Modeling the interaction of DNA with Terahertz fields.

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Today the use of non-ionizing radiation sources with frequencies on the THz range has spread in everyday life. The effects of this radiation on biological systems are interesting issues because biological functions may be altered and genotoxic effects may be generated. Particularly, the vibrational modes of DNA and others biomolecules are on the cited frequency range. Since THz photons do not carry enough energy to directly alter chemical reactions, nonlinear resonance effects may cause local changes of dynamics breathing in these systems. Motivated by this fact, Alexandrov et al. studied the influence of a THz field into dynamics of a homogeneous poly (A) DNA molecule with 64 base pairs (bp)[1,2]. To model the interactions of dsDNA with THz field, they used the Peyrard-Bishop-Dauxois (PBD) model citePBD. For this purpose, they studied periodic driving and frictional terms in the absence of thermal noise. It was found that breather modes (localized separations of the double strand) can be observed under certain conditions. Hence, it was concluded that the main effect of THz radiation is to resonantly influence into dynamical stability of the dsDNA. Later, Swanson showed that these breather modes can be eliminated changing the PBD model parameters or by including thermal noise[4]. He admitted that under assumptions concerning drag and drive forcing, breather modes can be generated at certain resonant frequencies.

On the other hand, Tapia et al. studied a homogeneous A-T sequence and the P5 virus promoter in the framework of the PBD model without applied external field and including thermal noise[5]. They enhanced this model with the inclusion of the solvent interaction through the addition of a Gaussian barrier to the Morse potential. They set suitable parameter values for the model and studied the formation and stabilities of bubbles in the system. They focused on the application of the principal component analysis (PCA) of the trajectories for P5 virus promoter under equilibrium conditions.

For these reasons we study the effect of the THz field in the dynamics of a heterogeneous sequence that has been widely studied in the framework of the PBD model[6], the P5 virus promoter. We included thermal noise to see the field influence under this condition. We use the PBD model with a solvation barrier. This barrier accounts for solvent interactions in the system and modifies the melting transition and the dynamics of molecule.

In this work we analyze the response of the system at different frequencies and field amplitudes. After that, we show the influence under some specific parameters of THz field in the melting transition and in the denaturation bubbles formation.

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[1] B. S. Alexandrov, V. Gelev, A.R. Bishop, A. Usheva, and K.O. Rasmussen, Phys. Lett. A 374, 1214 (2010).
[2] P. Maniadis, B. S. Alexandrov, A. R. Bishop, and K. O. Rasmussen, Phys. Rev. E 83(1), 011904 (2011).
[3] T. Dauxois, M. Peyrard, and A.R. Bishop, Phys. Rev. E 47, R44 (1993).
[4] Eric S. Swanson, Phys. Rev. E 83, 040901 (R) (2011).
[5] R. Tapia-Rojo, J. J. Mazo, and F. Falo, Phys. Rev. E 82, 031916 (2010).
[6] G. Kalosakas, K. O. Rasmussen, A. R. Bishop, C. H. Choi, and A. Usheva. Europhys. Lett. 68, 127-133 (2004).