Twist-radial oscillations resonance effects in double-stranded DNA chains

Germán Torrellas[1], Enrique Maciá[2]

[1]Dpto. Física de Materiales, Fac. CC. Físicas, Universidad Complutense de Madrid, 28040 - Madrid;
german_torrellas@hotmail.com
[2]Dpto. Física de Materiales, Fac. CC. Físicas, Universidad Complutense de Madrid, 28040 - Madrid;
emaciaba@fis.ucm.es

Studying the dynamics of the DNA double helix is a very complicated task, due to its complex structure and interactions between the nucleobases, the sugar-phosphate backbone and the environment [1].

In this work we study the canonical equations of motion and normal modes of a duplex DNA chain at low temperatures, taking into account the coupling between the H-bond radial oscillations and the twisting motion of each base pair through the helical backbone structure. This coupling is mediated by the stacking interaction between adjacent base pairs along the helix, as prescribed by the Peyrard-Dauxois-Bishop model [2].

This kind of coupling has been shown to be very important in biological processes (such as denaturation and transcription), given that an untwisting of the helix can cause the local aperture of the molecule (figure 2).

In order to provide a more realistic treatment, we explicitly consider different mass values for different nucleotides, hence properly extending previous works where the masses for A, T, G and C nucleobases were assumed to be identical [3]. A schematic view of the model is shown in figure 1.

In this way, we disclose several resonance conditions, which can be achieved via fine-tuning of the effective masses of the different nucleobases (which can be modified through metilation processes or the attachment of heavier molecules to the backbone), which lead to interesting particular solutions of the dynamical equations.

The role of these dynamical effects on the DNA chain charge transport properties is discussed.

References

[1] Chakarborty, T. Editor. *Charge Migration in DNA: Perspectives from Physics, Chemistry and Biology.* Springer, Berlin (2007) 1-288

[2] Peyrard M., *Nonlinearity,* **17** (2004) R1 – R40

[3] Maciá E., *Physical Review B,* **80** (2009) 125102-1 – 13

Figures

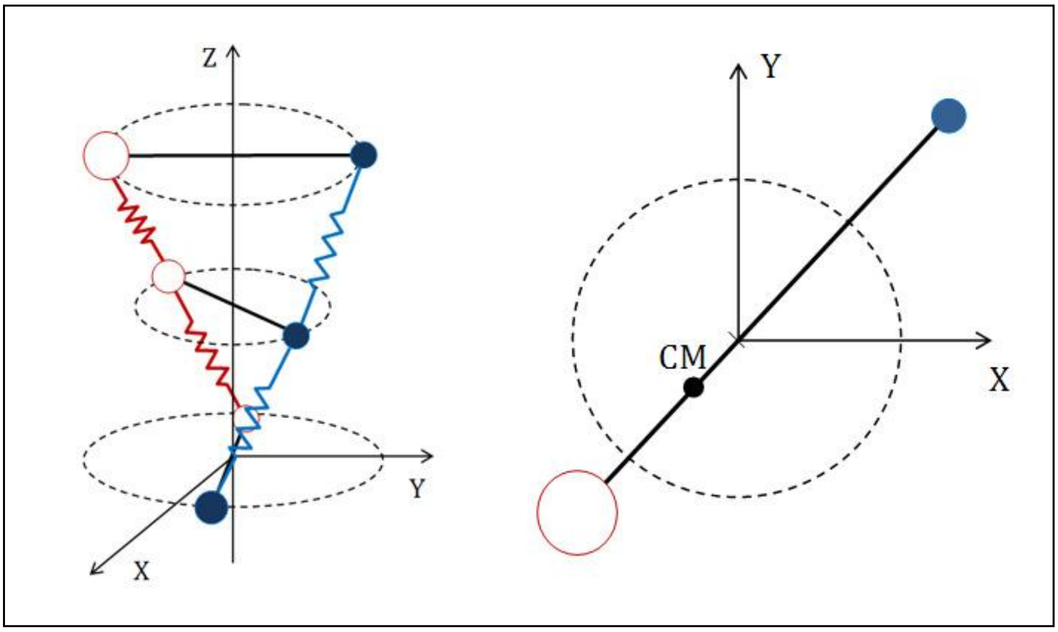

Figure 1. Schematic view of the model and detail of one of the base pair planes, where the mass difference effect is clearly visible.

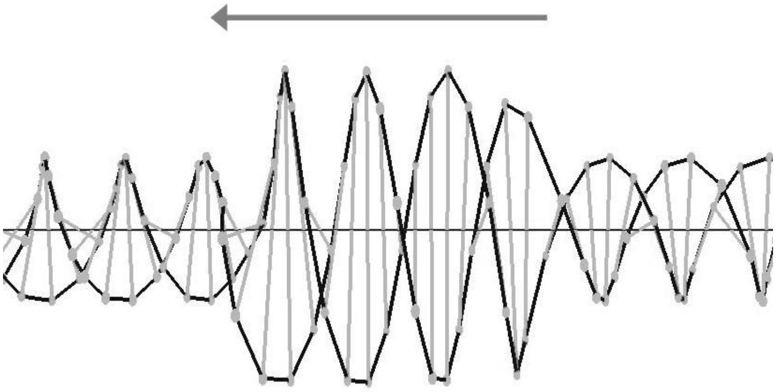

Figure 2. Radial opening of the molecule is only possible if accompanied by an untwisting.