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Quasi-crystalline model of DNA vibrational dynamics

L.A.Bulavin, S.M.Perepelytsya, A.D.Suprun

T.Shevchenko Kyiv National University, Department of Physics
64 Volodymyrska Str., UA-01033 Kyiv, Ukraine

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A model of DNA molecule vibrational dynamics has been constructed taking into account the system helical structure as well as the general case of nitrogen bases arrangement. An ideal model taking into account the molecule helicity but not its heterogeneity has been considered as a specific case. The vibrational frequencies have been determined analytically (two optical branches and one acoustic). The character of amplitudes and sound speed dependences on the wave vector has been determined and conclusions on the vibrational motions of the B-DNA double helix have been drawn using these data.

Построена модель колебательной динамики молекулы ДНК, которая учитывает спиральность системы, а также учитывает общий случай расположения азотистых оснований. Как частный случай, рассмотрена идеализированная модель, которая не учитывает гетерогенность, но учитывает спиральность молекулы. Найдены частоты колебаний в аналитическом виде (две оптические ветви и одна акустическая). Определен характер зависимости амплитуд и скорости звука от волнового вектора, на основе чего сделаны выводы о колебательных движениях двойной спирали В-ДНК.

The complete information on proteins and thus on an organism as a whole is known to be coded in DNA macromolecule [1], but the mechanisms of the genetic information transfer are not studied enough. To understand such mechanisms, it is necessary, inter alia, to determine the character of double helix dynamics dependence on the nitrogen bases sequence. That is why the results of the computer simulation attract a special interest. Using molecular dynamics simulation methods, Young, Beverige, McConnel, and others have shown that the binding sites for metal cations and the conformational mobility of DNA depend heavily on sequence of base pairs [2–4]. Their results correlate qualitatively with experimental data [5–7]. The vibrational dynamics of double helix was studied by Matsumoto and Olson using the normal mode method [8]. They have uncovered a correlation between bending vibrations and sequence of nitrogen bases.

But in spite of obvious successes of the computer simulation in this field, the models providing the determination of correlation between measured quantities and dynamical properties of the system are necessary for physical interpretation of the experimental data. This circumstance determines the actuality of this work. Today, there are several models describing the vibrational motions of double helix [9–11]. Each of them is intended to explain specific peculiarities of the structure dynamics. For example, the four mass model [9] describes intramolecular motions of double helix (the vibrations of nucleosides as penduli, the hydrogen bond stretching in base pairs). The models introduced in other papers [10, 11] were constructed to determine of the role of ions that neutralize the phosphate groups in the low-frequency (<250 cm^{-1}) vibrations of DNA molecule.

In this work, a model of DNA normal vibrations is developed. This model takes into account the general case of nitrogen bases localization. The object of the theoretical inves-