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Back of the Envelope Calculations Regarding Alexandrov, et al. 2009

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Concept Paper

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The paper entitled "DNA Breathing Dynamics in the Presence of a Terahertz Field" written by Alexandrov, Gelev, Bishop, Usheva, and Rasmussen that was posted on the Physics ArXiv on October 28, 2009, dealt with the effects of terahertz electromagnetic radiation on the DNA molecule. Figure 4 of the paper indicates that a segment of DNA that is between 60 and 70 base pairs in length will develop a "bubble" (i.e. separation of the hydrogen bonds between base pairs) at a location of about 45 base pairs, when exposed to 2 THz electromagnetic radiation for a time period of at least 40 picoseconds. Based upon assumptions regarding the model of biological quantum logic in DNA, some rapid calculations might provide insight into why such a specific change in the conformation of DNA occurs.

In a theoretical model of how such "bubble" formation takes place, it is postulated that the electromagnetic energy of the 2 THz radiation is absorbed by the phosphorus atoms of the DNA molecule, and that this effects a spin-pumping of energy in the form of spin angular momentum that is conducted longitudinally (as a spin current) along the pi-stacking interactions of the aromatic nucleotide bases of the DNA molecule to the point of "bubble" formation. "Bubble" formation occurs via the breaking of the hydrogen bonds between nucleotide bases, and it has been noted that naturally occurring "transcription bubble" formation tends to occur in areas of DNA that are rich in A-T (adenine-thymine) base pairs as opposed to C-G (cytosine-guanine) base pairs. This would make sense because the A-T base pairs are held together by two hydrogen bonds, and the C-G base pairs are held together by three hydrogen bonds, so the A-T base pairs would be easier to break.

The two hydrogen bonds that bond the A-T base pairs are an H-N bond that has a bond energy of 0.0824 eV, and an OH-N bond that has a bond energy of 1.258 eV. These two hydrogen bonds of the A-T base pair would have a combined total energy of 1.340 eV. If a phosphorus atom in a nucleotide were to absorb 2 THz radiation for 40 picoseconds it would be exposed to 80 wave cycles, with each wave cycle containing an energy of 0.00827 eV, which would supply a total energy to the phosphorus atom of 0.662 eV, and since there are two phosphorus atoms in the base pair di-nucleotide, the total energy absorbed by a particular base pair over 40 picoseconds would be doubled to 1.324 eV. This compares quite favorably to the total energy of the A-T hydrogen bonds of 1.34 eV. This could explain why "bubble" formation begins to take place after exposure to 40 picoseconds of 2 THz electromagnetic energy, but what would explain "bubble" formation at about the 45 base pair position on the DNA segment?

The spin filtering that takes place along the DNA molecule is distance dependent in that the further an electron (or its spin state) travels longitudinally along the DNA helix, the higher the spin motive force is on that electron (or its spin state). It is postulated that the point of "bubble" formation on the DNA segment depends upon the distance along the DNA molecule that would be necessary to develop enough of a spin motive force to spin filter the electron spin states at an energy that would break the hydrogen bonds of the A-T base pair. The work of Göhler, et al. ("Spin selectivity in electron transmission through self-assembled monolayers of double-stranded DNA" *Science.* 2011, 331, 894-897) indicated that the smallest distance necessary to spin filter an electron by DNA is between 10 and 20 base pairs, and a distance of 10 base pairs is necessary to make one complete turn of the B-DNA helix. Assuming the efficiencies of nature, an electron (or its spin state) would need to traverse one complete turn of the B-DNA helix, or a distance of 10 base pairs, to develop enough spin motive force to spin filter out an electron that would overcome the energy barrier between the C2-endo and C3-endo deoxyribose enantiomers. This assumes that as part of the model of biological quantum logic in DNA, the energy barrier between the C2-endo and C3-endo deoxyribose enantiomers represents the Landauer limit of a biologically perceptible bit of information. The Landauer limit of 0.0172 eV would thus be developed by the 10 base pair distance of a complete turn of B-DNA. If 0.0172 eV is developed by the electron spin filtering distance of 10 base pairs, then the number of base pairs of spin-filtering distance necessary to develop the energy necessary to break the first hydrogen bond of the A-T base pair (0.0824 eV) would be 48 base pairs (0.0824 x 10 ÷ 0.0172 = 47.9), which compares favorably to the "bubble" formation distance of about 45 base pairs indicated in Figure 4 of Alexandrov, et al.

In conclusion, the DNA effect of 2 THz radiation for 40 picoseconds is to create "bubble" formation at a distance of about 45 base pairs along the DNA molecule, and this effect might be understood through consideration of the quantum mechanics involved in the emergent quantum logic of the DNA molecule.

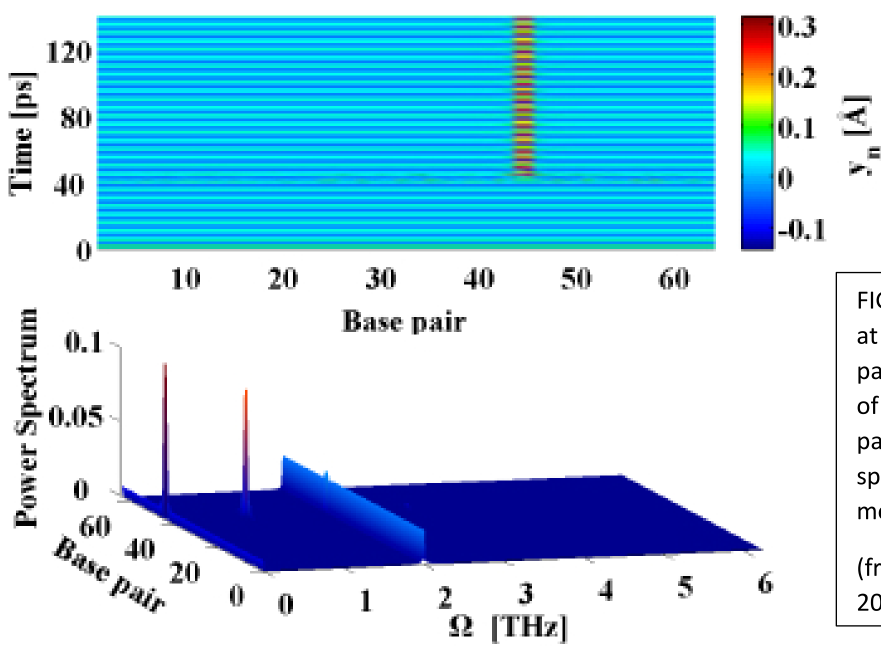

FIG. 4: Breather formation at Ω = 2.00 THz. The upper panel shows the evolution of the breather. The lower panel shows the power spectrum of the breather motion.

(from Alexandrov, et al. 2009 as cited above)