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Peculiarity of electron density calculation during interaction of ultrashort laser pulse with nitrogenous base of DNA molecule adenine

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Abstract. Today, ultrashort laser pulses are used to study and analyze biomolecules. Their advantages over X-rays lie in the speed of measurement and accuracy, which allows studying the structure of a molecule on a time scale commensurate with the time of various biochemical processes in it. However, the practical possibility of studying chemical and biological processes in facilities using existing and promising X-ray free-electron lasers requires the development of a theory of the interaction of laser pulses with matter. In this article we will consider the interaction of an ultrashort laser pulse (USPs) with the base of the DNA (Deoxyribonucleic acid) molecule - adenine. In more detail we will consider the calculation of the photon birth probability, after the interaction of the pulse with the molecule. We will build a model of the base of the molecule and propose a method for calculating the electron density for the case when the substance has a different elemental composition.

Keywords: Deoxyribonucleic acid, ultrashort laser pulse, photon, electron density, elemental composition

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Материалы конференции

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Особенность расчета электронной плотности при взаимодействии ультракороткого лазерного импульса с азотистым основанием молекулы ДНК аденином

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Аннотация. Сегодня применяются для изучения и анализа биомолекул ультракороткие лазерные импульсы. Их преимущества по сравнению с рентгеновским излучением заключается в быстроте измерения и точности. Однако, практическая возможность изучения химических и биологических процессов требует разработки теории взаимодействия лазерных импульсов с веществом. В данной статье мы рассмотрим взаимодействие ультракороткого лазерного импульса (УКИ) с основанием молекулы ДНК - аденином. Подробнее рассмотрим расчет вероятности рождения фотона, предложим способ расчета электронной плотности для случая, когда вещество имеет разный элементный состав.

Ключевые слова: Дезоксирибонуклеиновая кислота, ультракороткий лазерный импульс, фотон, электронная плотность, элементный состав

Финансирование: Исследование выполнено при поддержке государственного задания Российской Федерации № FSRU-2020-0008.

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Introduction

Imaging techniques from diffraction data obtained using ultrashort laser pulses are being actively developed for applications in nanotechnology and structural biology. Methods of X-ray diffraction analysis of matter (XRD) as well as X-ray crystallography (XRC) are well studied and underlie many modern discoveries in physics, chemistry, biology, medicine [1,2]. The structure of a molecule is determined from the time-domain infinite plane wave scattering spectrum [1,2]. But recently scientists have started to apply ultrashort laser pulses for investigation. In this case the scattering spectrum moves into the femto and atto-second time range, which is poorly understood up to now.

The use of (USPs) to analyze the structure of molecules is a very promising area of research. As noted, ultrashort laser pulses (USPs) operate on a small time scale. This is very convenient for the description of organic structures, as such materials can be both stationary and non-stationary. Non-stationary objects, such as DNA, for example, can only be studied using (USPs), because the characteristic time in such systems is smaller or comparable to the femtosecond time scale. The non-stationarity in them may be caused by the formation and rearrangement of chemical bonds, intra-atomic and molecular processes, etc. [3].

Experimental studies of molecules using (USPs) on European X-Ray Free Electron Laser (XFEL) are already in progress [3]. The technique of introducing the molecules into the X-ray beam (e.g. XFEL) is being actively researched and improved. In order to analyse the experimentally obtained data, theoretical descriptions of the interaction processes between (USPs) and biostructures are urgently needed.

So far, a lot of theoretical studies on the specificity of scattered (USPs) on various multi-atomic systems have been carried out. However, despite this fact the theoretical base is still weak and does not take into account all specific features of diffuse (USPs).

In this paper we will consider the DNA molecule as a promising and poorly studied biomolecule at the atomic level. The molecule stores biological information in the form of a genetic code consisting of a sequence of nucleotides. Consequently, a defect on a nucleotide can indicate the presence of a defect in the molecule. In [4] we considered the interaction of an ultrashort laser pulse with a DNA molecule in a simplified form, considering each nucleotide as a separate unit of matter, within the whole molecule. We now focus in detail on a single nucleotide with the nitrogenous base adenine. The difficulty of the new calculation is that now it is necessary to take into account the elemental composition of the molecule. It is possible to take it into account through the electron density of the molecule, which we will consider in this work.

In the following, the atomic system of units will be used, where $\hbar = 1$, $|e| = 1$, $m_e = 1$.

Materials and Methods

A nucleotide is a compound of a phosphate group, a carbohydrate, and a nitrogenous base – adenine. Let us imagine it as an arbitrary polyatomic system, on which the (USPs) falls in the direction n_0 . The duration of such a pulse will be considered much less than the characteristic atomic time $\tau_a = 1$, i.e., $\tau/\tau_a = 1$. This will allow us to use the sudden perturbation approximation.



In this approximation, the proper Hamiltonian of the system can be neglected, since the electron in the atom does not have time to evolve under the action of the atom's field due to the too fast interaction of the momentum with the electron in the atom [5]. It should be added that the condition $\tau/\tau_a = 1$ for using our approximation is not strict. To do this, it is sufficient to assume, as was shown in [5], that, $\omega_0\tau_a = 1$, where ω_0 is the carrier frequency of the incident (USPs). Obviously, the condition $\omega_0\tau_a = 1$ holds for X-ray frequencies. The intensity of the electromagnetic field of the (USPs) $\mathbf{E}(\mathbf{r},t)$ is considered in general terms, i.e., we will consider it to depend on the coordinates and time. We are interested in electromagnetic fields that are not strong enough to account for relativistic effects. As was obtained in [6], taking into account these approximations, the probability of the birth of a photon W of a given frequency ω per unit solid angle Ωk with the simultaneous transition of the polyatomic system from the ground state to all possible final states (hereinafter, the scattering spectrum of the USPs)

$$\frac{d^2W}{d\omega d\Omega} = \frac{1}{(2\pi)^2} \frac{1}{c^3\omega} (N_a N_b G(\omega, \mathbf{n}, \mathbf{n}_0) + \delta_N(\mathbf{p})(N_b - 1)F(\omega, \mathbf{n}, \mathbf{n}_0)), \quad (1)$$

where N_a is the total number of atoms in the system, N_b is the number of electrons in the atom, \mathbf{n} is the speed of light, $G(\omega, \mathbf{n}, \mathbf{n}_0)$ is the direction of escape of the born photon, $F(\omega, \mathbf{n}, \mathbf{n}_0)$ and the mean values expressed in terms of electron density $\rho(\mathbf{r})$ as

$$G(\omega, \mathbf{n}, \mathbf{n}_0) = \frac{1}{N_b} \int \rho(\mathbf{r}) |\mathbf{f}(\mathbf{r})|^2 d\mathbf{r}, \quad (2)$$

$$F(\omega, \mathbf{n}, \mathbf{n}_0) = \frac{1}{N_b} \left| \int \rho(\mathbf{r}) \mathbf{f}(\mathbf{r}) e^{-i\mathbf{k}\mathbf{r}} d\mathbf{r} \right|^2, \quad (3)$$

where $\mathbf{k} = \mathbf{n}\omega/c$, $\mathbf{f}(\mathbf{r}_a) = [\tilde{\mathbf{E}}(\omega) \times \mathbf{n}]$,

$$\tilde{\mathbf{E}}(\omega) = \int_{-\infty}^{+\infty} \left(\mathbf{E}(\mathbf{r}_{a,e}, t) - \frac{1}{2} \nabla_a \left(\frac{\mathbf{E}(\mathbf{r}_{a,e}, t)}{c} \right)^2 \right) e^{i\omega t} dt,$$

where $\nabla_{a,e} = \partial/\partial \mathbf{r}_{a,e}$.

Furthermore, $\delta N(\mathbf{p})$ in (2) is a factor which completely determines the geometrical arrangement of the atoms in the target, which is calculated in general form

$$\delta_N(\mathbf{p}) = \sum_{a,b} e^{i\mathbf{p}(\mathbf{R}_a - \mathbf{R}_b)} = \left| \sum_a e^{i\mathbf{p}\mathbf{R}_a} \right|^2. \quad (4)$$

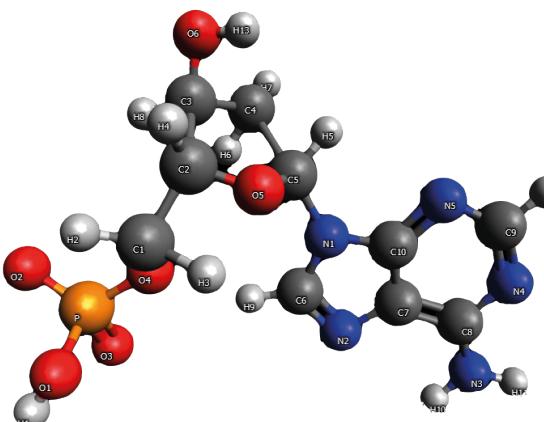


Fig. 1. 3D model of the nucleotide: C corresponds to carbohydrate, N to nitrogen, O to oxygen, P to phosphorus, H to hydrogen
[source: Avogadro software]

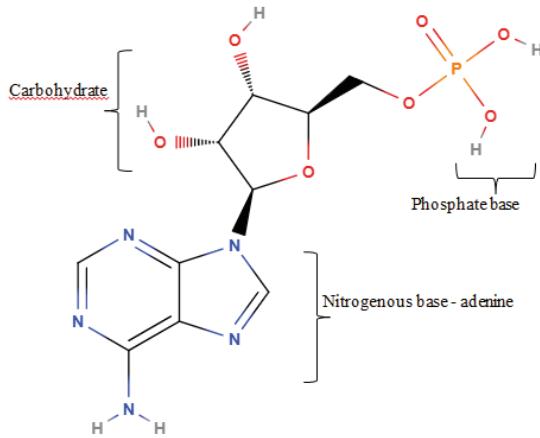


Fig. 2. Arrangement of atoms in a nucleotide: C corresponds to carbohydrate, N to nitrogen, O to oxygen, P to phosphorus, H to hydrogen
[source: Avogadro software]

The summation in (3) is carried out for all atoms of the system in question. The electron density can be taken in different models. We will use the Dirac–Hartree–Fock–Slater model from [7]:

$$\rho(\mathbf{r}) = \frac{N_e}{4\pi r} \sum_{i=1}^3 A_i \alpha_i^2 e^{-\alpha_i r},$$

where A_i , α_i are the table coefficients giving the electron density in the atom [7]. In our case we cannot use this form of electron density since the base of the molecule consists of different elements. Let us present a 3D model of the nucleotide (Fig. 1.). Using the given distances of 1.372 Å between the elements and their coordinates in space we will find the electron density.

In general, phosphate consists of 5 atoms bonded together by covalent bonds. The covalent radius of oxygen is 73 pm, the radius of the atomic nucleus is 3.27 fm, for phosphorus respectively 106 pm and 3.27 fm. The radius of the atomic nucleus is calculated as , where A is the number of nucleons. We can assume that the nuclei of atoms are at a distance many times larger than their own radius.

Results and Discussion

Let us set in Avogadro the coordinates of all elements. Then the electron density of the phosphate group will take the form.

$$\rho(\mathbf{r}_{ph}) = \rho_1(\mathbf{r}_1) + \rho_2(\mathbf{r}_2) + \rho_3(\mathbf{r}_3) + \rho_4(\mathbf{r}_4) + \rho(\mathbf{r}_i), \quad (5)$$

where is the electron of the relevant element

$$\rho_1(\mathbf{r}_1) = \frac{N_e}{4\pi(r)} A_p \alpha_p^2 e^{-\alpha_p r}. \quad (6)$$

We will use the following data for further calculations (Table 1).

Then the expression $G_i(\omega, \mathbf{n}, \mathbf{n}_0)$ for each atom, taking formula (4) into account, will take the form:

$$G_i(\omega, \mathbf{n}, \mathbf{n}_0) = \frac{1}{N_e} \int \rho_i(\mathbf{r}) |\mathbf{f}(\mathbf{r})|^2 d\mathbf{r}, \quad (7)$$

For the whole phosphate group, let us do the summation:

$$G_{ph}(\omega, \mathbf{n}, \mathbf{n}_0) = \sum_{i=1}^5 G_i(\omega, \mathbf{n}, \mathbf{n}_0), \quad (8)$$

Using this model it is possible to find expressions $G_i(\omega, \mathbf{n}, \mathbf{n}_0)$ for and go on to further calculate the interaction of USPs with the molecule.



Table 1
Distribution of atoms at the base
of adenines by coordinates

Number	Element	X(A)	Y(A)	Z(A)
Atom 1	H	-1.547	9.377	-1.216
Atom 2	O	-1.44	8.896	-0.401
Atom 3	P	0.038	8.907	0.116
Atom 4	O	0.220	10.175	0.734
Atom 5	O	0.790	8.733	-1.239
...				
Atom 34	H	2.147	0.165	2.718
Atom 35	H	1.815	6.312	5.385

Conclusion

The paper considers the probability of photon emission of a given frequency during the interaction of USPs with the nitrogenous base of DNA molecule, adenine. The peculiarities of the calculation of complex molecule with different elemental chemical composition were pointed out. A method of quantitative finding of electron density to refine the probability calculation is proposed.

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