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Acoustic phonon generation by intrinsically localized vibrational modes in double-helices of DNA macromolecules and transition from inter-strand energy exchange to nonlinear self-trapping

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We study ultrafast dynamics of intrinsically localized vibrational modes (breathers) in a double helix of two weakly coupled chains of nonlinear oscillators. With this we model nonlinear dynamics of DNA-type macromolecules, which can be studied by means of femtosecond infrared pump-probe laser spectroscopy similar to the case of protein α-helices [1]. We show that there are two regimes of coupled breathers: the time-periodic wandering of low-amplitude breather between the chains, and the one-chain-localization (self-trapping) of high-amplitude breather. We also find bound states of two breathers, localized in different chains, with different positions in the chains. The helix symmetry of the system results in a specific chiral mode which accomplishes the interaction between torsional and longitudinal acoustic modes in the constituent chains. In both nonlinear regimes, the inter-strand energy exchange gives rise to acoustic phonon generation in the coupled chains, and the generation is much stronger in the wandering-breather regime. Ultrafast acoustic phonon generation can be detected by means of optoacoustics, which can therefore provide a tool to study in time domain the inter-strand energy exchange and the transition to nonlinear self-trapping in DNA-type macromolecules.

1. J. Edler, R. Pfister, V. Pouthier, C. Falvo, and P. Hamm, 2004, Phys. Rev. Lett. v. 93, 106405.