

# Calculation of the Interference Coefficient of the Polyatomic Molecular Structure of DNA

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**Abstract.** This paper shows the calculation of the DNA interference coefficient and uses it to obtain the spectrum of the interaction of an ultrashort laser pulse with a molecule. The calculation is based on a simplified model of the molecule.  
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**Keywords:** laser pulses; molecule; DNA; radiation spectrum.

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## 1 Introduction

Currently, much attention is focused on the study of complex molecular structures using ultrashort laser pulses [1, 2]. This is due to the difficulties of analyzing unsteady molecular structures using other methods [3, 4]. Methods from the field of chemistry, the Slinger method, for example, give accurate results, but the study is long and time-consuming. X-ray irradiation does not give accurate results. That is why scientists are now interested in the use of ultrashort laser pulses [5, 6]. With their help in the future it is possible not only to determine the structure of multi-atomic objects, but also to study of molecular processes in it [7, 8], because ultrashort pulses operate in a very small time range, corresponding to atto and femtosecond scales.

The problem with using ultrashort lasers today is primarily the lack of a theoretical apparatus for interpreting the results obtained experimentally. Deciphering the interaction spectra is complicated without theoretical calculations of the process of irradiating a molecule with laser pulses. There are ways to calculate the interaction of pulses with one target, one atom or molecule consisting of atoms of one substance. However, there are molecular objects, interesting for research and consisting of many atoms. The calculation in this case is complicated by the number of atoms, different electron density, over-radiation, etc. Such an object can be calculated on a qualitative level, using simulation methods, specifying the coordinates of the atoms included in the system [9]. However, the calculation of the system defined by a real-DNA number of coordinates requires a large amount of time for processing (more than a day), which is inconvenient for analysis. To simplify, it is necessary to move away from the use of coordinates and introduce an analytical

formula for the spectrum of interaction of ultrashort pulses with the object. The main component of the spectrum formula is the interference factor. It changes depending on the spatial position of the elements in the system. It is impossible to describe it analytically for a real molecule, consisting of many atoms. This paper proposes a simplified model of a DNA molecule, which is used to calculate the interference factor.

## 2 Theory

In this work, we will use a single helix of DNA as the object of study; this will facilitate the process of considering the atomic model of the molecule. We use a DNA helix with alternating nitrogenous bases: cytosine and guanine (Fig. 1).

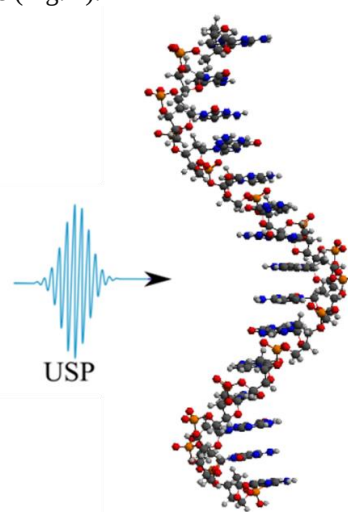


Fig. 1 The helix of a DNA molecule irradiated by an ultrashort laser pulse (USP). Performed in the Avogadro program.

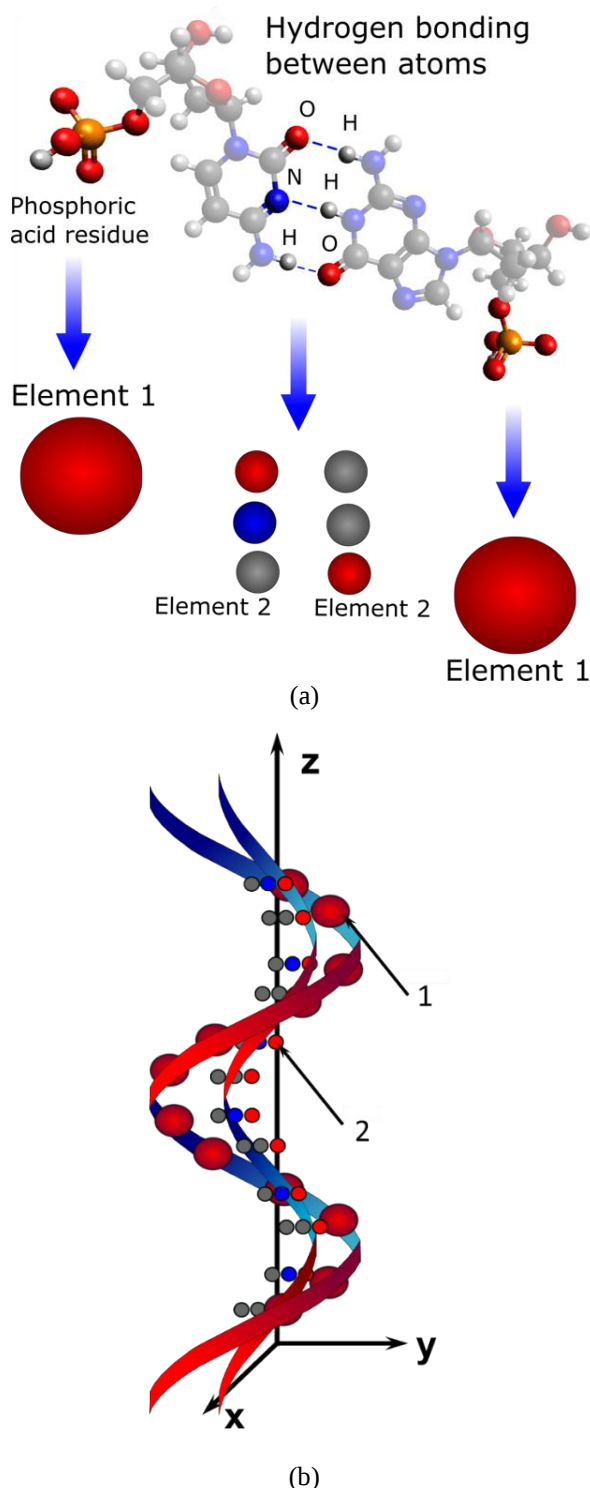


Fig. 2 A simplified model of a single turn of the DNA helix. Atoms involved in hydrogen bonding: gray – hydrogen, red – oxygen, blue – nitrogen. a) An illustration of how the elements were formed. b) One turn of the spiral built with the elements.

According to the principle of complementarity, only they can interact with each other, so the presence of adenine and thymine next to each other is excluded. Suppose an ultrashort laser pulse falls on a molecule. In this case, there are many atoms in the radiation path that

have some symmetry and periodicity. The periodicity of the structure of the molecule makes it possible to simplify the model and move from a polyatomic structure to a system consisting of simpler elements.

Each nitrogen base of the molecule is connected to the opposite one by three hydrogen bonds. The DNA helix consists of a phosphoric acid residue and a monosaccharide. Thus, these elements perform an important function, they “form” a molecule. The remaining atoms from the analysis can be omitted. Thus, the outer part of DNA turns into a periodic set of elements as shown in Fig. 2, where 1 denotes monosaccharide + phosphoric acid residue and 2 denotes the inner: nitrogenous base atoms involved in hydrogen bonding. The remaining atoms that make up the molecule are not considered, we believe that in the absence of elements 1 and 2, the remaining elements are also missing, because the “connection” function is not performed.

Based on the calculations given in Refs. [9, 10], we write down an expression for the interference factor:

$$g_N(p) = \left| \sum_a e^{i \cdot p R_a} \right|^2, \quad (1)$$

where  $p$  – scattering pulse, i.e. the pulse received by an electron when scattering an ultrashort laser pulse,  $a$  – system atoms,  $R_a$  – radius-vector of the atom. In the case of simplification, the atom is replaced by an element and we consider elements of two varieties 1 and 2.

In general terms, the radius vector is represented by the following expression:

$$R_a = xi + yj + zk, \quad (2)$$

$$\begin{cases} x = \rho \cos \varphi \\ y = \rho \sin \varphi, \\ z = z \end{cases}$$

where  $\rho = R_a = const$  is a radius of the plane of rotation of a single element,  $\varphi \in [0; 2\pi \times T]$  – rotation angle. The nucleotide rotates in one plane on a circle, so the angle can be written as  $\varphi = 2\pi \frac{a}{N_T}$ , where  $a$  – sequence number of the nucleotide,  $N_T$  – their total number for the period.  $z = C \cdot 2\pi \frac{a}{N_T}$ , where  $C$  is the geometric

parameter of the spiral. Then we change from a system consisting of atoms to a system consisting of elements and replace the radius vector designation  $R_a$  with  $R_l$ .

In the case of simplification, we get two spirals, external and internal. They differ only in the number of elements and radius-vectors. Let us locate both spirals in the xyz coordinate system (Fig. 3).

In Fig. 3,  $R_1$  is the radius-vector of external elements (monosaccharides + phosphoric acid residues) and  $R_2$  is the radius-vector of internal elements (nitrogenous bases).

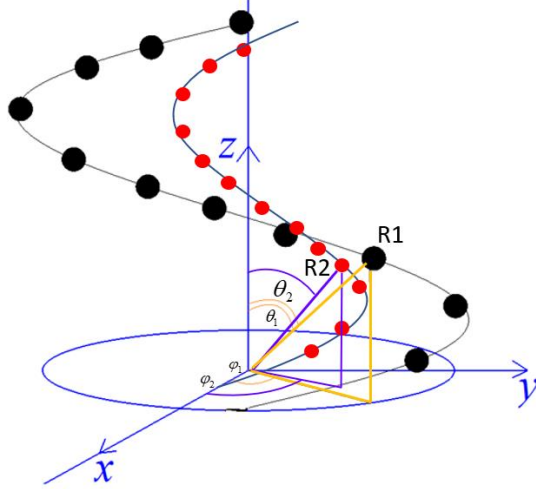


Fig. 3 DNA spirals in the xyz coordinate system. Red indicates internal elements – nitrogenous base atoms, black shows external elements – monosaccharide + phosphoric acid residue.

The calculation of the interference factor of one helix of a molecule was carried out in Ref. [10]. We use the formula obtained in this work:

$$g_N(p) = \left( \frac{N}{2\pi} \right)^2 \left| \int_0^{2\pi} e^{ipR \sin \theta \cos z + ip \cos \theta \times \alpha \times z} dz \right|^2. \quad (3)$$

In the model under consideration, the number of spirals doubles, so the interference factor changes:

$$\left| \sum_{a=0}^N e^{ipR_a} \right|^2 = \left( \frac{1}{2\pi} \right)^2 \left( \left| \int_0^{2\pi} N_1 e^{ipR_1 \sin \theta_1 \cos z + ip \cos \theta_1 \cdot \alpha \cdot z} dz \right|^2 + \right. \quad (4)$$

$$\left. + \left| \int_0^{2\pi} N_2 e^{ipR_2 \sin \theta_2 \cos z + ip \cos \theta_2 \cdot \alpha \cdot z} dz \right|^2 \right),$$

where  $N$  – number of elements in the system,  $\alpha = 2\pi \cdot CT$  – parameter of the spiral, which depends on its period. Adding two interference factors together is a big simplification. In this case, we consider the system rather roughly, neglecting the interaction of secondary scattering from elements 1 and 2. We believe that the distance between groups of elements inside the same chain. This model takes into account interference between nearby atoms directly involved in hydrogen bonding and phosphodiester bonding. This approach should test the very idea of using a two-element model.

Next, we calculate the scattering spectrum using the form obtained in the work [11]:

$$\begin{aligned} \frac{d^2W}{d\omega d\Omega_k} = & \frac{1}{(2\pi)^2} \frac{f(\omega)}{c^3 \omega} (N_a N_b G(\omega, n, n_0) + \\ & + N_a N_b (N_b - 1) F(\omega, n, n_0) + \\ & N_b^2 Q(\omega, n, n_0) g_N(p)), \end{aligned} \quad (5)$$

where  $Q(\omega, n, n_0)$ ,  $G(\omega, n, n_0)$ , and  $F(\omega, n, n_0)$  – atomic form factor,  $d\Omega_k$  – solid angle,  $n$  – direction of the scattered pulse,  $n_0$  – direction of the incident pulse.

Using Eq. (5), let us simulate the scattering of an ultrashort laser pulse within a simplified model of Eq. (4). The simulation results are presented in Fig. 4, which demonstrates a cross-shaped scattering spectrum, which is similar to classical experiments with X-ray radiation.

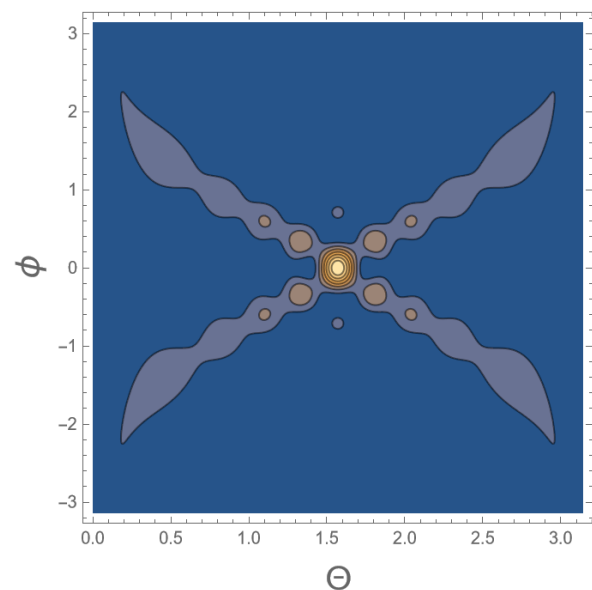


Fig. 4 Contour plot of the scattering spectrum of an ultrashort laser pulse on a simplified model of a molecule:  $\theta$  – angle between the helix axis and the scattering direction,  $\varphi$  – is the angle between the x-axis and the projection on the plane perpendicular to the helix axis (spherical coordinates).

The simulation was performed in Wolfram Mathematica 13.0. Specified parameters for the simulation: the pulse falls on the system at an angle of  $90^\circ$ . All spectra are normalized to one. A 3D contour plot of the spectrum is shown in Fig. 5, which illustrates the difference between the considered model and the model of paper [10].

As can be seen from Fig. 5(b), the spectrum obtained in Ref. [10] is asymmetric, which indicates that the analytical formula was erroneous. The helix of the DNA molecule has a periodicity, from which it could be assumed that the spectrum of interaction of radiation with it should be symmetrical. After processing of Eq. (3), we obtained a model of the diffraction pattern in Fig. (4), which is symmetrical and similar to X-ray images of a DNA molecule.

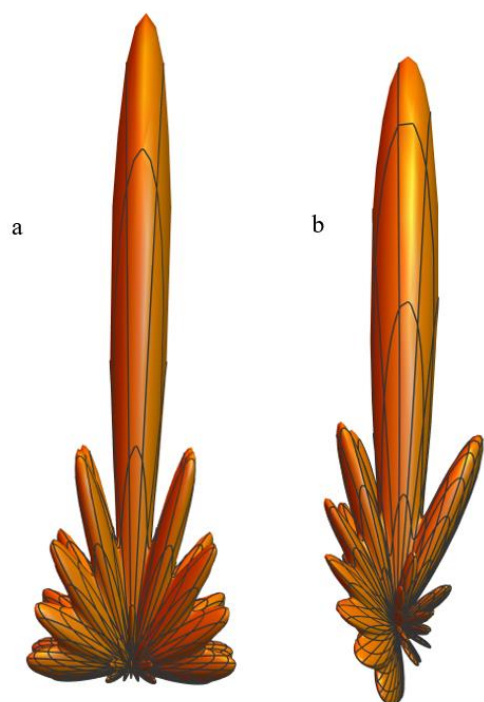


Fig. 5 Contour plot of the scattering spectrum of an ultrashort laser pulse on a simplified model of a molecule: (a) obtained on the basis of calculations of Eq. (4); (b) obtained on the basis of calculations from Ref. [10].

### 3 Conclusion

The article describes the idea of a new simplified calculation of the interference coefficient for the case of a polyatomic molecular structure when it is irradiated with ultrashort laser pulses. The object of the study is a DNA molecule and a femtosecond laser pulse impinging on it. A simplified model of the system under study is constructed, on the basis of which the formula of the interference coefficient is derived. The results are compared with the previously obtained spectra of the interaction of an ultrashort pulse with a single turn of the molecule without taking into account the internal nitrogenous bases. The simulation results demonstrate that such a way of describing DNA by dividing it into elements is feasible and it is possible to continue working on the theory, complicating it by taking into account repeated emissions.

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### Disclosures

The authors declare no conflict of interest.

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