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Article

Scattering of Ultrashort Laser Pulses on DNA and RNA Trinucleotides

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Abstract: X-ray diffraction (XRD) analysis of complex poly-atomic systems, especially of biomolecules, using ultra-short laser pulses (USP), is currently one of the most important fields of modern physics. The basis for interpreting and "deciphering" experimental data is the well-known theory of X-ray scattering, where the main parameter of USPs - its duration - is not taken into account. In the present work it is shown that for scattering of attosecond USPs on DNA and RNA trinucleotides the pulse length is the most important scattering parameter. In this case the diffraction pattern significantly changes with respect to the previously known scattering theory. The results obtained are extremely important in XRD when using attosecond pulses to study trinucleotides of DNA and RNA because using the previously known scattering theory which does not take into account the duration of USPs one can not correctly interpret and therefore "decode" DNA and RNA structures.

Keywords: X-ray scattering; DNA; RNA; X-ray diffraction; ultrashort pulse; trinucleotides; CCG, CGG, CAG, CUG

1. Introduction

It is well known that X-ray diffraction analysis (XRD) is the primary method of determining the structure of matter [1–4]. The structures of most crystals and complex biomolecules such as deoxyribonucleic acid (DNA) and ribonucleic acid (RNA) have been determined using this method. The theoretical basis for diffraction analysis dates back to the work of Max von Laue, who won the Nobel Prize in Physics in 1914 for the discovery of how X-rays can diffract on crystals [2]. The importance of this area can be estimated by the number of Nobel Prizes awarded for work related to X-ray crystallography, of which there are now more than 20. The key quantity in X-ray scattering is the scattering spectrum which is related to the Fourier transform of the electron density distribution $\rho(\mathbf{r})$ in matter as follows [5,6]

$$\frac{d\varepsilon}{d\Omega} = \frac{d\varepsilon_e}{d\Omega}\left|\rho(\mathbf{r})e^{i\mathbf{pr}}d^3r\right|^2, \tag{1}$$

where $\frac{d\varepsilon_e}{d\Omega}$ is the scattering spectrum of a free electron (Thomson scattering), $\mathbf{p}$ is the momentum transferred to the electron during light scattering (otherwise $\mathbf{p} = \frac{2\pi}{\lambda}(\mathbf{n} - \mathbf{n}_0)$ is the scattering vector, where $\mathbf{n}$ is the direction of scattered radiation, $\mathbf{n}_0$ is the direction of the primary radiation), Ω is the solid angle at which scattering occurs. Using known methods [7] it is possible to determine $\rho(\mathbf{r})$ from the scattering pattern of X-rays. The surprising result is that Eq. (1) can be derived from the classical description of electromagnetic radiation scattered by stationary electron density $\rho(\mathbf{r})$, which gives a result identical to that obtained with the quantum electrodynamic description of scattering [5]. The simplicity of the Eq. (1) has given it wide distribution in XRD using not only conventional X-ray sources, but also sources generating ultra-short X-ray pulses (USPs). Although one can see that the Eq. (1) does not contain values characterizing USPs and this question deserves a separate consideration. Indeed, particular attention is now being paid to the physics of ultrashort pulses, namely, the methods for generating such pulses and their interaction with matter [8–10]. Using such USPs, one can investigate the structure of complex substances with an advanced structure with high temporal and spatial resolution. Moreover, it is now technically possible to carry out such studies, e.g. using XFELs [11] free electron lasers. Such lasers can generate USPs not only of femtosecond but also of attosecond duration [12,13]. Despite this, old theoretical approaches for "deciphering" polyatomic system structures based on the use of Eq.(1), which do not take into account the features of interaction of such USPs with complex polyatomic structures are currently used [6,14–17].

Recently it has been shown in [18–20] that there are important cases where the specific scattering of USPs must be taken into account and consequently the use in diffraction analysis of Eq. (1) gives large errors. Basically such errors appear in scattering of attosecond USPs on certain kinds of structures. Such structures have been shown to include DNA and RNA nucleotides etc. Thus, it is important to study structures where previously known diffraction analysis theory would give wrong results. By using such erroneous results when "deciphering" structures, it is possible to incorrectly identify the structures of the object under study. An interesting system to study scattering is DNA and RNA molecules. The spatial position of atoms in it carries information about an organism's genome, its possible diseases and development programme. This data is stored as a code - a specific sequence of nucleotides. Let us look at some of the trinucleotides in DNA and RNA: CCG, CGG, CAG, CUG. Trinucleotides or triplets are repetitive regions in a molecule. The arrangement of triplets indicates the presence or absence of DNA and RNA mutations [21]. The mechanism of repeat formation is not fully known, but research in this area is actively pursued [22,23]. Excessive repetition of trinucleotide repeats causes various neurodegenerative diseases that are currently considered incurable: mental retardation (CCG repeats >200), Baratella-Scott syndrome (CGG repeats > 100), Huntington's disease, etc. [24,25]. Changes in the number of triplet repeats should be reflected in scattering spectra. Therefore, it is highly relevant to know the exact structure of such triplets, as well as the disruption of these structures in DNA and RNA molecules.

This paper shows that the duration of USPs when scattered on trinucleotides DNA and RNA: CCG, CGG, CAG, CUG is one of the most important features when using attosecond pulses. If the pulses are much longer than attosecond pulses the duration parameter is not essential in the scattering picture and Eq. (1) can be used. The results obtained indicate that to use Eq. (1), on the basis of which complex molecules and biomolecules are "decoded", should be used with great caution in the case of attosecond USPs.

Next, we will use the atomic system of units: $\hbar = 1$; $|e| = 1$; $m_e = 1$, where $\hbar$ is the Dirac constant, e is the electron charge, m_e is the electron mass.

2. Scattering of ultra-short laser pulses

Consider the DNA and RNA trinucleotides: CCG, CGG, CAG, CUG, on which the USP falls in the $\mathbf{n}_0$ direction, see Figs 1-4. We will use the sudden perturbation approximation to find the scattering spectra of USPs. It is assumed that the duration of the ultrashort pulse τ is many times shorter than the characteristic atomic time $\tau_a \sim 1$, i.e. $\tau \ll \tau_a$. As has been shown in [26] that the condition of applicability of the sudden interaction approximation $\tau \ll \tau_a$ need not be fulfilled in the case of X-ray USPs. It has also been shown [26,27] that for X-ray USPs it is sufficient to assume that $\omega_0 \tau_a \gg 1$, where ω_0 is the carrier frequency of incident USPs, to extend the sudden perturbation theory to the case of X-ray USPs. In other words, it is sufficient to consider USPs as multi-cycle. We will consider the USP as spatially inhomogeneous, i.e. the USP electromagnetic field strength should be chosen as $\mathbf{E}(\mathbf{r}, t) = \mathbf{E}_0 h(t - \mathbf{n}_0\mathbf{r}/c)$, where $\mathbf{E}_0$ is the field amplitude, $h(t - \mathbf{n}_0\mathbf{r}/c)$ is the arbitrary function defining the USP shape, c is

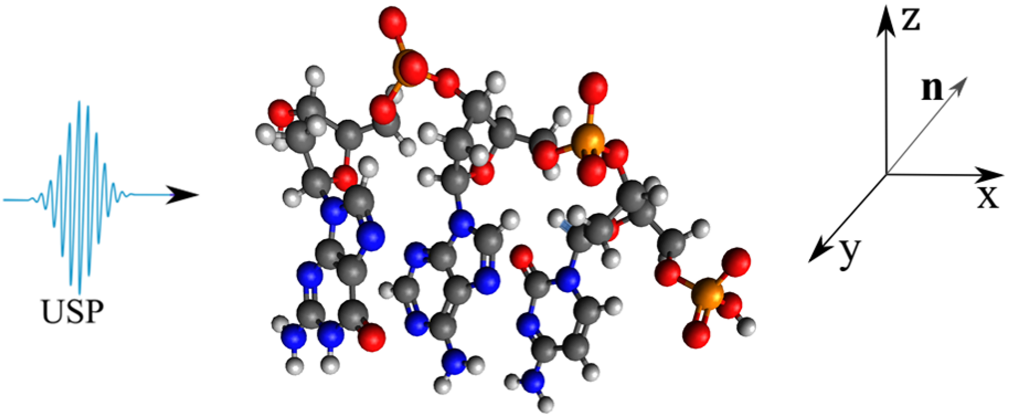

Figure 1. The CAG trinucleotide on which the USP falls is depicted, along with the selected coordinate system. The scattering spectra were calculated in the spatial orientation of the CAG with respect to the USP in the selected coordinate system shown in this figure. The red balls are oxygen atoms (*O*), the yellow ones are phosphorus (*P*), the blue ones are nitrogen (*N*), the light grey ones are hydrogen (*H*) and the dark grey ones are carbon (*C*).

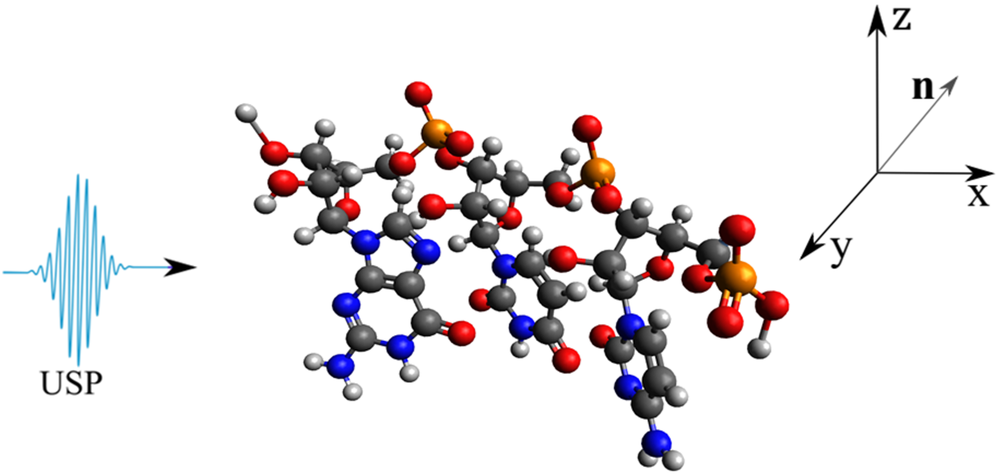

Figure 2. The same as in Fig. 1, but only for trinucleide CUG.

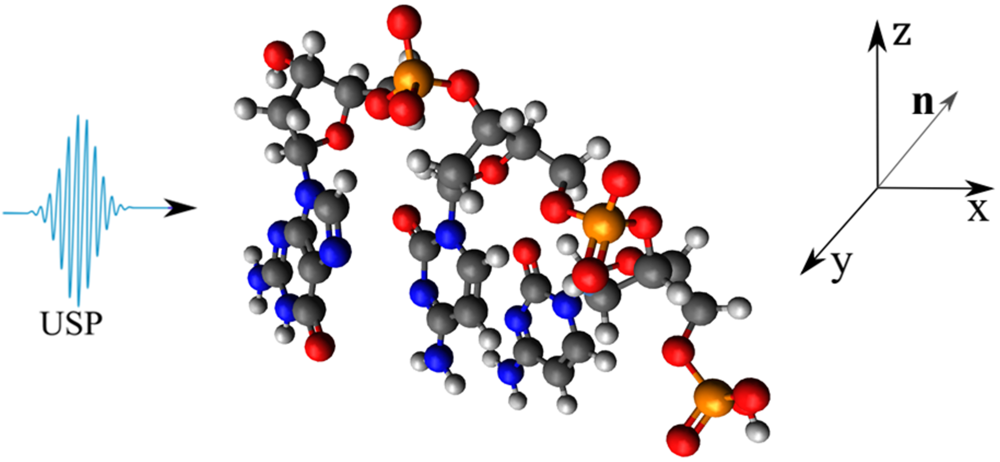

Figure 3. The same as in Fig. 1, but only for trinucleide CCG.

the light speed (in a. e. $c \approx 137$). Currently, the USPs intensities at the most powerful XFELs where matter structure studies are carried out do not exceed $10^{23} W/cm^2$. In this case (more correctly said at I $\ll 10^{25}$W/cm^2), as shown in [18,19,27], the magnetic component of the USP can be neglected. In this case, the scattering spectra (scattered

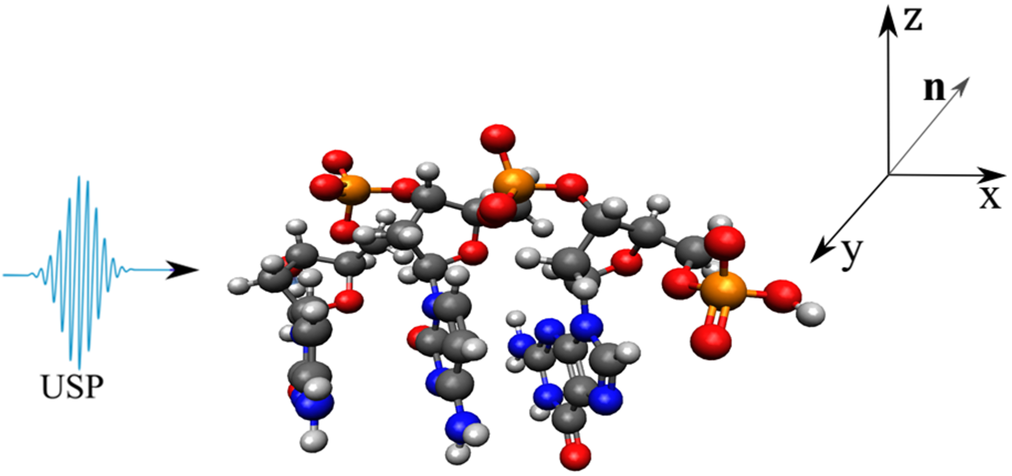

Figure 4. The same as in Fig. 1, but only for trinucleide CGG.

energy USPs per unit solid angle in the unit frequency interval) can be represented as [18,19,27,28]

$$\frac{d^2\varepsilon}{d\Omega_{\mathbf{k}}d\omega}=\frac{[\mathbf{E}_0\mathbf{n}]^2}{(2\pi)^2}\frac{|\tilde{h}(\omega)|^2}{c^3}\left[\sum_{i=1}^{s}N_{e,i}N_{A,i}(1-|F_i(\mathbf{p})|^2)+\sum_{i,j=1}^{s}\delta_{i,j}N_{e,i}N_{e,j}F_i(\mathbf{p})F_j^*(\mathbf{p})\right], \quad (2)$$

where $N_{A,i}$ is the number of atoms i variety; $N_{e,i}$ is the number of electrons in the atom i variety; summing over all atoms (i,j) up to s; $\tilde{h}(\omega)=\int\limits_{-\infty}^{+\infty}h(\eta)e^{i\omega\eta}d\eta$, and $\mathbf{p}=\frac{\omega}{c}(\mathbf{n}-\mathbf{n}_0)$ has the meaning of recoil momentum when a USP is scattered on a bound electron; $F_i(\mathbf{p})=\frac{1}{N_{e,i}}\int\rho_{e,i}(\mathbf{r})e^{-i\mathbf{pr}}d^3\mathbf{r}$ is the form factor of the i atom of the variety with electron density $\rho_{e,i}(\mathbf{r})$. In Eq. (2) factor $\delta_{i,j}=\sum_{Ai,A'j}e^{-i\mathbf{p}(\mathbf{R_{Ai}}-\mathbf{R_{A'j}})}$ is a crucial quantity in USPs scattering since it depends only on the position of atoms in space, i.e., on the coordinates of the atoms i of the variety (with number Ai) whose position in space is determined by the radius vector $\mathbf{R}_{Ai}$ It is known that the case of main interest for XRD is at $\tau\omega_0\gg1$, i.e. USP and is multicycle. If we make the assumption that $\tau\to\infty$, then we obtain the previously well known XRD theory where the radiation source is continuous. For the calculation we will use the so-called Gaussian USP, which is the USP where the shape has a Gaussian envelope, i.e. i.e. $h(t)=e^{-i(\omega_0t-\mathbf{k}_0\mathbf{r})}e^{-\alpha^2(t-\mathbf{n}_0\mathbf{r}/c)^2}$, where $\alpha=1/\tau$, $\mathbf{k}_0=\mathbf{n}_0\omega_0/c$. It should be added that such a USP is one of the best known for describing the shape of USPs and is often used in theoretical analysis. For example, in [29], based on exact solutions of the electromagnetic field equations, it was shown that at $\omega_0/\alpha\gg1$, the solution takes the form of a simple Gaussian USP. In this case it is not difficult to show that $\tilde{h}(\omega)=\frac{\sqrt{\pi}}{\alpha}e^{-(\omega-\omega_0)^2/4\alpha^2}$. The condition $\omega_0/\alpha\gg1$ is exactly the same as the multi-cycle USP mainly used in XRD. In this case it is not difficult to obtain the full scattering spectrum using Eq. (2) in the form

$$\frac{d\varepsilon}{d\Omega_{\mathbf{k}}}=\frac{[\mathbf{E}_0\mathbf{n}]^2}{4c^3\alpha\sqrt{2\pi}}\left[\sum_{i=1}^{s}N_{e,i}N_{A,i}(1-|F_i(\mathbf{p}_0)|^2)+\sum_{i,j=1}^{s}\gamma_{i,j}(\mathbf{p}_0,\mathbf{p}_\tau)N_{e,i}N_{e,j}F_i(\mathbf{p}_0)F_j^*(\mathbf{p}_0)\right],$$

$$\gamma_{i,j}(\mathbf{p}_0,\mathbf{p}_\tau)=\sum_{Ai,A'j}e^{-i\mathbf{p}_0(\mathbf{R}_{Ai}-\mathbf{R}_{A'j}))}e^{-\frac{1}{2}(\mathbf{p}_\tau(\mathbf{R}_{Ai}-\mathbf{R}_{A'j}))^2}. \quad (3)$$

where $F_i(\mathbf{p}_0),\delta_{i,j}(\mathbf{p}_0)$ at $\mathbf{p}_0=\frac{\omega_0}{c}(\mathbf{n}-\mathbf{n}_0)$ and $\mathbf{p}_\tau=\frac{1}{c\tau}(\mathbf{n}-\mathbf{n}_0)$. The electron density of the atoms $\rho_{e,i}$ variety i will be chosen in the independent atom model [30]. In this case we get $\rho_{e,i}(\mathbf{r}) = \frac{N_{e,i}}{4\pi r}\sum_{k=1}^{3} A_{k,i}\alpha_{k,i}^{2}e^{-\alpha_{k,i}r}$, where $A_{k,i}, \alpha_{k,i}$ are constant coefficients defined in [30].

In Eq. (3) contains characteristics which are responsible for the duration of the τ USP, and hence the specificity of the USP scattering on the system under study is taken into account. In doing so, one can see that if in Eq. (3) increase $\tau \to \infty$, we get the well-known Eq. (1), see eg [19]. This is not difficult to show if $\tau \to \infty$, with $\mathbf{p}_\tau = \frac{1}{c\tau}(\mathbf{n} - \mathbf{n}_0) \to 0$ and Eq. (3) becomes proportional to τ (Fermi's golden rule). And Eq. (1) in this case, exactly corresponds to the golden Fermi rule. It can be shown qualitatively that the pulse duration τ becomes an important scattering parameter only for attosecond and shorter pulses. For this purpose one can see that in the parameter $\gamma_{i,j}(\mathbf{p}_0, \mathbf{p}_\tau)$ in Eq. (3) there is an important factor $e^{-\frac{1}{2}(\mathbf{p}_\tau(\mathbf{R}_{Ai}-\mathbf{R}_{A'j}))^2}$ which is close to unity for small $\mathbf{p}_\tau(\mathbf{R}_{Ai} - \mathbf{R}_{A'j}) \ll 1$. A small value of $\mathbf{p}_\tau(\mathbf{R}_{Ai} - \mathbf{R}_{A'j}) \ll 1$ will almost always be if the pulses are many times longer than attosecond pulses, since in this case $\mathbf{p}_\tau \lesssim 10^{-4}$. If we choose shorter attosecond pulses, then $\mathbf{p}_\tau \gtrsim 10^{-2}$, which leads to considerable values of $\mathbf{p}_\tau(\mathbf{R}_{Ai} - \mathbf{R}_{A'j})$ for multi-atomic systems. In this case, the duration of the USP cannot be neglected. Of course, this is a qualitative analysis and one can only say more accurately about the effect of pulse duration after calculations using Eq. (3) . Although one can quite confidently state that the duration of USPs must be taken into account only for attosecond and shorter pulses. It is also possible to explain qualitatively in terms of physics why the duration of USPs can significantly affect the scattering spectra and why Eq.(1) is not always correct. When some fraction of atoms in the matter fall into a spatial region of USP size ($\sim c\tau$), the emission is coherent from this region. Accordingly, if the duration of the USP is large, i.e. $\tau \gg 1$, then the region where emission occurs coherently is also large. In Eq.(1) such a region where radiation occurs coherently is infinitely large. This will indeed be true in the case of USP when the region ($\sim c\tau$) captures the whole system (molecule, nanosystem, etc.) under study. If, on the contrary, when the $\sim c\tau$ region captures a smaller region than the size of the system being studied, there will be no coherent emission from that whole system. That is why the study of USP scattering by bimolecules, especially DNA and RNA, will be relevant, since such molecules are quite large and the size of the attosecond pulse $\sim c\tau$ becomes smaller than the size of the molecule itself. This is a very important refinement because when using attosecond pulses in XRD one must take into account the duration of the USP, which is not taken into account in Eq. (1). This in turn leads to incorrect determination of the matter structure using Eq. (1).

3. Results: Scattering of USPs on trinucleotides of DNA and RNA.

Let us perform USP scattering calculations on the systems shown in Figs.1-4 and show that for such systems the use of Eq. (1) introduces large errors. Calculations of scattering spectra using Eq. (3) are shown in Figs.5-8. In the calculations, the USP was assumed to fall as shown in Figs.1-4 with photon energy $\hbar\omega_0 = 7.46\ keV$, pulse duration $\tau = 1$(as). From the Figs. 5-8 we can see that the scattering spectra in the case of using Eq. (3) and Eq. (1) are significantly different. The central peaks, no matter how the calculations were carried out, are always close to each other and this is well explained, since this peak is directed in the direction of the incident USP $\mathbf{n}_0$. Indeed, it is quite obvious that most of the USP will scatter in the direction $\mathbf{n}_0$. Other diffraction peaks already differ essentially from each other, and when scattering to more angles they differ even qualitatively, i.e. the scattering is different. At this it is possible to notice the same regularity at scattering irrespective of investigated trinucleotides is the reduction of peaks in a diffraction picture at the big angles of scattering in case of using Eq. (3). This reduction of peaks in the diffraction pattern can be explained by the influence of the pulse duration on the scattering spectra.

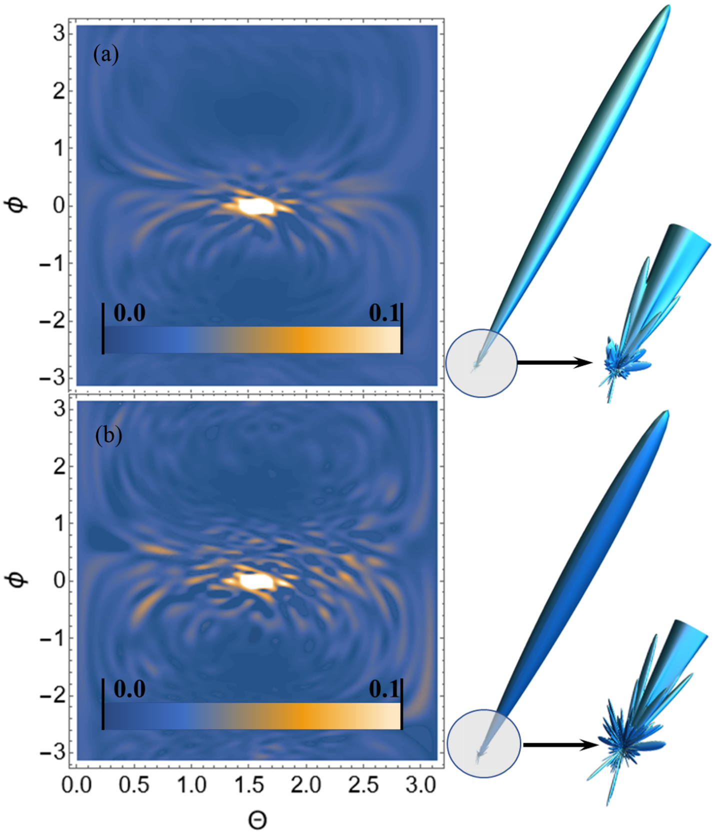

Figure 5. USP scattering spectra on the CAG trinucleotide: (a) calculated using the formula Eq. (3), (b) calculated by Eq. (1). The spectra are presented as 2D (left) and 3D (right) plots. The 2D plots are presented in dimensionless units and normalised to the maximum value of the spectrum. The angles ϕ, θ are spherical angles in the coordinate system shown in Fig. 1.

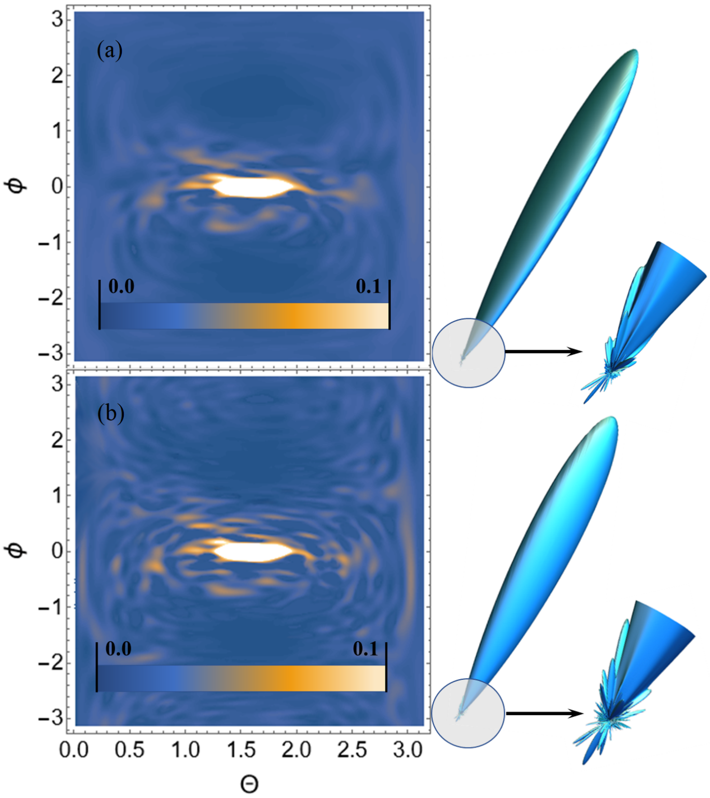

Figure 6. The same as in Fig. 5, but only for trinucleide CUG.

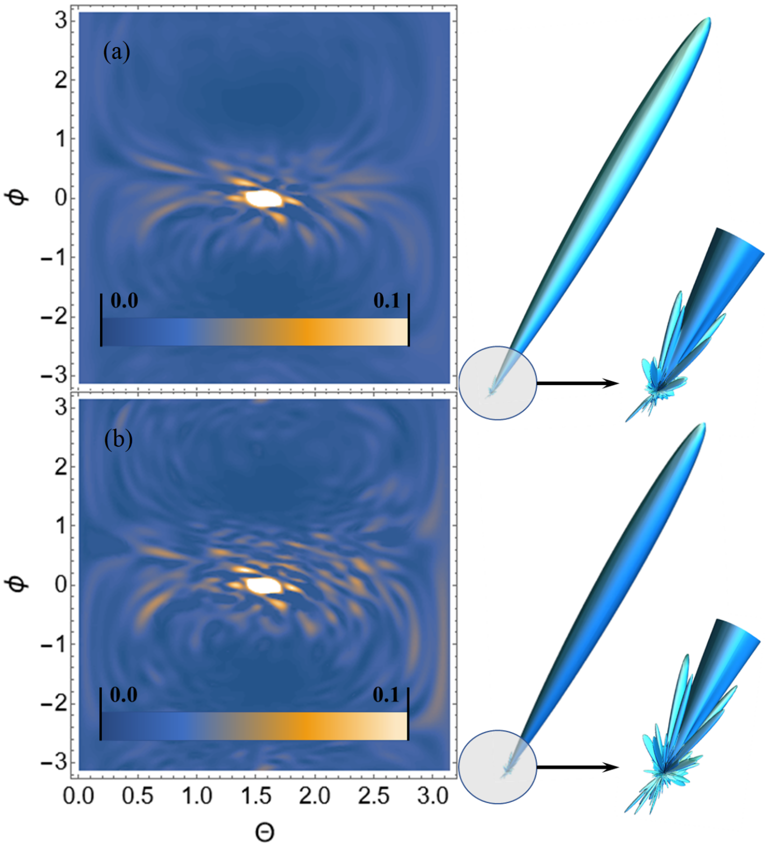

Figure 7. The same as in Fig. 5, but only for trinucleide CCG.

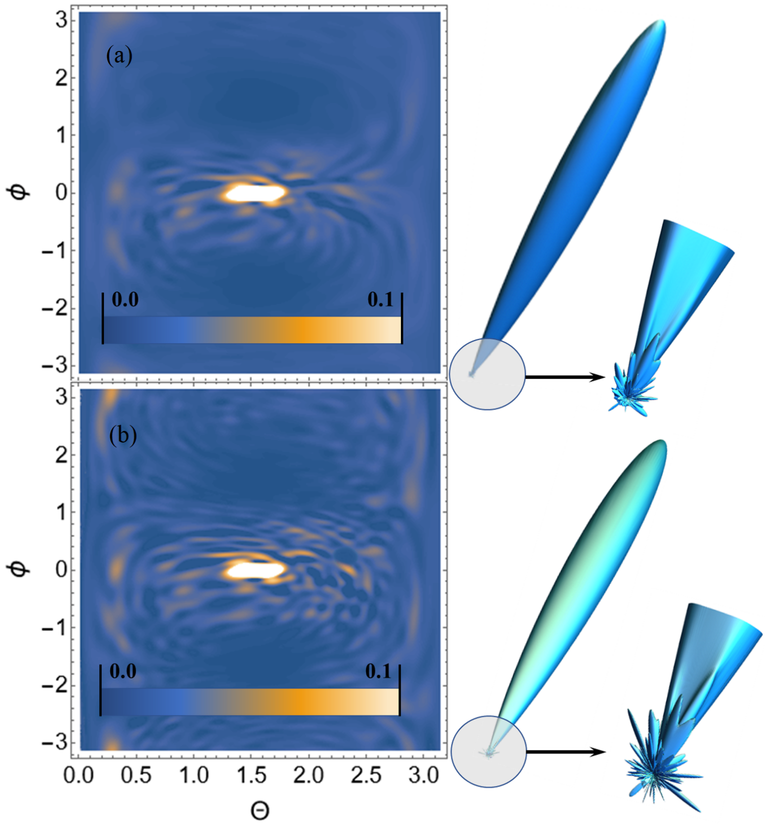

Figure 8. The same as in Fig. 5, but only for trinucleide CGG.

4. Conclusion

Thus, comparing the results of the calculations and the analysis of Eq. (3) we obtained an important conclusion. In the case of attosecond USPs scattering on DNA and RNA trinucleotides: CCG, CGG, CAG, CUG, the duration of the USPs is an important parameter in scattering and to use the previously known Eq. (1) in XRD is not correct. It should be added that this conclusion would have even more significance if we consider that the use of Eq. (1) in XRD has been some standard for many years. Our approach, presented here, for a sufficiently long USP and a multi-atom system, passes to the previously known theory, i.e. Eq. (3) becomes equal to Eq. (1). Thus Eq. (3) is more general in XRD theory, where the previous theory is a special case of the theory presented here. Obviously, in the case of using attosecond pulses, as explained above, to determine structures of more complex molecules than those considered here, the conclusions may be the same.

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