

Delocalization of longitudinal acoustic-like excitations in DNA due to structural effects

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Submitted 14 August 2020
Resubmitted 9 September 2020
Accepted 10 September 2020

DOI: 10.31857/S1234567820190088

Terahertz-frequency phonon-like modes in DNA have been widely studied in recent years [1–3]. However, current theoretical models turn out to fail to reproduce some basic properties of these modes [2, 3]. In the present work, we consider the dynamics of longitudinal acoustic-like modes in DNA on a length scale corresponding to a wave number region between $\sim q_{\max}/2$ and $\sim q_{\max}$, where q_{\max} is the position of the major peak of the static structure factor $S(q)$. This region corresponds to the wave number region where structural effects due to wave number-dependence of the static structure factor become especially important. The dynamics of terahertz longitudinal acoustic-like modes in DNA can be described by a hydrodynamic theory generalized to high wave numbers (up to $\sim 30 \text{ nm}^{-1}$) [1]. Generalized hydrodynamic models are typically based on retaining the formal structure of the classical hydrodynamic theory and replacing macroscopic thermodynamic and transport coefficients with appropriate wave number-dependent memory functions. We approximately consider the heat mode to be decoupled from the sound mode for the parameters under study.

Using a generalized hydrodynamic approach [4, 5] and the results of inelastic X-ray scattering measurements [1], we propose a model to describe structural effects due to wave number-dependence of the static structure factor in the dynamics of longitudinal acoustic-like excitations in DNA. In the linear approximation, the generalized hydrodynamic equations are reduced to the following dynamic structure factor [4–6]

$$S(q, \omega) \propto \frac{\Gamma(q)\omega_0^2(q)}{(\omega^2 - \omega_0^2(q))^2 + 4\Gamma^2(q)\omega^2}.$$

Here, $\Gamma(q)$ is the damping factor and

$$\omega_0^2(q) = \frac{k_B T q^2}{mS(q)}$$

is the excitation frequency squared, with $S(q)$, k_B , T , and m being the static structure factor, the Boltzmann constant, the absolute temperature, and the mass of the particle, respectively. The dispersion relation for the excitation frequency $\omega_0(q)$ for longitudinal acoustic-like modes shows a typical behavior for liquids at mesoscopic scales: $\omega_0(q)$ is linear for small wave numbers q , reaches a maximum near $q_{\max}/2$, then decreases to a sharp minimum at $q \sim q_{\max}$, and again increases ($q_{\max} \approx 18.6 \text{ nm}^{-1}$) [1]. Accordingly, we use the following approximation for $\omega_0^2(q)$ up to wave numbers corresponding to $\sim q_{\max}$:

$$\omega_0^2(q) \approx k_1 q^2 - k_2 q^4 + k_3 q^6, \quad (1)$$

with the coefficients k_1 , k_2 , and k_3 being positive constants (the approximation given by Eq. (1) is valid only for wave numbers less than $\sim q_{\max}$). We estimate the values of k_1 , k_2 , and k_3 from a least-squares fit to the dispersion curve for ω_0 obtained in [1] for samples in the B conformation of DNA at ambient temperature. Accordingly, in the framework of generalized hydrodynamic approach, we consider the following free energy of the system

$$F = \frac{1}{2\rho_0} \int \left[k_1 \delta\rho^2 - k_2 (\nabla\delta\rho)^2 + k_3 (\nabla^2\delta\rho)^2 + \frac{\alpha}{3} \delta\rho^3 + \frac{\gamma}{6} \delta\rho^4 \right] d\mathbf{r},$$

where $\delta\rho$ is the fluctuation of the mass density, ρ_0 is the average mass density, α and γ are constants, and obtain

$$\frac{\partial^2 \delta\rho}{\partial t^2} = k_1 \frac{\partial^2 \delta\rho}{\partial x^2} + k_2 \frac{\partial^4 \delta\rho}{\partial x^4} + k_3 \frac{\partial^6 \delta\rho}{\partial x^6} + \alpha \frac{\partial}{\partial x} \left(\delta\rho \frac{\partial \delta\rho}{\partial x} \right) +$$

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$$+ \gamma \frac{\partial}{\partial x} \left(\delta \rho^2 \frac{\partial \delta \rho}{\partial x} \right) + \nu_L \frac{\partial^2}{\partial x^2} \frac{\partial \delta \rho}{\partial t} - \frac{\partial \delta S}{\partial x^2}, \quad (2)$$

where ν_L is a constant reflecting viscous dissipation and δS satisfies the following relations

$$\begin{aligned} \langle \delta S(x, t) \rangle &= 0, \quad \langle \delta S(x_1, t_1)^* \delta S(x_2, t_2) \rangle = \\ &= 2k_B T \rho_0 \nu_L \delta(x_1 - x_2) \delta(t_1 - t_2) \end{aligned}$$

(the bracket $\langle \rangle$ implies a thermal ensemble average).

Structural effects, reflected by the q -dependence of the static structure factor, are represented in our model by the terms with fourth- and sixth-order spatial derivatives in Eq. (2). The form of the dispersion relation (1) is essentially different from that typically used for modeling of longitudinal acoustic-like excitations in DNA in the low-wave number region [7],

$$\omega_0^2(q) \approx k_1 q^2 - k_2 q^4. \quad (3)$$

For the dispersion relation (3), a non-linear acoustic mode model with longitudinal waves along DNA molecule based on the well-known Boussinesq equation, was proposed. The fourth-order Boussinesq equation possesses solutions corresponding to monotone (sech-like) shapes which can be interpreted as non-linear localized excitations in DNA [7]. As for the sixth-order equation (2), when the dispersion coefficients k_2 and k_3 are positive, as in our case, two dispersions act in opposition to each other which causes the occurrence of spatially non-local regimes, while the soliton-like regimes disappear [8]. Thus the sixth-order derivative term qualitatively changes the behavior of the solutions. Our numerical simulations confirmed that a tendency of delocalization for DNA acoustic-like excitations may occur, at least in the case of large-amplitude density variations and for sufficiently short time scales. It should be emphasized that the dynamics on subpicosecond time scale are potentially important for biological function of DNA since, for example, initial steps of base pair opening can be associated with delocalized phonon-like modes on the

time scale $1/\Gamma \sim 0.1-0.2$ ps, as has been experimentally shown in [1]. We showed also that the nonlinearity in Eq. (2) influences amplitude limiting but can preserve the tendency of delocalization. Thus, our analysis qualitatively suggests that on a length scale corresponding to a wave number region between the positions of the maximum and the minimum of the dispersion relation for the excitation frequency, structural effects could induce a tendency of delocalization of the dynamics of acoustic-like excitations in DNA.

We are grateful to the anonymous referees for their critical comments and suggestions. We also thank O. S. Volodko for help in numerical simulations.

The reported study was funded by Russian Foundation for Basic Research, Government of Krasnoyarsk Territory, Krasnoyarsk Regional Fund of Science, to the research project 19-41-240003 “Mathematical modeling of collective atomic dynamics of biomacromolecules in non-equilibrium conditions on a picosecond time scale”.

Full text of the paper is published in JETP Letters journal. DOI: 10.1134/S0021364020190030

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