \left\{ \frac{2\hbar^2}{Lq_e^2} \sin^2 \frac{q_e}{2\hbar} \phi_m + \frac{1}{2C}(q_m - q_{m-1})^2 \right\} (6)$$

where the index m describes the cell (circuit) at position m, containing an inductance L and capacitance C. The conjugate operators, charge q and pseudoflux ϕ, satisfy the usual commutation rule

$$\left[q_m, \phi_{m'}\right] = i\hbar \delta_{m,m'} \text{ and } \left[q_m, q_s\right] = \left[\phi_m, \phi_s\right] = 0. \qquad (7)$$

A spatially extended solution of Eq. (6) corresponds to the quantization of the classical electric transmission line with discrete charge (i.e. elementary charge q_e). Note that in the formal limit $q_e \to 0$ the above Hamiltonian gives the well-known dynamics related to the one-band quantum transmission line, similar to the phonon case. The system described by Eq. (10) is very cumbersome since the equations of motion for the operators are highly nonlinear due to charge discreteness. However, this system is invariant under transformation $q_k \to q_k + q$, that is, the total pseudo flux operator $\phi = \sum \phi_m$ commutes with the Hamiltonian; simplifying the study of this system.

$$H_m = \frac{2\hbar^2}{Lq_e^2} \sin^2 \frac{q_e}{2\hbar} \phi_m - \frac{1}{2C}(q_{m+1} - \phi_m)^2 \qquad (8)$$

where H_m represents the Hamiltonian density operator for the fields. From the above Hamiltonian we find the equations of motion (Heisenberg equations) for the field operators:

$$\frac{\partial}{\partial t}\phi_m = \frac{1}{C}(q_{m+1} + q_{m-1} - 2q_m) \qquad (9)$$

$$\frac{\partial}{\partial t} q = \frac{\hbar}{Lq_e} \sin\left(\frac{q_e}{\hbar}\phi\right) \qquad (10)$$

and from eq. (6), the dispersion relation is given by

$$\omega = 2\frac{|\sin k/2|}{\sqrt{LC}} \qquad (11)$$

If $k \ll 1$, $\omega = k/\sqrt{LC}$, from here we can obtain

$$v_p = \frac{\omega}{k} = 1/\sqrt{LC}, \; v_g = \frac{\partial \omega}{\partial k} = 1/\sqrt{LC} \qquad (12)$$

III. WAVEFRONT SOLUTION

In real seismic applications there is always the presence of damping. We shall consider the effect of its simplest form, small viscous damping. Eq. (3) is extended by adding a linear damping term λ :

Now we consider a homogeneous classical transmission line, assumed infinite, where the every cell is constituted of a LC circuit with series inductance L and shunt capacitance C per unit length . The approach is based on the mapping of field components (i.e., E and H) in the medium to the voltages and currents of the equivalent distributed L-C network [15, 17]. It is well known that dielectric properties like permittivity and permeability can be modeled using distributed L-C networks. To illustrate how these material parameters relate the distributed series impedances and shunt admittances of the network, 1-D distributed L–C network is depicted in Fig. 1. The network consists of a series per-unit-length impedance Z ' in z direction and a shunt per-unit-length admittance Y' in y direction.

https://dx.doi.org/10.22161/ijaers.4.5.33 ISSN: 2349-6495(P) | 2456-1908(O)

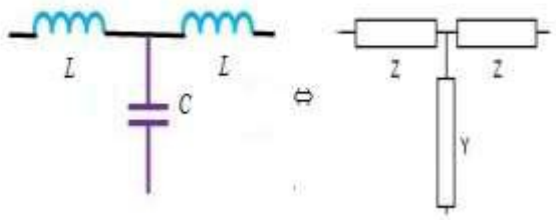

Fig.1: Transmission line model with L, C per unit length.

For the conventional homogeneous isotropic RHM with positive permittivity ε and permeability μ, Eqs.(1, 2) implies a network of a low-pass topology with series inductor L ' = μ (H/m) and shunt capacitor C ' = ε (F/m), or *Z=jωL* ' and *Y* = *jωC* ' , both of which are positive quantities. The negative permittivity and permeability [16, 17] in LHM leads to the question whether the parameters Z ' and Y ' in the network representation can also be made negative. From the impedance perspective, a negative L ' and C ' can be realized by exchanging their inductive and capacitive roles, which means the series inductor becomes a series capacitor, and the shunt capacitor becomes a shunt inductor. In this paper we are interested in the normal RHM transmission line which in the limit $q_e \to 0$ becomes the usual one band transmission wave equation.

$v^2 = \omega^2 / k^2 = 1/LC$. In general the dispersion relation from Eqs. (9) and (10) is

$$\frac{\omega^2 LC}{k^2} = \cos(q_e \phi / \hbar)\left(\frac{\sin(k/2)}{k/2}\right)^2 \quad (13)$$

where v is the phase velocity given by

$$v = \sqrt{\frac{\omega^2 LC}{k^2}} = \sqrt{\cos(q_e \phi / \hbar)}\left(\frac{\sin(k/2)}{k/2}\right) \quad (14)$$

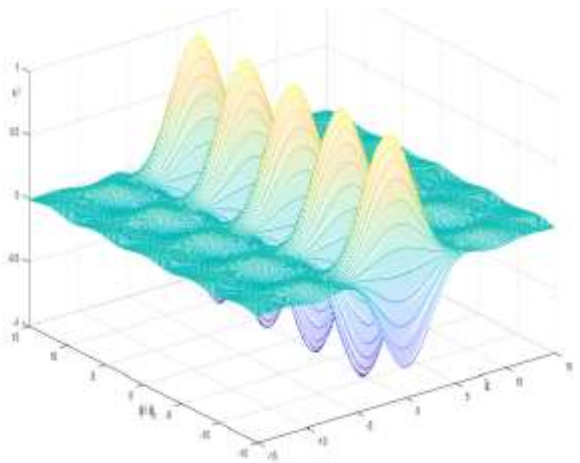

Fig.2:. The normalized expression (17) v^2 *is shown as a function of* ϕ / ϕ_0 *and k*

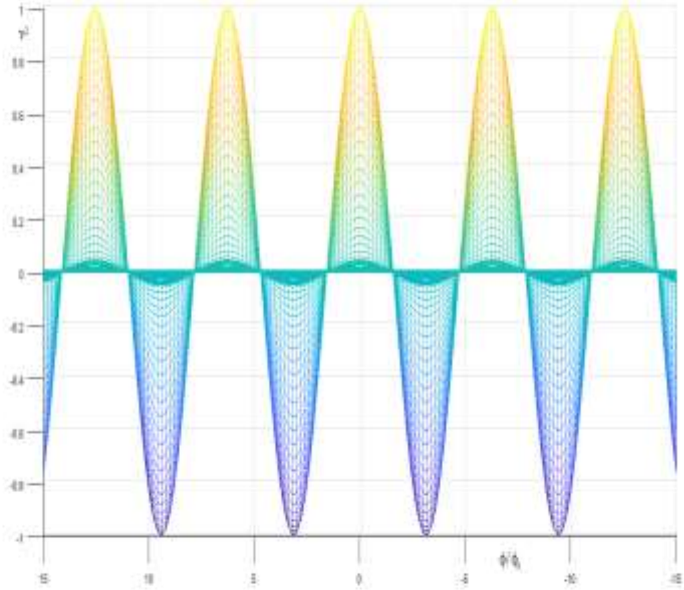

Fig.3: Profile of v^2 *as a function of* ϕ / ϕ_0 *with* $k = \text{cte}$

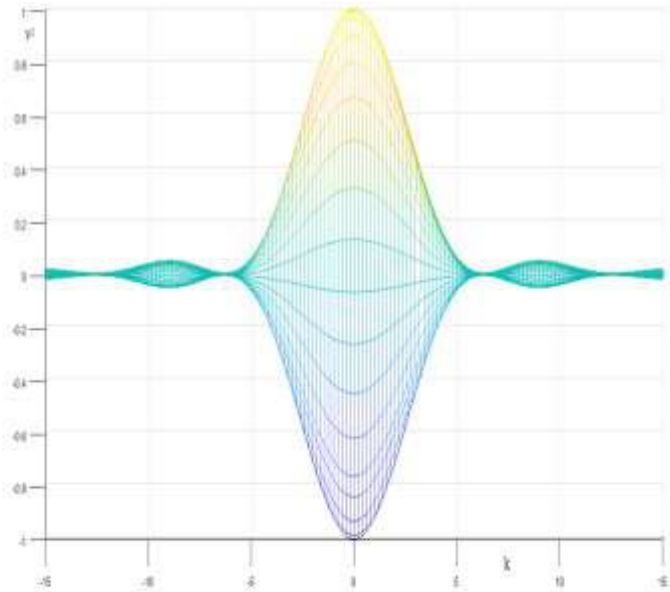

Fig.4: Profile of v^2 *as a function of k with* $\phi / \phi_0 = \text{cte}$

Figures 2-4 show the normalized v^2 of the charge migration in a transmission line where we can see that the velocity of wavefront which has bands and gaps. To see this in a clearer way we know that always v^2 must be positive ($v^2 LC > 0$), so the two equations (13), (14), are satisfied simultaneously when $\phi / \phi_0 = 2n\pi$, $n = \pm 1, \pm 2...$ that means that $\phi = 2n\pi\phi_0 = nh / q_e$.

Let

$$f(k) = v^2 LC = \frac{\omega^2 LC}{k^2} = \cos(pk)\left(\frac{\sin(k/2)}{k/2}\right)^2 \quad (15)$$

https://dx.doi.org/10.22161/ijaers.4.5.33 *ISSN: 2349-6495(P) | 2456-1908(O)*

Where we define $pk = q_e \phi / \hbar = \phi / \phi_0$, so we have the factor p as a free parameter to analyze the quantum circuit.

In figure 5 we present the case with $\phi / \phi_0 = 0$ where $f(k) \geq 0$ and there is not a structure of bands and gaps because $q_e \to 0$. In figure 6 we have a structure of bands and gaps because $pk = q_e \phi / \hbar = \phi / \phi_0 \neq 0$

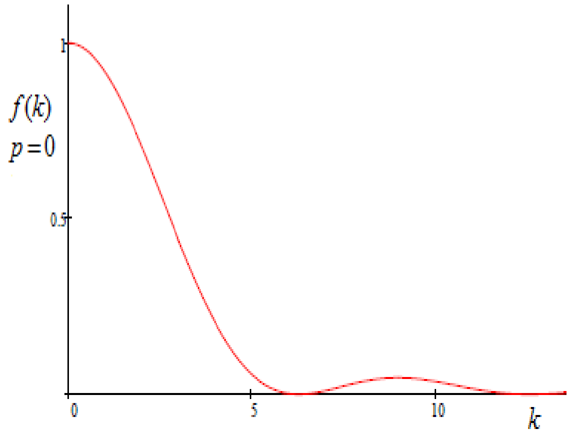

Fig.5: Plot of the velocity of the wavefront, as a function of k with the magnetic flux as the parameter p.

As specified by Eq. (18), if p=0, there is only a structure of bands because $pk = q_e \phi / \hbar = \phi / \phi_0 = 0$, that is $q_e \to 0$.

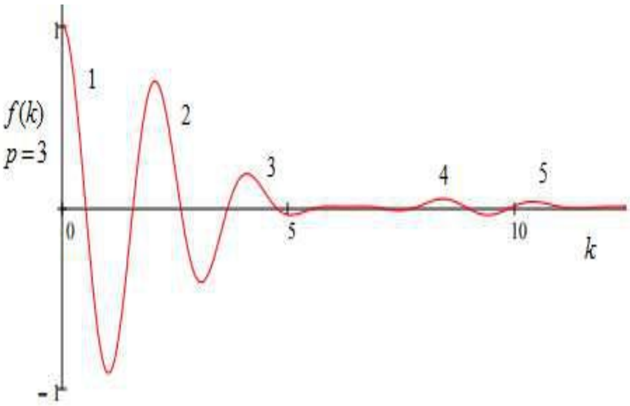

Fig. 6. Plot of the velocity of the wavefront, as a function of k with the magnetic flux as the parameter p.

As specified by Eq. (18) there is a structure of bands and gaps because $pk = q_e \phi / \hbar = \phi / \phi_0 \neq 0$ with p=3 , so that have five bands where there is wave propagation and charge migration as are shown in Figure 7.

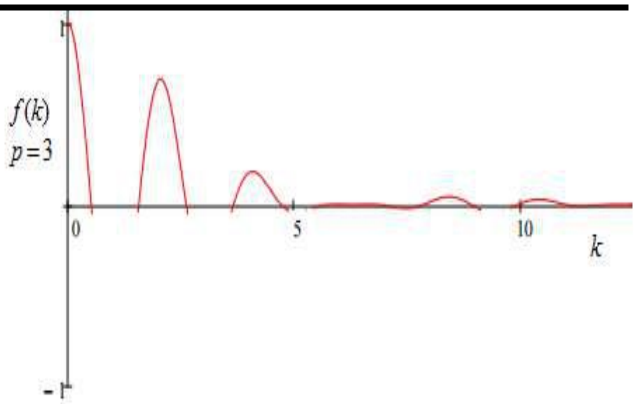

Fig. 7. $v^2 LC \geq 0$ *where there are wave propagation.*

As we have seen from these graphs, the condition $v^2 \geq 0$ on the wave-front velocity gives the band-gap conditions on the system. In fact, from (16) the restriction

$$v^2 = \frac{1}{LC} \cos(q_e \phi / \hbar) \left(\frac{\sin(k/2)}{k/2} \right)^2 \geq 0$$

means that there exists a sequence of bands and gaps.

The nonlinearity of the system becomes be deeply related to charge discreteness or in terms Of discrete values of quantum flux $\phi_0 = \hbar / q_e$. The wavefront velocity is found to depend on a step discontinuity on the (pseudo) flux variable, p, displaying allowed and forbidden regions (gaps), as a function of p.

Defining, $\phi / \phi_0 = pk$, any complex function Ψ can be written as $\psi = \psi_0 \exp(ipk)$ where ψ_0 is the amplitude and θ is the phase. It is obvious that changing the phase pk by $2n\pi$ will not change ψ and, correspondingly, will not change any physical properties in this quantum transmission line. However, in the superconductor of non-trivial topology, e.g. superconductor with the hole or superconducting loop/cylinder, the phase pk may continuously change from some value pk_0 to the value $pk_0 + 2\pi n$ as one goes around the hole/loop and comes to the same starting point. If this is so, then one has n magnetic flux quanta trapped in the hole/loop, [18, 19], In the case of charge migration in DNA, charge discreteness is the statement that charge comes in packets which are of size 1 electron charge. These results enable the investigation of charge migration as quantum charge in both longitudinal and transverse configurations and stimulate theoretical interpretations [20-24]. Some of these studies are concerned with the issues of the charge migration induced by environmental factors, among which ionizing radiation or RF fields are of great interest.

Charge migration through DNA has been the focus of considerable interest in recent years because DNA is the

https://dx.doi.org/10.22161/ijaers.4.5.33 ISSN: 2349-6495(P) | 2456-1908(O)

molecule that contains all of the information required to build and maintain the cell . A deeper understanding of the nature of charge transfer and transport along the double helix is important in fields as diverse as physics, chemistry and nanotechnology. It has also important implications in biology, in particular in DNA damage and repair. In this context this paper can be a contribution in the study of this topic.

IV. CONCLUSIONS

A charge migration in a chain of DNA molecules is simulated with the quantum electric transmission line with charge discreteness described by the Hamiltonian (12), and equations of motion (13-14), Wavefront solution was found.. One condition on the velocity generates a band-gap structure dependent on the pseudo flux parameter, namely, there exist regions for which a solitary wavefront propagates with constant speed according the value of ϕ/ϕ_0. The main results of this work are the existence of the band-gap structures for $0<\phi/\phi_0<1$. Charge migration under radiation is possible when $v^2 \geq 0$.

REFERENCES

[1] S. Datta, Lessons from Nanoelectronics, a Lecture Notes Series (Volume 1, Publication, Singapore :World Scientific Press, 2012).

[2] S. Lyshevski, Nano and Molecular Electronics Handbook, CRC Press. Taylor & Francis Group, 2016.

[3] H. J. de Los Santos, Principles and Applications of Nano MEMS Physics. Springer, Berlin, 2005.

[4] David K. Ferry and Stephen M. Goodnick, Transport in Nanostructures. (Cambridge University Press, 2009).

[5] W. D. Heiss (Ed.), Quantum Dots: Doorway to Nanoscales Physics. (Springer, Berlin 2005).

[6] Y. Q. Li and B. Chen, Phys. Rev. B 53, 4027 (1996).

[7] B. Chen et al, Phys. Lett. A 335, 103 (2005), and references therein.

[8] J. C. Flores, Phys. Rev. B 6 , 235309 (2001).

[9] J. C. Flores, Europhys. Lett. 69, 116 (2005).

[10] T. Lu and Y. Q. Li, Mod. Phys. Lett. B, 16, 975 (2002).

[11] S. A. Gurvitz, Phys.Rev.Lett.85, 812 (2000).

[12] C. A. Contreras and D. Laroze, Physica B, 476, 77-81, (2015).

[13] N. V. Grib et al, Distance-dependent coherent charge transport in DNA: crossover from tunneling to free propagation, Journal of Biophysical Chemistry, Vol.1, No.2, 77-85 (2010).

[14] J. C. Flores et al, Phys. Rev. B 74, 193319, (2006), and references therein.

[15] H. Torres-Silva, "A Transmission Line Model with Metamaterial Effects in Gamma Ray Bursts", Journal of Electronics and Communication Engineering Research, Volume 3, Issue 5, P 12-17, (2016).

[16] H. Torres-Silva, D. Torres-Cabezas and J. López-Bonilla, Charge discreteness in LC quantum circuit, Open Journal of Technology & Engineering Disciplines (OJTED), Vol. 2, No. 3, September 2016, pp. 01-06.

[17] H. Torres-Silva, Metamateriales, Actualidad y Desarrollo, Dyna, vol 92, nº 3, Cod 8244, 2017, and references therein.

[18] S. Frankel, National Mathematics Magazine, Vol. 11, No. 4, pp. 177-182 (1937)

[19] D. Bascom; F. William , Review Letters. **7** (2): 43–46, (1961)

[20] R. Doll, N. Näbaue, (July 1961).. Physical Review Letters. **7** (2): 51–52, (1961).

[21] B. Giese B, S. Wessely, M. Spormann, U. Lindemann, E. Meggers and M.E. Michel-Beyerle, On the mechanism of long-range electron transfer through DNA, Angewandte Chemie International Edition **38** (1999), 996-998.

[22] V.D. Lakhno, Soliton-like solutions and electron transfer in DNA, Journal of Biological Physics **26** (2000), 133-147.

[23] S. Eh. Shirmovsky and D.L. Boyda, Study of DNA conducting properties: Reversible and irreversible evolution, Biophysical Chemistry **180-181** (2013), 95-101.

[24] C.T. Shih, Sequence and energy dependence of electric transport properties of DNA –A tight-binding model study, Chinese Journal of Physics **45** (2007), 703-707.