



## LIFETIME OF QUANTUM BREATHERS FOR DNA MACROMOLECULES

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### ABSTRACT

In this paper a non-periodic boundary condition and number conserving approach, apart from various techniques available, only the temporal evolution of the number of quanta (i.e. phonons) in more sites, i.e. in more domains, is detailed in this present investigation for a generalized Klein-Gordon system with important application in macromolecules such as DNA. The temporal evolution spectra are also presented. From the approximate meeting point of different quanta, we also derive the 'time of redistribution' or 'critical time' of quanta that is proportional to the lifetime of quantum breathers (QBs) in femtoseconds (fs).

**Keywords:** Quantum Breathers Life Time, Femto-Second Responses, DNA, K-G Equation.

### I. INTRODUCTION

Localization is an important aspect for a variety of devices under the broad field of applied physics. It plays a crucial role in qualifying and quantifying a systems' operations. The extent of localization in the quantum regime assumes more importance for very small-structured materials, e.g. for nano-structured devices. Now, the question comes, how do we get localization in a system or a lattice? Localization is evolved mainly either by disorder in the lattice (Anderson Localization) [1] or by the systems' interplay of nonlinearity and discreteness [2], i.e. our attention is diverted towards discrete breathers (DBs) or intrinsic localized modes (ILMs). Here, we shall discuss mainly about the localization due to nonlinearity by adding some nonlinear components in the governing equation and discreteness.

Now, the bulk system characterizing DBs, or classical DBs [4], were the right tool, but when we are dealing with the systems that are very small, the laws of classical mechanics are not valid, and we have to use a different tool of study i.e. quantum physics, and hence it brings us to the quantum breathers (QB) [5,6]. These QBs are observed in many systems viz. ladder array of Josephson junction for superconductors [7,8,9], BEC in optical lattices/nonlinear photonic lattices [10], interacting optical waveguides [11,12], cantilever vibrations in micromechanical arrays [13], macromolecules such as DNA [14], splitting resonator (SRR) based metamaterials in antenna arrays [15], two-magnon bound states in antiferromagnets [16,17], two-phonon bound states (TPBS), i.e. quantum breathers due to charge defects in ferroelectrics, as

investigated by Fourier Grid Hamiltonian method [18].

Nanotechnology and molecular electronics based on electronic transport through biomolecules have recently attracted great interest [19]. DNA has a fundamental physical interest for the development of DNA-based molecular technologies, as it possesses ideal structural and molecular recognition properties for use in self assembling nano-devices with a definite molecular architecture [20]. Moreover, the robust, malleable one-dimensional structure of DNA can be used to design electronic devices [21, 22], serving as a wire, transistor switch or rectifier depending on its electronic properties [23, 24], and in quantum computation [25]. In addition, electronic transport plays an important role for some biological functions of DNA, such as biosynthesis and DNA repair after radiation damage. This is of great importance as some mutations in living systems and radical migrations are critical issues in carcinogenesis studies, and may yield insights into damage prevention or repair processes [26].

However, DNA is nonlinear [27]. At biological or room temperatures, DNA undergoes large amplitude localized opening of the base pairs, which can even exist in homopolymers. Although the base pair dynamics are detected in some Raman scattering experiments, the standard analysis of Raman vibrational modes cannot be used to analyze the experiments because they are based on harmonic or weakly anharmonic modes that are not localized. As we are primarily focused on quantum localization that depends on discreteness and nonlinearity, we are inclined to take DNA as a good example for the purpose. Thus, the model must include the nonlinearities which are associated with the large amplitude motions of the bases.

## II. THEORETICAL MODEL

The simplest model is a model at the scale of a base pair originally introduced to study the thermal denaturation process of DNA by Peyrard and Bishop (PB) [28, 29]. It considers a single variable for each base pair, i.e. the

stretching of the bond ( $y$ ) connecting the two bases. It is defined by the Hamiltonian:

$$H = \sum_n \left[ \frac{1}{2m} \dot{y}_n^2 + \frac{k}{2} (y_n - y_{n-1})^2 + D(e^{-by_n} - 1)^2 \right] \quad (1)$$

Here, the first term is the kinetic energy of the nucleotide of mass  $m$  at the  $n$ th site of the chain,  $y_n$  is a variable denoting the transverse stretching of the hydrogen bond connecting the bases at the  $n$ th site, the second term includes the interaction or coupling constant ( $k$ ), and finally the third term is the on-site Morse potential that represents the interaction energy due to the hydrogen bonds within the base pairs and the term  $D$  denotes the well-depth representing the ‘dissociation’ energy of a base pair. It has to be noted that on Euler expansion, this potential term gives rise to Landau type of anharmonic potential, and as per Cuevas et al [30], the PB model with Morse potential will lead to a Klein-Gordon type of equation. Therefore, this model can be safely considered as that of Klein-Gordon lattice. Thus, the classical equation of motion is again described in terms of nonlinear Klein-Gordon equation. Although the above concept has been modeled by many researchers [31], wherein an extra term for dipole-dipole forces has been added. However, in terms of approximated Bose-Hubbard model, here we directly employ second-quantization method with bosonic operators by using Eq. (1) leading to:

$$H = \sum_n -\frac{1}{2m} (a_n^{+2} + a_n^2 - 2a_n^+ a_n - 1) + \frac{k}{4} (a_n^{+2} + a_n^2 + 2a_n^+ a_n + a_{n-1}^{+2} + a_{n-1}^2 + 2a_{n-1}^+ a_{n-1} + 2) - \frac{k}{2} (a_n^+ a_{n-1}^+ + a_n a_{n-1} + a_n^+ a_{n-1} + a_n a_{n-1}^+) + D(e^{-b\left(\frac{a_n^+ + a_n}{\sqrt{2}}\right)} - 1)^2 \quad (2)$$

The general Hamiltonian for the Klein-Gordon equation for order parameter ( $y_n$ ) at  $n$ th site is written as:

$$H = \sum_n \frac{p_n^2}{2m} + \frac{A}{2} y_n^2 + \frac{B}{4} y_n^4 + k(y_n - y_{n-1})^2. \quad (3)$$

The first term is momentum at  $n$ th site ( $p_n$ ), the second and third terms are nonlinear potential formulation and the last term contains an interaction constant ( $k$ ). Here,  $A$  and  $B$  are two constants. The classical equation of motion is given by:

$$\dot{y}_n = \frac{1}{m} p_n \quad (4)$$

$$\ddot{y}_n = -\frac{A}{m} y_n - \frac{B}{m} y_n^3 - \frac{k}{m} (2y_n - y_{n-1} - y_{n+1}) \quad (5)$$

Now, we rescale time as follows:

$$t = \frac{1}{\alpha} \tau \quad (6)$$

and we take  $\alpha^2 = \frac{A}{m}$ , where  $m$  the electronic mass. Now Eq. (5) can be rewritten as:

$$\frac{\partial^2 y_n}{\partial \tau^2} = -y_n - \frac{B}{A} y_n^3 - \frac{k}{A} (2y_n - y_{n-1} - y_{n+1}) \quad (7)$$

$$\tilde{H} = \sum_n \frac{1}{2} p_n^2 + \frac{1}{2} y_n^2 + \eta y_n^4 + \lambda (y_n - y_{n-1})^2 \quad (8)$$

where  $\eta = \frac{B}{4A}$ ,  $\lambda = \frac{k}{2A}$ .

Next, let us introduce creation ( $a^+$ ) and annihilation ( $a$ ) Bosonic operators at the  $n$ -th site as follows:

$$a_n^+ = \frac{(y_n - ip_n)}{\sqrt{2}}, \quad a_n = \frac{(y_n + ip_n)}{\sqrt{2}} \quad (9)$$

$$H = \sum_n \frac{1}{2} + a_n^+ a_n + \frac{\eta}{4} (a_n^{+4} + 4a_n^{+3} a_n + 4a_n^+ a_n^3 + 6a_n^{+2} a_n^2 + a_n^4) + \frac{\lambda}{2} (a_n^{+2} + a_n^2 + 2a_n^+ a_n + a_{n-1}^{+2} + a_{n-1}^2 + 2a_{n-1}^+ a_{n-1} + 2) - \lambda (a_n^+ a_{n-1}^+ + a_n a_{n-1} + a_n^+ a_{n-1} + a_n a_{n-1}^+). \quad (10)$$

First we should discuss the physics of the terms appearing in some of the above equations, since the meaning of the linear terms is clear, we comment mainly on the nonlinear terms as follows:

The terms  $a_n^{+4}$ ,  $a_n^{+2} a_n^2$ ,  $a_n^{+3} a_n$  are the bosonic operators that represent creation of four particles at site  $n$ , then simultaneous ‘creation’ and ‘annihilation’ of two quanta at site  $n$ , and finally creation of three quanta and annihilation of one quanta at site  $n$  respectively. Here, the first and the third terms are non-number conserving because same number of particles are “not” created and annihilated. Other similar terms can be explained in this way.

Again, the terms  $a_n^+ a_{n-1}$ ,  $a_n^+ a_{n-1}^+$ ,  $a_n a_{n-1}$  represent simultaneous tunneling of one quanta between neighboring sites i.e. simultaneous creation of one quanta at site  $n$  with a simultaneous annihilation of one quanta at site  $(n-1)$ , then creation of only one quanta at sites  $n$  and  $n-1$  respectively, and finally annihilation of one quanta at site  $n$  and  $n-1$  respectively. Other similar terms can be explained in this manner.

After having done the second quantization as described above, to account for the above mentioned terms in a proper way, a general basis with non-number conserving of particles needs to be formed. Therefore, next, let us introduce the basis as follows:

$$\psi_i = |n_{k1}, n_{k2}, \dots, n_{kn}\rangle = \prod_k \frac{[a_k^+]^{n_k}}{(n_k!)} |0\rangle \quad (11)$$

where  $n_{k1} + n_{k2} + \dots + n_{kn} = N$  is the total number of particles, and  $k_1, k_2, \dots, k_n$  denotes the sites. So, a given number of particles on a given number of sites can be generated by the mathematical module “compositions” in mathematica. However, with increasing number of particles and lattice sites, the Hilbert space dimension grows rapidly. Next, let us define the creation and annihilation operators as follows:

$$a_i |n_{k1}, n_{k2}, \dots, n_{ki}, \dots, n_{kn}\rangle = \sqrt{n_{ki}} |n_{k1}, n_{k2}, \dots, n_{ki} - 1, \dots, n_{kn}\rangle \quad (12)$$

$$a_i^+ |n_{k1}, n_{k2}, \dots, n_{ki}, \dots, n_{kn}\rangle = \sqrt{n_{ki} + 1} |n_{k1}, n_{k2}, \dots, n_{ki} + 1, \dots, n_{kn}\rangle \quad (13)$$

In an important work done by Proville [32], the non-number conserving methods for four sites and an arbitrary number of particles are shown. However, the method presented above gives a generalized way to solve the system for arbitrary number of particles on arbitrary number of sites. So, our method is clearly distinguished from the other investigations.

For the characterization of quantum discrete breathers, we need to make the Hamiltonian time-dependent. Let us take the help of temporal evolution of number of bosons at each site of the system  $\langle n_i \rangle(t) = \langle \Psi_t | \hat{n}_i | \Psi_t \rangle$ . We take  $i$ -th eigenstate of the Hamiltonian, and then we make it time dependent as follows:

$$|\Psi_i(t)\rangle = \sum_i b_i \exp(-iE_i t / \hbar) |\psi_i\rangle, \quad (14)$$

where  $\psi_i$  and  $E_i$  is the  $i$ -th eigenvector and eigenvalue respectively, and  $t$  is time. The Planck's constant ( $\hbar$ ) is taken as unity and  $b_i = \langle \psi_i | \Psi(0) \rangle$  for each site  $i$  and for a given range of  $t$ , where  $\Psi(0)$  stands for the initial state.

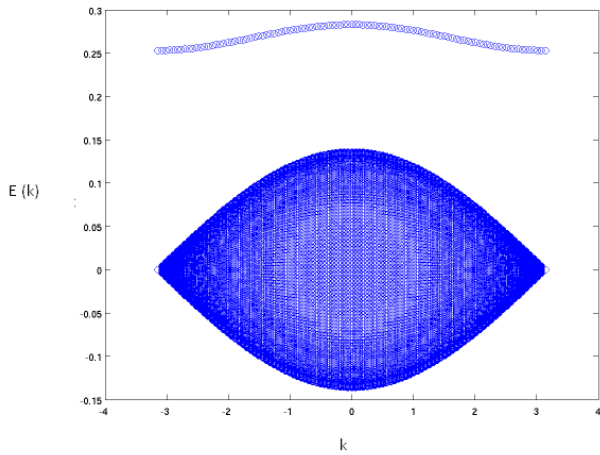
It is pertinent to mention that in contrast with the Discrete Non-Linear Schrodinger (DNLS) equation, where complete energy transfer takes place [33], in case of nonlinear K-G lattice, complete energy transfer does not take place between the anharmonic oscillators and there is a critical time of redistribution for the quanta. With the above methodology, we can now proceed to deal with some applications of non-periodic boundary condition approach in different types of materials.

### III. RESULTS AND DISCUSSION

As said earlier, here our main focus is on the temporal evolution of the number of quanta in different types of materials based on a generalized Hamiltonian in Klein-Gordon lattice. It is not possible within the present scope of the paper to discuss various aspects

of different types of materials. However, we briefly mention about the Hamiltonian needed to describe a given material, e.g. ferroelectric, then based on the second quantization, as shown in the ref [34]. From the approximate meeting point of different quanta, we also derive the 'time of redistribution' or 'critical time' of quanta that is proportional to the lifetime of quantum breathers (QBs) in femtoseconds (fs). This information thus derived will have consequences in the femtosecond response of DNA macromolecules. For the benefit of the readers, appropriate references are given to introduce the subject very briefly and then the relevant spectra are shown in order to highlight the 'application' of our above methodology to these materials to remain within the main focus of this paper that has implication in the field of applied physics for THz applications.

In the vast ocean of good literature, DNA stands apart from any other material both for scientific innovation as well as technological creation. However, a very brief introduction is given here on DNA, particularly in the context of denaturation, wherein our method of quantum calculations could be applied with an eye on future technology development. In recent years, biomolecular modeling has received an increasing amount of attention, especially focused on the DNA molecule as well as protein structures. The basic structure of DNA is fairly well understood since the discovery of Crick and Watson [35], but it is becoming increasingly apparent that structure alone does not sufficiently explain its functionality that is immensely complex. An example is the mechanism leading to bubble generation in DNA, in which the two polypeptide strands open to allow replication of the molecule, processing of proteins or complete strand separation (denaturation) [36]. The latter issue is of importance vis-à-vis the applicability of our generalized technique of temporal evolution of the number of quanta.



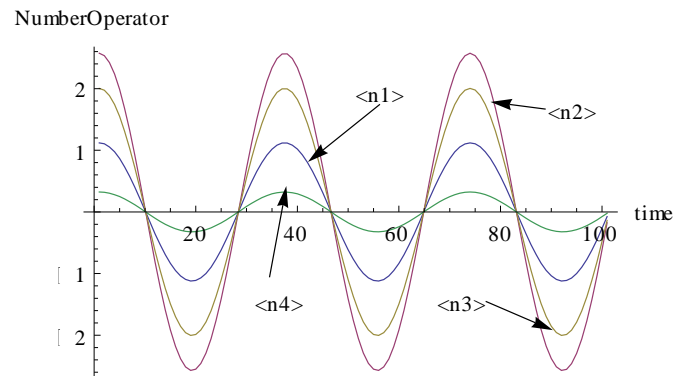
**Fig. 1:** Two-phonon bound state (TPBS) of DNA at a low value of interaction constant  $k=0.01$

Again as a preamble before showing the temporal behaviour of a multi-particle system that might be relevant to the DNA system of macromolecules in a non-periodic boundary condition approach, it may be pertinent to show two-phonon bound states (TPBS) or quantum breather states in a periodic boundary condition shown in fig 1.

It is pertinent to mention that in our earlier work on quantum breathers, the variability of lithium niobate system was “impurity” content. For our DNA system, although no such attempt has been made here, the microbiologists might find a relevant structural parameter for DNA to be useful for comparison purpose with TPBS parameters, such as energy gap ( $E_g$ ) between the continuum and the localized breather band, phonon hopping coefficient ( $\mu$ ), etc. Moreover, the variation of interaction constant or coupling in the DNA macromolecular system, the single-phonon spectrum width ( $W_{ph}$ ) can also be correlated again to derive some important information. Such a variation of TPBS parameters with those of DNA, such as dissociation energy of the base pair, transverse stretching of the hydrogen bond connecting the bases, the depth of the anharmonic potential wells, etc. will be the future directions of study. Here, it is simply emphasized that our Hamiltonian upon quantization gives rise to certain parameters for QB in the DNA macromolecules that are

possible to be related to some quantum parameters to shed light on DNA.

Following Eq.(14) for  $D = 0.08$  eV,  $b = 4.5$  Å,  $m = 350$  amu (see Dauxois et al [29]),  $k = 1$ , the temporal evolution is shown for 7 quanta on 4 sites  $|\Psi(0)\rangle = |6,1,0,0\rangle$ , as seen in Fig.2.



**Fig. 2:** For DNA, the temporal evolution spectra for 7 particles on 4 sites with  $|\Psi(0)\rangle = |6,1,0,0\rangle$  with the parameters values as:  $D = 0.04$  eV,  $b = 4.45$  Å,  $m = 300$  amu,  $k = 1$ .

This indicates that with an increase in the number of quanta, the QB’s lifetime decreases and hence while analyzing femtosecond response of DNA for a particular application, the temporal evolution spectra could be useful in deriving the critical time of redistribution of quanta and its relation with the number of quanta. This micro-level information on such an important macromolecule is of great importance in the application of DNA.

#### IV. CONCLUSION

The temporal variation of such number of quanta or phonons in more number of sites (i.e. subunits or domains) is detailed in this investigation for a generalized Klein-Gordon system with application in interesting macromolecules like DNA. As per a non-exhaustive literature search, it appears that there has not been an adequate amount of study on the quantum (nonlinear) localization of energy and its transfer using DNA. So our work with an inclination towards applied research paves the way for a direct method to study and utilize this DNA denaturation

phenomenon to investigate a particular medicinal effect on tissues more vividly. One could study the effect of such medicines, a diet or so, by knowing its  $D$ ,  $b$  and other coefficients used in the Hamiltonian and after studying its temporal-evolution, the composition of the medicines can actually be varied so that the cells of a particular animal or human may denatured

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