Physics Letters A ••• (••••) •••–•••

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Physics Letters A

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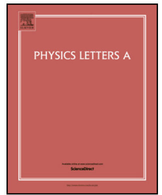

Water-mediated correlations in DNA-enzyme interactions

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ARTICLE INFO

Article history:
Received 31 March 2017
Received in revised form 25 September 2017
Accepted 18 October 2017
Available online xxxx
Communicated by Z. Siwy

Keywords:
Aromatic networks
Dipole oscillations
Water dipole field
EcoRI restriction endonuclease
Taq DNA polymerase
Quantum biology

ABSTRACT

In this paper we consider dipole-mediated correlations between DNA and enzymes in the context of their water environment. Such correlations emerge from electric dipole-dipole interactions between aromatic ring structures in DNA and in enzymes. We show that there are matching collective modes between DNA and enzyme dipole fields, and that a dynamic time-averaged polarization vanishes in the water dipole field only if either DNA, enzyme, or both are absent from the sample. This persistent field may serve as the electromagnetic image that, in popular colloquialisms about DNA biochemistry, allows enzymes to “scan” or “read” the double helix. Topologically nontrivial configurations in the coherent ground state requiring clamplike enzyme behavior on the DNA may stem, ultimately, from spontaneously broken gauge symmetries.

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1. Introduction

In a recent paper [1], the dipole structure of DNA has been studied by examining the molecular dipole components induced due to van der Waals (vdW)-type dispersion forces between base pairs. In particular, delocalized electrons in the base pairs of DNA were analyzed and theoretically shown to stimulate dipole formation at the molecular level. These dipole networks generate collective modes that are suitably fine-tuned for enzymatic activity resulting in double-strand breaks in the DNA helix. This class of enzymes rapidly scans the DNA [2] searching for target recognition sequences, which exhibit a marked palindromic mirror symmetry between one DNA strand and its complement. Specific binding of target sequence produces conformational changes in the enzyme and DNA, with characteristic release of water and charge-countering ions from the DNA-protein interface. Under optimum biological conditions, concerted cutting of both strands then occurs without producing intermediate single-strand cuts [3–6], which requires, in order to occur, synchronization of dipole vibrational modes between spatially separated nucleotides and enzymatic molecular subunits. The dipolar correlations between DNA and enzyme are required in order for these enzymes to cleave DNA in a manner that preserves the palindromic symmetry of the double-stranded substrates to which they bind.

Although the evolution from sequence recognition to catalysis is perhaps the least understood aspect of the enzymology, the synchronous long-range correlations over distance are a hallmark of collective molecular dynamics [7,8]. However, the study of the chemistry of DNA-enzyme interactions, and perhaps the whole range of biomacromolecular interactions, is still fraught with the lacuna in our understanding between the intrinsically stochastic molecular kinematics and the high efficiency and precise targeting of enzymatic catalytic activity [9,10]. This highly efficient, ultraprecise coordination has been shown to confound the explanatory reach of statistical methods for describing average regularities in bulk matter [11]. What is needed is of course not in opposition to the current state of knowledge derived from biochemistry. On the contrary, what we propose to shed light on is the quantum dynamical basis of the molecular interactions so as to provide a solid physical foundation for the biochemistry results. Such inquiry develops in many respects along the same path of the traditional study of the molecular dipole and multipole dynamical structure of the electronic quantum conformational shells determining the properties of interacting molecules in chemistry.

By following such a line of thought, our aim in the present paper is to deepen the understanding of DNA-enzyme interactions

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https://doi.org/10.1016/j.physleta.2017.10.038
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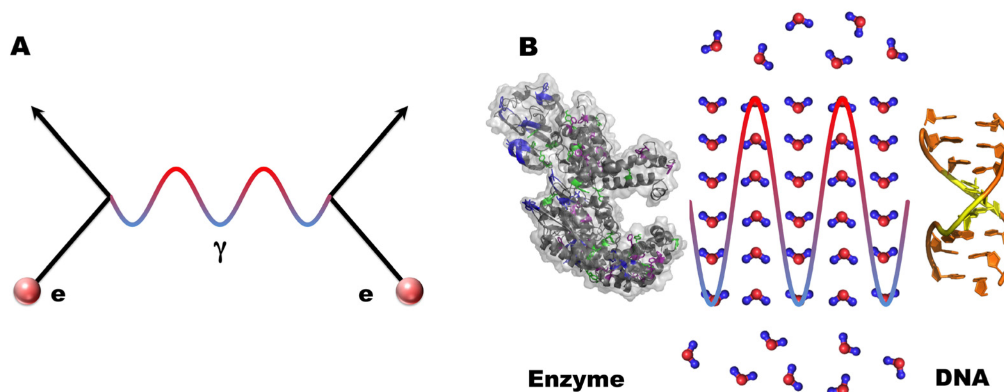

Fig. 1. Mediating wave fields or quanta in subatomic and biological physics. (A) Electron–electron correlations are mediated by photons in quantum field theory. (B) Analogously, long-range correlations in the molecular water field between DNA and enzymes may be mediated by dipole waves. Note that these are schematic renderings, neither drawn to scale nor representative of the actual orientations of water molecules.

by characterizing quantitatively the nature of long-range correlations between DNA and enzyme in water. Water is the matrix of all known living systems and constitutes about 65% of the human body by mass and about 99% by number of molecules. On the one hand, we exploit the basic feature of any statistically oriented analysis, namely the fact that biomolecules are not isolated from their environment of water molecules. Thus, we have to face the complexity arising from dealing with a large number of molecular components and the quantum vibrational modes of their dipoles, which brings us to consider the quantum field theory (QFT) formalism. On the other hand, the generation of collective mode dynamics derived in the framework of spontaneously broken gauge symmetry theories can explain the observation of highly ordered patterns characterizing the catalytic activity, in space and in time (time ordered sequences of steps in the chemical activity). In a rather natural way we are thus led to adopt in the study of DNA-enzyme interactions the QFT paradigm of gauge theories, namely that the interaction between two systems is realized through the exchange between them of a mediating wave field or quantum, in analogy with the photon exchanged by two electric charges in quantum electrodynamics (see Fig. 1). Due to the relevant role played by electric dipoles in the molecular interactions under study, we center our investigation on a generalized model of the radiative dipole wave field mediating the molecular interactions between DNA and enzyme in water. This model is discussed in Sections 3 and 4.

The paper is organized as follows. In Section 2 we discuss and partially review the molecular dipole structure of DNA and enzyme. To connect with previous work, we consider the case of the type II restriction endonuclease *Eco*RI and, for generality, we similarly analyze the *Taq* DNA polymerase, which is widely used in polymerase chain reaction (PCR) processes for the amplification of DNA sequences. In Section 3 we study the collective dipole dynamics of water molecules in the presence of the DNA radiative dipole field. In Section 4 we examine how the water dipole wave field interacts with the enzyme radiative dipole field. The water dipole field is identified as the mediating wave field in the DNA-enzyme interaction. Concluding remarks are presented in Section 5. The appendix reports some further details on the DNA and enzyme systems, including polarizability data and other model parameters.

2. Dipole networks in DNA sequence and enzyme systems

In this section we present the computation of the collective dipole behavior in the DNA and enzyme molecules by considering the interactions between their constituent aromatic rings. These rings, present in both DNA base pairs and enzyme amino acids as well as a host of other biomolecules, contain conjugated planar ring systems with delocalized π electrons shared across the structure, instead of permanent, alternating single and double bonds. Benzene is the canonical example of such a ring. This confers on aromatic compounds an unusual stability and low reactivity, but also provides an ideal structure for the formation of electric dipoles, which can interact to produce electromagnetic couplings in biology.

2.1. DNA sequence

We consider first the linearized DNA sequence, with polarizability data for its four bases given in Table 1 in the appendix. The symmetry and regularity of the molecule about its helical axis simplifies the calculation relative to the one for enzyme aromatic networks. By resorting to the results of Ref. [1], we observe that in DNA the delocalized electrons belong to the planar-stacked base pairs that serve as "ladder rungs" stepping up the longitudinal helix axis. The dipole formation is generated by Coulombic interactions between electron clouds.

By considering a molecule of length N nucleotides, following Ref. [1], we can exploit the natural symmetry of the linearized DNA sequence about the longitudinal z axis. Such symmetry is not available for the considered enzymes, so we have employed a simplified approach using the effective average polarizability in Section 2.2. The DNA collective oscillations can thus be decoupled into longitudinal z and transverse xy modes, which correspond to different potential matrices $\mathbf{V}_j$ to be used in the characteristic equation for the DNA eigenfrequencies: $det(\mathbf{V}_j - \Omega^2_{s,j}\mathbf{T}_j) = 0$, where $\mathbf{T}_j$ are the diagonal kinetic matrices containing only the electron mass m_e in each element. We thus obtain the standard diagonalized Hamiltonian

$$H_{DNA} = \sum_j H_j = \sum_j \sum_{s=0}^{N-1} \hbar\Omega_{s,j}\left(a^\dagger_{s,j}a_{s,j} + \frac{1}{2}\right), \quad (1)$$

with eigenstates given by

$$\left|\psi_{s,j}\right\rangle = a^\dagger_{s,j}\left|0\right\rangle, \quad (2)$$

where $s = 0, 1, \ldots, N-1$ for the $j = xy, z$ potential.

Of course, DNA has no observed electronic transitions—meaning absorption spectra of individual chromophores leading to electronic excitation and fluorescence—in the 0.1–1.7 eV range calculated in Table 2 in the appendix. However, the type of processes we describe here are coherent oscillations that arise from long-range dipole-dipole correlations between constituent aromatic rings. These dipolar correlations do not require photoabsorption-induced electronic excitation. This coherent behavior stems from van der

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