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Towards the control of photo-ionization with electron wave-packet interferences

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Contents

Abstract

In this work the photoelectric effect is explored through simulations of the phase shift that an IR-field can induce into an electron wave packet and the photoelectron distribution over frequency components that is produced in the photoionization of an atom with a attosecond pulses made of XUV photons. The IR-field is sent along two attosecond pulses made of XUV photons towards a 3D momentum spectrometer were there is a gas that can be photoionized and the photoelectrons can be measured. The IR-field gives a phase shift to an electron wave packet (photoelectron). The XUV attosecond pulses can be Fourier transformed from time to frequency domains enabling to know the temporal structure and the spectrum of light fields. The kinetic energy distribution of the photoelectron is closely related to the XUV light field distribution in the frequency domain (spectrum), by applying the Einstein equation. However the intensity of the kinetic energy distribution follows the rules of quantum mechanics, and not the rules of optics. This study shows that analogies can be done within the framework of the strong field approximation.

The simulated photoelectron distribution over frequency components were simulated with an IR-field with a wavelength of 820 nm, an intensity of 10^{12} W/cm^2, a momentum of 1.9 $\cdot 10^{-24}$ kg·m/s and a standard deviation of 0.3 PHz. The attosecond pulses made of XUV photons were set to have a standard deviation of 30 PHz and a frequency of 100 PHz. The separation between the attosecond pulses made of XUV photons was set to 1.3 fs. The phase shifted attosecond pulses made of XUV photons were plotted in order to give a picture of them. Then there Fourier transform was presented together with the phase shifts that was put into each XUV attosecond photon pulse. In the case with two attosecond pulses made of XUV photons the Fourier transform had to be shifted in time in order to make the result reasonable. In the case of two attosecond pulses made of XUV photons interesting patterns in the photoelectron distribution over frequency components occur. In order to explore the photoelectron distributions deeper more phase shifts have to be used in attosecond pulses made of XUV photons and then Fourier transformed. Thus giving more photoelectron distributions that can be studied.

1   Motivation

The phenomenon of photoionization was first discovered by the physicist Heinrich Rudolf Hertz, in 1887. In 1905, Albert Einstein proposed an explanation to this phenomenon, connecting the discovery of H.R. Hertz to the work of Max Planck. Later in 1916, the physicist Robert Millikan performed the first experiment that could confirm the prediction of A. Einstein by measuring the Planck constant, h, with photoionization [5]. With the emergence of extreme ultraviolet (XUV) attosecond (10^{-18} s) pulses at the beginning of the millennium, the possibility to control photoionization was envisioned. In recent years, experiments made in Lund [6] achieved control over photoinization by combining the XUV radiation with an Infra-Red (IR) laser beam.
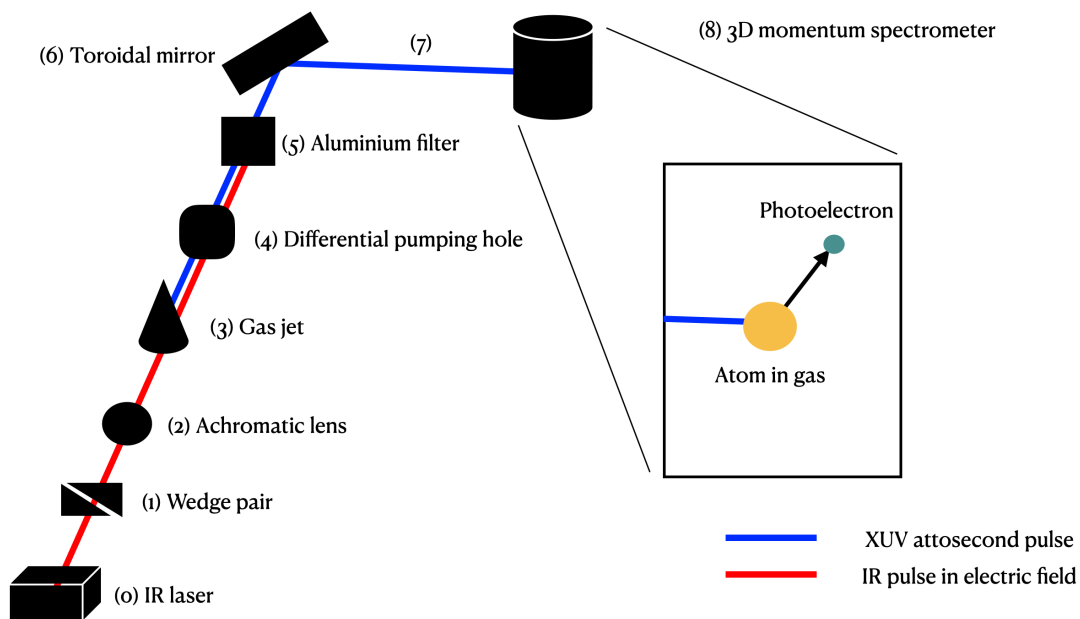

Figure 1: Set-up used in the experiment referred to in this work. Before the wedge pair there is a pulses-shaped electric field indicated, here IR-pulses are coming from the laser (0). (1) Wedge pair which an Infra-red (IR) laser goes into. (2) Achromatic lens which focuses the light. (3) High pressure jet of argon gas, where XUV attosecond pulses are generated. To separate the XUV and IR fields, the beams are sent into (4) which also acts as a differential pumping hole. After that an Al (aluminium) filter (5) is there to take completely away the IR field. (6) Toroidal mirror which focuses the XUV attosecond pulses in the experimental chamber where a 3D momentum spectrometer (8) is used to study the ionization of helium. It is the photoionization in (8) that is simulated in this work but the IR-field is then let in to (8) along with the XUV attosecond pulses. [6]

Here is a short summary of the important parts shown in Fig.1, that is relevant for this work:

- Before the wedge pair (1) there is a laser (0) sending a pulse in the IR-field (infra-red electric field) into the experimental setup. Different values for this electric field will be varied in the beginning of this work giving different phase shifts to an electron wave packet.

- In (3) the attosecond pulses made of XUV photons are created and together with the IR-field they can travel into the toroidal mirror (6) and be focused. Giving that in the ray of light that is (7) there can be attosecond pulses made of XUV photons together or not together with an IR-field (the IR-field can be filtered out).

- The electric field that is in (7) then travels into (8) where the attosecond pulses made of XUV photons photoionize the gas that is in there. This process produces electrons that can be phase shifted by the IR-field.

In the following figure three electron wave packets along with an IR-field is shown.
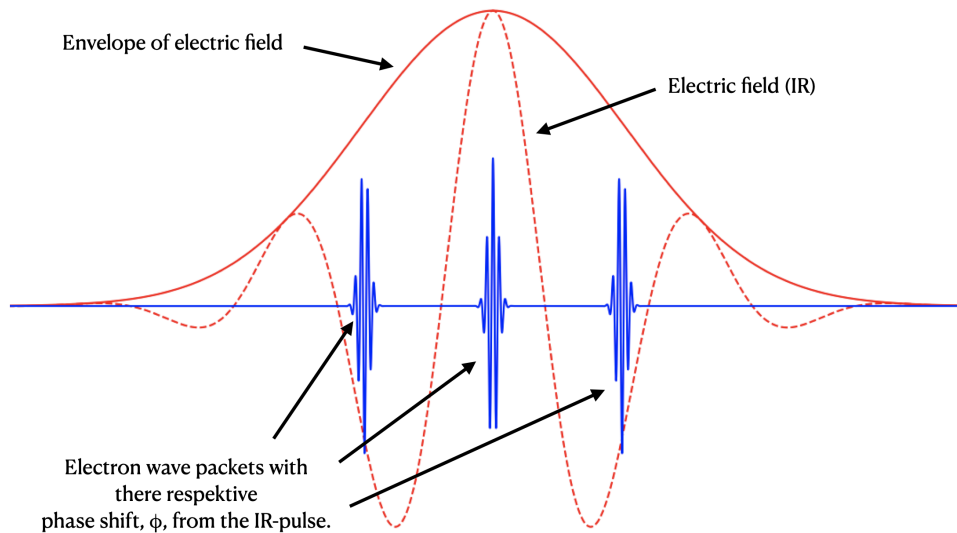

Figure 2: In this figure three electron wave packets together with an IR-field is shown. The amplitude of the electron wave packets, EWPs, is different from the one for the IR-field to point out that they are describing different particles.

For different positions in time the EWP gets a phase shift corresponding to the amplitude of the IR-field. The phase shift is calculated through a formula that will be presented later. More importantly is that the EWP is created at the time when a XUV photon attosecond pulse photoionize an atom. Having two XUV photon attosecond pulses with a separation of 1.3 fs (which will be looked at later) would in the figure above correspond to having two EWPs. Each EWP separated by 1.3 fs and each EWP at the same position in time as the corresponding XUV photon attosecond pulse.

The process of photoionization and the electron wave packet picking up the phase shift from the IR-field can be formulated as follows.

- Step 1: Atom + h·f$_{XUV}$ $\Rightarrow$ Atomic Ion + Electron Wavepacket

- Step 2: Atomic Ion + Electron Wavepacket+ h·f$_{IR}$ $\Rightarrow$

    Atomic Ion + Phase modulated Electron Wavepacket

The XUV attosecond pulses originates from high-harmonic generation in gases using an ultra-short near infra-red laser. Fig.1 illustrates this process, where the carrier-to-envelope phase of the laser is adjusted (1) before being focused (2) into an argon gas jet (3). The XUV radiation is spatially filtered from the Infrared laser at (4) and (5) and then refocused (6) in the experimental chamber (8) where an electron spectrometer allows to study the interaction of XUV attosecond pulses with an atomic target in a gas.

2   Theory

The formulas used in this report will be presented in this section. There will be subsections to group the formulas in order to keep a better overview of them. The first section being "Light field".

2.1   Light field

Starting with some basic but important relations used through out the work. Through the following formula the electric field is given.

$$E(t) = -\frac{\partial}{\partial t}A(t) \tag{1}$$

where E is the electric field only dependent on time t and A is the vector potential [1]. This means that the vector potential is calculated through integrating the electric field, as follows.

$$A(t) = -\int_{\mathcal{O}}^{t} E(t')dt' . \tag{2}$$

Where $\mathcal{O}$ is a point in time where the primitive function to $E(t')$ is 0.

In this work the following formula relating the averaged intensity to the magnitude of the electric field will be used.

$$I = \frac{1}{2}c\epsilon_0 E_0^2 \Rightarrow E_0 = \sqrt{\frac{2I}{c\epsilon_0}} \tag{3}$$

where c is the speed of light, ϵ_0 is the permittivity of vacuum and E_0 is the magnitude of the electric field [1].

Below is the electric field of a train of pulses with the amplitude from Eq.3.

$$E(t) = \sqrt{\frac{2I}{c\epsilon_0}} \cdot \sum_{j=1}^{n} e^{i(\omega t + \phi_j)} e^{-\frac{1}{2}a^2(t-jT)^2} \tag{4}$$

where n is the number of pulses, i is the imaginary unit, ω is the angular frequency, ϕ_j is the phase shift for the j:th pulse, $a = 1/\sigma$ where σ is the standard deviation and T is the time between the pulses [4]. When using one pulse, ϕ_j and T could be set to 0.

For pulses that are separated in time, which is the case for the XUV attosecond pulses used later in this work, the following would be the case extrapolating from Eq.4.

$$E(t) = \sqrt{\frac{2I}{c\epsilon_0}} \cdot \sum_{j=1}^{n} e^{i(\omega(t-jT)+\phi_j)} e^{-\frac{1}{2}a^2(t-jT)^2} \tag{5}$$

In Fig.3 and Fig.4 some of the fundamental equations and electric fields used in this work are presented as graphs.
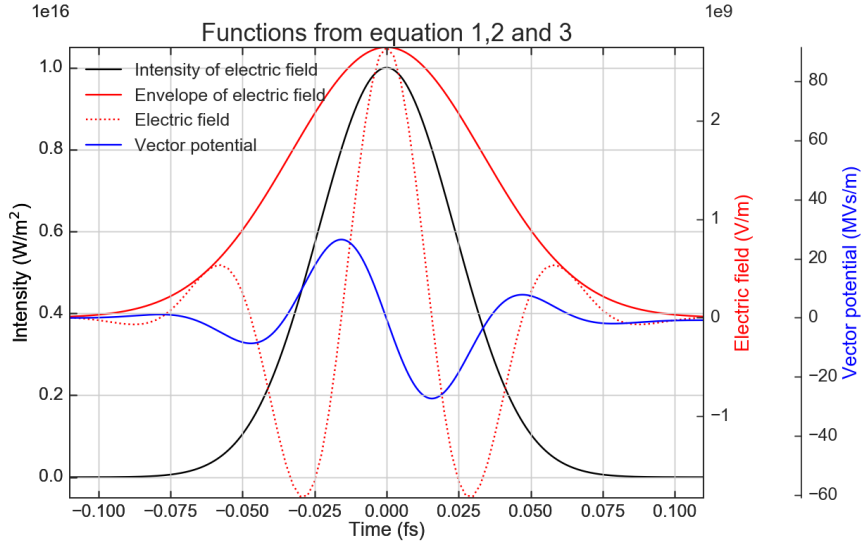
Figure 3: In this figure the vector potential that through Eq.1 gives the electric field and its envelope and through Eq.3 gives the intensity. The electric pulse has a frequency of 100 PHz (approximately a wavelength of 3 nm) and its inverse standard deviation from Eq.4 has been set to 30 PHz. The electric pulse with these values will be used in the result section of this work later.

Figure 4: In this figure an IR-filed and a XUV-filed both being pulses are shown. The XUV-field is the same as the electric pulse in Fig.3 but three of them instead of one and the IR-field has a wavelength of 820 nm and an inverse standard deviation of 0.5 PHz. The three attosecond pulses made of XUV photons are separated in time with 1.3 fs.

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2.2 Electron wave-packet

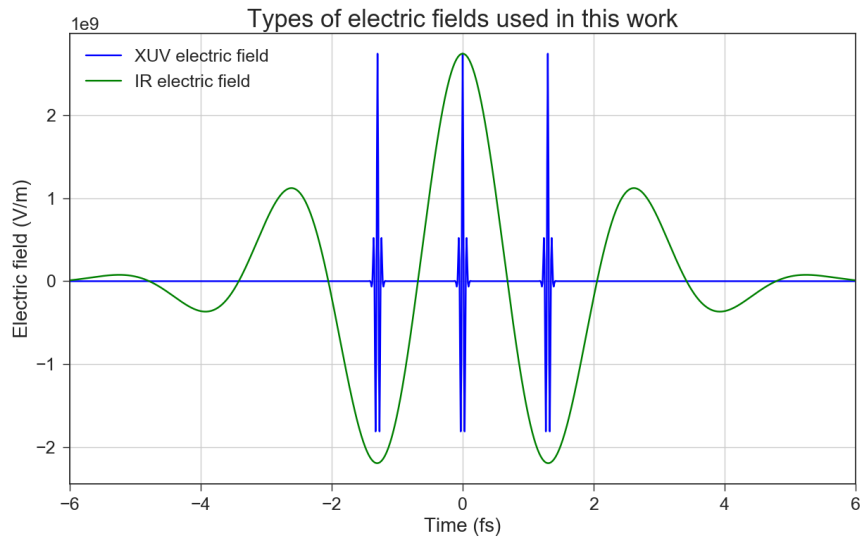An electron wave-packet is a way of describing an electron with a wave-packet. A wave-packet is composed of more than one wave. The waves build up the wave-packet together through superposition – also known as interference.

In this work XUV attosecond pulses will photoionize an atom and thus produce photo-electrons which also can be thought of as electron wave packets because of the wave-particle duality.

The following equation

$$i\frac{\partial}{\partial t}\psi(\bar{r},t) = \left[\frac{\hat{p}^2}{2} + \bar{A}(t)\cdot\hat{p} + \frac{\bar{A}(t)^2}{2}\right]\psi(\bar{r},t) \tag{6}$$

has a solution called the Volkow wave which describes a free electron interacting with an electric field. The Volkow wave is given by Eq.7.

$$\psi_V(\bar{r},t) = \frac{1}{(2\pi)^{3/2}}e^{i\left[\bar{q}\cdot\bar{r}-\int_0^t\left(\frac{q^2}{2}+\bar{A}(t')\cdot\bar{q}+\frac{\bar{A}(t')^2}{2}\right)dt'\right]} \tag{7}$$

where $\bar{q}$ is a wave vector, $\bar{r}$ is the spacial position as a vector, $\bar{A}$ is the vector potential and $\hat{p}$ is the momentum operator. [8]

2.3 Electron wave-packet phase modulation due to a laser field

When an atom or a molecule gets extra energy the electron can be emitted from the atom or molecule. If the energy given to the atom during photoionization is higher than the ionization potential, I_p, the electron gets free from the Coulomb field of the atom or molecule. The energy is given from a photon with energy hf, where h is the Planck constant and f is the frequency of the photon. The electrons kinetic energy is the difference between the energy of the photon and the energy of the ionization potential, $E_k = hf - I_p$. The kinetic energy, E_k, of the electron is connected to the electron velocity, v, as follow:

$$E_k = \frac{m_e v^2}{2} . \tag{8}$$

where m_e is the rest mass of the electron. Introducing the momentum of an electron

$$p = m_e v \,, \tag{9}$$

and inserting in into Eq.8, it gives how the momentum depends on the kinetic energy:

$$p = \sqrt{2E_k m_e} \,. \tag{10}$$

As discussed earlier, the electron will be influenced by a strong laser field, and will acquire a phase shift, Φ_{IR}, that is related to its travel in the oscillating electrical field[6]. This phase shift can be calculated as follows:

$$\Phi_{IR}(\bar{p}, t) = -\frac{e}{m_e \hbar} \int_t^\infty \bar{p} \cdot \bar{A}(t') dt' \tag{11}$$

where e is the electric charge of the electron, $\hbar$ is the reduced Planck constant divided by $\bar{p}$ is the momentum of the electron and $\bar{A}$ is the vector potential. This expression can be simplified to a 1-dimensional problem in the case of linearly polarized light and the electron emitted along this polarization axis.

An analytical expression can be found for this phase shift, in the case of a Gaussian pulse

$$\int_t^\infty e^{-\frac{1}{2}a^2 t'^2} \cos(\omega t') \, dt' = -e^{-\frac{1}{2}a^2 t^2} \sin(\omega t) \cdot \frac{1}{\omega} + 2\frac{a^2}{\omega^2} t \cos(\omega t) e^{-\frac{1}{2}a^2 t^2} \,. \tag{12}$$

On the left-hand side of Eq.12 the exponent of e has a t'^2 which can be changed to t'^{2n}, where n is an integer. This will give a new result on the right-hand side of Eq.12. The result will start with the same term as in the right-hand side of Eq.12 except for the exponent of e. Then there will be new terms which will all have a $1/\omega$ of order two ($(1/\omega)^2$) or higher. The angular frequencies, ω, when using XUV are on the order of PHz. Which means that the second term on the right-hand side in Eq.12 is on the order of 10^{-15} smaller than the first term on the same side in Eq.12. This would lead to the following – for XUV – good approximation up to 10^{-15}.

$$\int_t^\infty e^{-\frac{1}{2}a^2 t'^{2n}} \cos(\omega t') \, dt' \approx -e^{-\frac{1}{2}a^2 t^{2n}} \sin(\omega t) \cdot \frac{1}{\omega} \,. \tag{13}$$

2.4 Goal - Time Frequency analysis

In this work the phase shift from an applied IR-field (infrared) was one part of what was looked upon. This was to see how the phase shift varies over time but firstly the integrator that was used in the code was investigated to see what error it had. The test of the integrator was done through taking a function much like those that were used later for the phase shifts. This function was then differentiated by hand and then integrated with the integrator. The original function and the result of the integration was then plotted in one plot with the difference between the two functions in a plot below the first plot, section 3.2 Calculation of the phase modulation.

In the next step when plotting the phase shifts, parameters like wavelength, momentum and intensity was varied in order to visualize how the phase shift is dependent on them. Then the idea was to send in two XUV attosecond pulses. The XUV attosecond pulses got each their own phase shift shaped like the phase shift from an IR-field induced into an electron wave packet at the position that they were at with respect to the IR-filed. Through photoionization these phase shifted XUV attosecond pulses produce photoelectrons. The distribution of photoelectrons over frequency components was calculated through the Fourier transform of the phase sifted XUV attosecond pulses.

A complex function $f(t)$ can be defined as follows according to the Fourier theorem.

$$f(t) = \int_{-\infty}^{\infty} F(\nu) e^{i2\pi\nu t} d\nu \,. \tag{14}$$

Where $F(\nu)$ is the Fourier transform of $f(t)$, ν is the frequency, i is the imaginary number and t is time. [3]

The Fourier transform to $f(t)$ can then be calculated to be as follows.

$$F(\nu) = \int_{-\infty}^{\infty} f(t) e^{-i2\pi\nu t} dt \,. \quad [3] \tag{15}$$

The time spent on different parts of this project was the following. The first month was spent on reading up on this field of physics, learning formulas and concepts important for this project. During the next month the code was started on. It was understood that not all integrators work equally good. Which resulted in the testing of the integrator which can

be seen in the method section 3.1 Numerical integration. After that the phase shifts were worked more upon. The resulting figures that were produced through the code for the phase shifts are presented in the section 4 Results and Discussion. After that the phase shifts were used in the XUV photon attosecond pulses and then Fourier transformed in order to show the photoelectron distribution over frequency components which also can be seen in the section 4 Results and Discussion. While the phase shifts and Fourier transforms where looked at the written part of the work was started. Which all together resulted in this work which in the next section will be about the method.

3   Method

The phase shifts were used for 2 and 3 attosecond pulses made of XUV photons. For different positions with respect to the IR-field the attosecond pulses made of XUV photons got different phase shifts. They each had a separation of 1.3 fs between each other as they were put at different positions again with respect to the IR-field. The attosecond pulses made of XUV photons were thus separated in time and got the phase shifts at different times or positions (they are the same quantity in the sense that the speed of light is c, the XUV-field and IR-filed travel with the same speed). The phase shifted XUV photon attosecond pulses were Fourier transformed in order to see the photoelectron distribution over frequency components that they would create for each time if they were to interact through photoionization.

First the attosecond pulse made of XUV photons is presented in order to give a picture of it. The phase shifts were also presented in order to illustrate what was coming. Then, for both the 2 and 3 pulse cases, the electric field over time was plotted. In the end the intensity of the Fourier transformed electric field (attosecond pulses made of XUV photons) was plotted together with the phase shifts specific for those pulses.

3.1   Numerical integration

In order to check the integrator used to calculate the phase shifts a test function

$$E(t) = 2e^{-t^2}\cos(10t) \tag{16}$$

was defined. Which corresponds to an electric field with an amplitude of 2 units of V/m, an angular frequency of 10^{16} Hz since the time is measured in units of 10^{-15} s, fs.

The test function was differentiated and then through the integrator integrated. This new function was plotted together with the original test function. The difference was plotted in another plot. A difference suitable for this project was assumed to be achievable. It was achieved with the code in 6.1 Code for Fig.5. The figures, Fig.5 and Fig.6, show the quality of the numerical integrator used for the code in order to calculate the phase shifts and the Fourier transforms.

3.2   Calculation of the phase modulation

In order to calculate the integral in Eq.11 the integrator in 6.1 Code for Fig.5 was used. In the plots the envelope of the phase shifts and a color map of the phase shifts were plotted. Thus giving a view over the smaller variations of the phase shift with the color map and a bigger view independent of the smaller variations with the envelope.

All numerical values to evaluate the phase shifts were calculated using Eq.11 with the following values for the constants.

$$e = 1.60218 \cdot 10^{-19}\,\text{C}, \ m_e = 9.10939 \cdot 10^{-31}\,\text{kg}, \ \hbar = \frac{6.62608 \cdot 10^{-34}\,\text{Js}}{2\pi}$$

$$\text{and } c = 299792458\,\text{m/s} \ .$$

4   Results and Discussion

4.1   Phase Modulation due to the external laser field

In the following plots in this section different parameters will be varied. If their value is not stated in the figure or in the description of the figure, then the following values have been used.
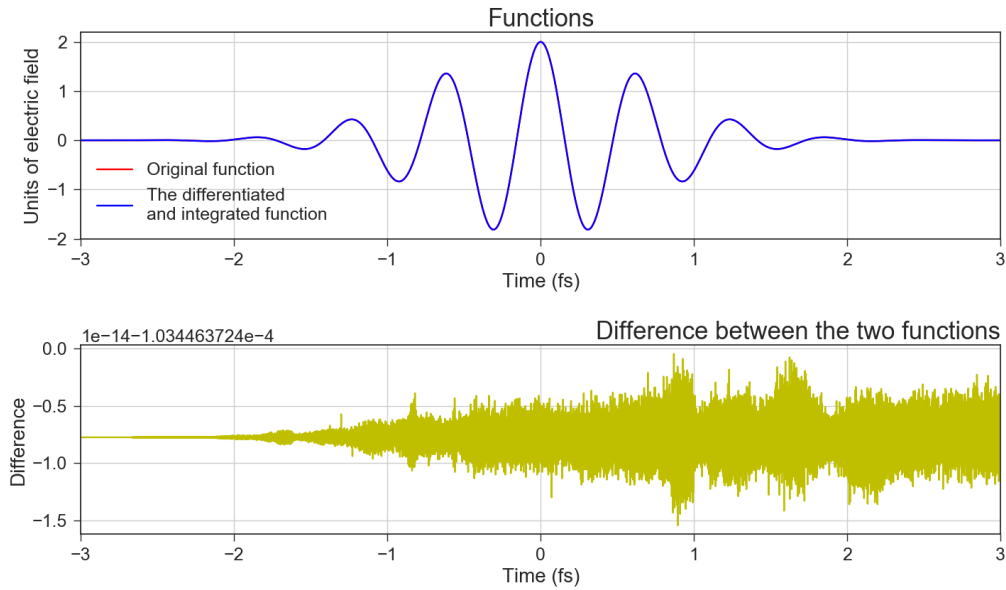
Figure 5: Here is the result of a numerical integral that also shows the difference between the real and the differentiated and then integrated version of the same function, Eq.16. The limit where the primitive function to the differentiated function should be 0 has been set to $-\pi$. The difference is around $-1.034 \cdot 10^{-4}$ with its exact value and variation shown in this figure.
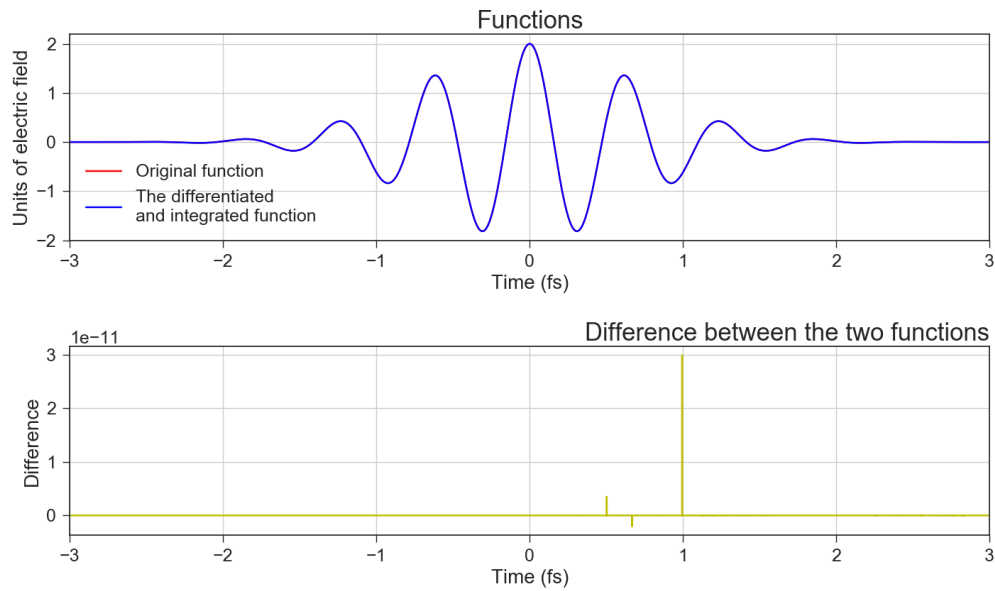

Figure 6: Here is the result of a numerical integral that also shows the difference between the real and the differentiated and then integrated version of the same function, Eq.16. The limit where the primitive function to the differentiated function should be 0 has been set to $-10 \cdot \pi$ and is the limit used in the rest of the codes. The difference is in this case nearly always 0.

$$I = 10^{12}\,\mathrm{W/cm^2}, \ \lambda = 820\,\mathrm{nm}, \ p_e = 1.9 \cdot 10^{-24}\,\mathrm{kg \cdot m/s}, \ n = 2. \tag{17}$$

4.1.1 One pulse case

In the two figures below, Fig.7 and Fig.8, the phase shift is dependent on the momentum of the electron according to Eq.11. The momentum was varied between $(0 \text{ to } 2) \cdot 10^{-24}$ kgm/s because that had been done in a figure in the paper referred to in Fig.1, and time was varied from -6 fs to 6 fs because that will include all the phase shifts.
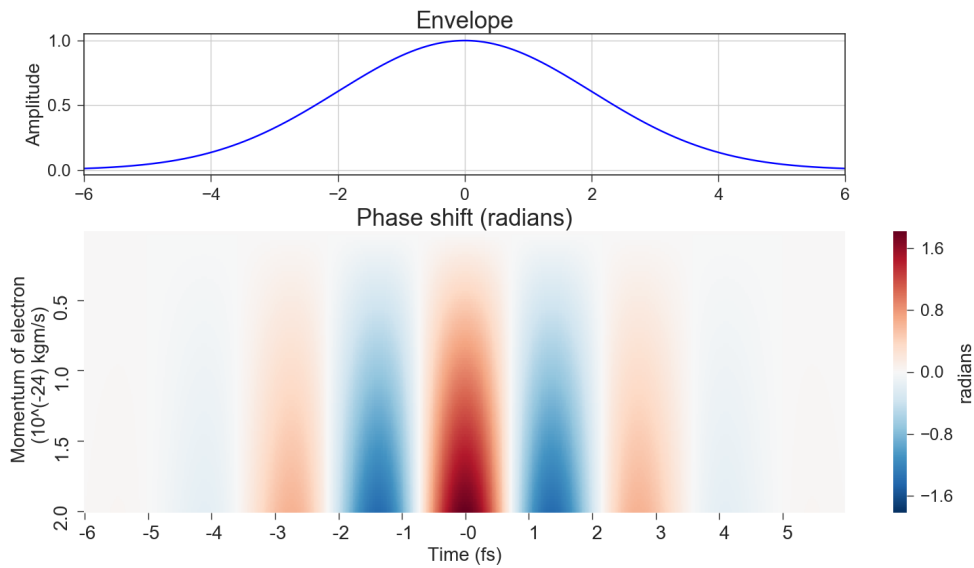

Figure 7: In this figure the result from when the momentum of the electron and time has been varied is presented. The integer n from Eq.13 has been set to 1. The inverse standard deviation from Eq.4 has been set to $a = 0.5$ PHz. The envelope in the upper part of the graph show how much the phase shift has been magnified. When the amplitude of the envelope is 1 the phase shift is what it would be without an envelope and if the amplitude of the envelope is 0 the phase shift is also 0.
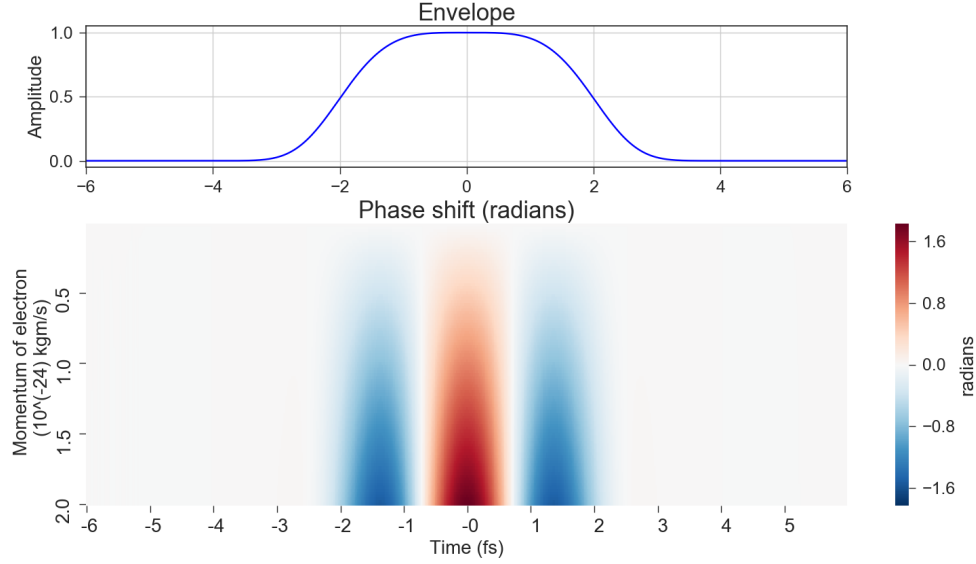
Figure 8: In this figure the result from when the momentum of the electron and time has been varied is presented. The integer n from Eq.13 has been set to 2. The inverse standard deviation from Eq.4 has been set to $a = 0.3$ PHz.

In figure, Fig.9, the wavelength of the IR-field has been varied between 700 nm and 1.7 μm and the time has been varied between -6 fs and 6 fs.

In the next figure, Fig.10, how the phase shift varies with time is plotted with different values for n. It gives an intuitive sense of why to choose $n = 2$. $n = 1$ is too spread out in time and has a too smooth decrease in amplitude. $n = 3$ is too sharp thus it might be hard to produce in a lab. n would correspond to how the IR-filed that is sent out from the laser looks.
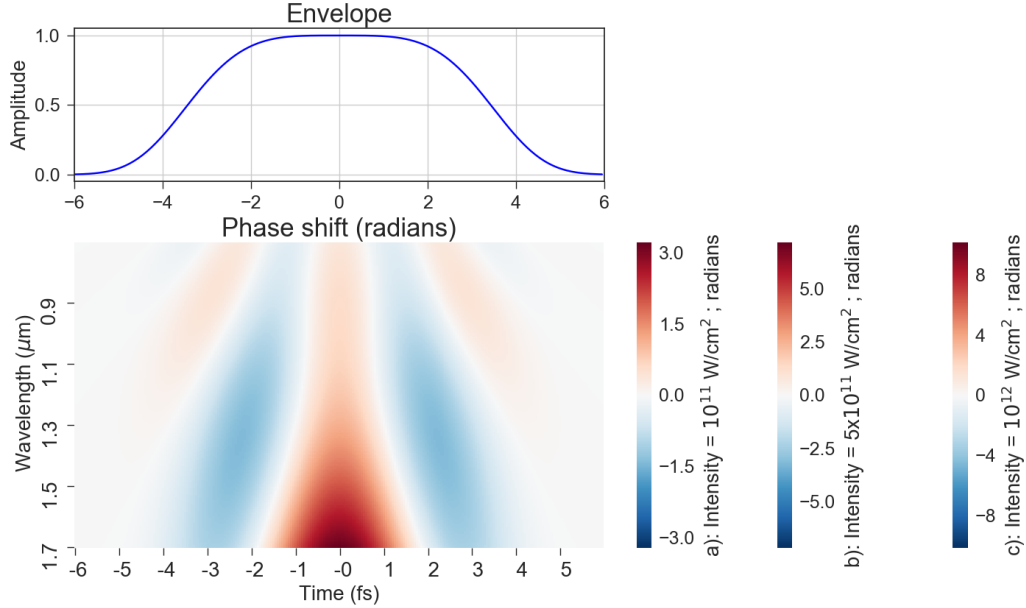
Figure 9: In this figure the result from when the wavelength and time has been varied is presented. For the left most colourbar, a), the intensity has been set to 10^{11} W/cm^2. For the colourbar in the middle, b), the intensity has been set to $5 \cdot 10^{11}$ W/cm^2. For the right most colourbar, c), the intensity has been set to 10^{12} W/cm^2. The intensities are set to these values so that the high harmonic generation can happen which is important for the experiments referred to in Fig.1. The inverse standard deviation from Eq.4 has been set to 0.1 PHz. We can see that for higher wavelengths there will be less fluctuations in the IR-field which gives the phase shift in this figure. For the intensity it can be seen that a higher intensity gives a bigger span between the biggest and the smallest phase shift.
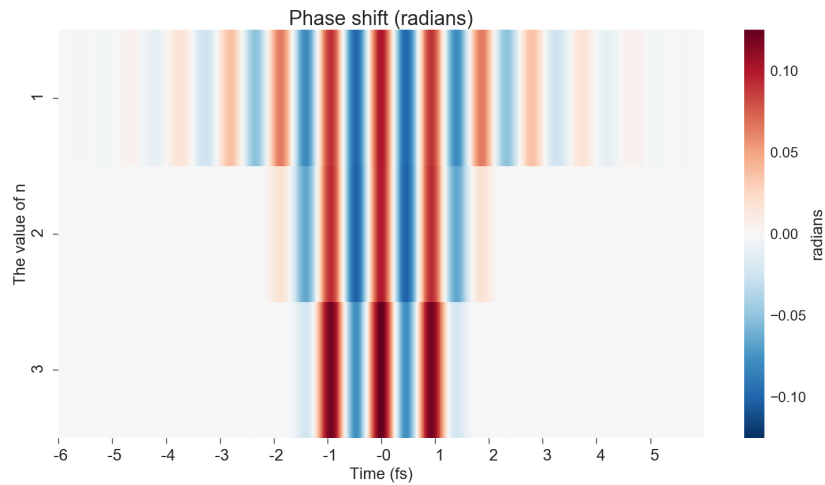

Figure 10: In this figure a comparison between different values on the integer n from Eq.13 is presented. In the experiments the integer $n = 2$ is used. A value of 0.5 PHz has been used for the inverse standard deviation a from Eq.4.

4.1.2 A Pulse train composed of three pulses

In the following figure, Fig.11, the momentum of the electrons and time has been varied as in Fig.8 but now for a Pulse train composed of three pulses. They have a separation of 2 fs between each other.
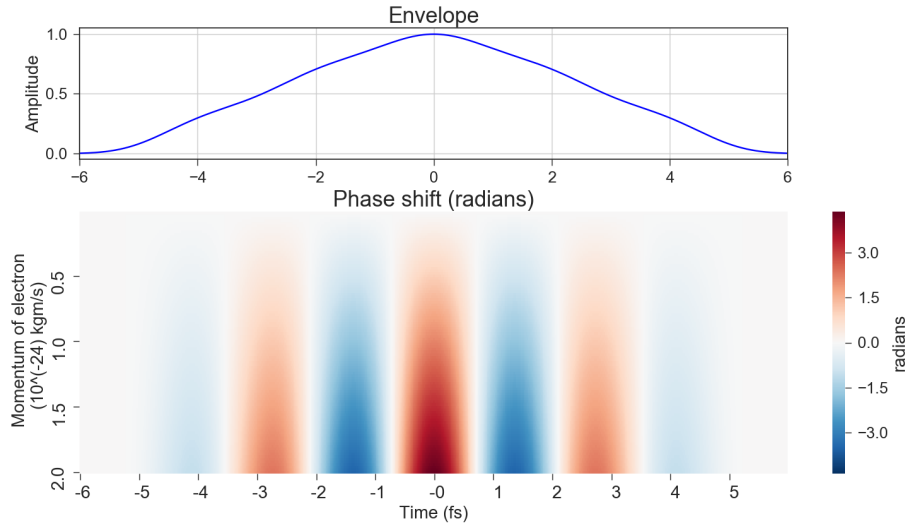
Figure 11: In this figure the result from using the same values as in Fig.8 but for three pulses is presented. One pulse is shifted with -2 fs, one pulse at 0 fs (the same as in Fig.8) and one pulse shifted with +2 fs. The inverse standard deviation from Eq.4 has been set to $a = 0.2$ PHz. When the amplitude of the envelope is 1 the phase shift is what it would be without an envelope and if the amplitude of the envelope is 0 the phase shift is also 0.

In the following figure, Fig.12, the wavelength and time has been varied for the same situation as in Fig.11.
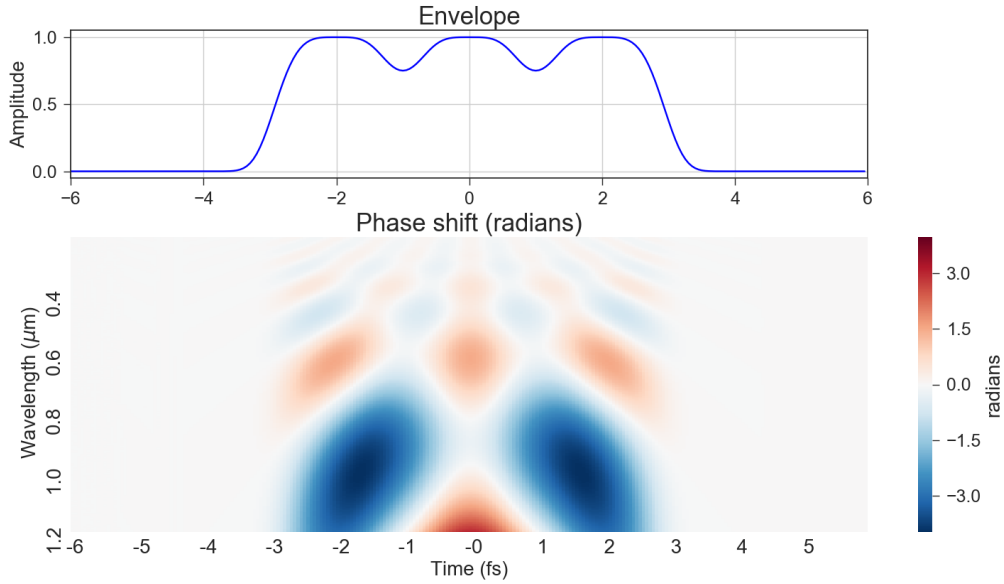
Figure 12: In this figure the result for the same situation as in Fig.11 is presented but here the wavelength and time has been varied. The inverse standard deviation from Eq.4 has been set to $a = 1.4$ PHz. When the amplitude of the envelope is 1 the phase shift is what it would be without an envelope and if the amplitude of the envelope is 0 the phase shift is also 0.

4.2 Temporal-Frequency analysis

This subsection will start with showing the XUV photon attosecond pulse in the following figure, Fig.13, which will be used for the simulations.

Figure 13: In this figure the attosecond pulse made of XUV photons that will be used in the following simulations is presented. It has a frequency of 100 PHz and its inverse standard deviation from Eq.4 has been set to 30 PHz.

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In the following figure, Fig.14, the phase shifts used in this section are plotted.
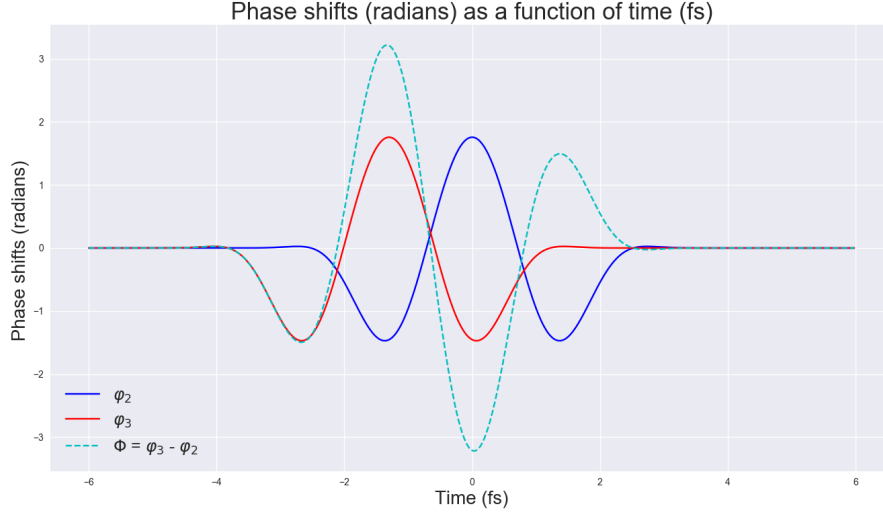
Figure 14: In this figure the different phase shifts are plotted. φ_2 and φ_3 are both originating from the phase shift in Fig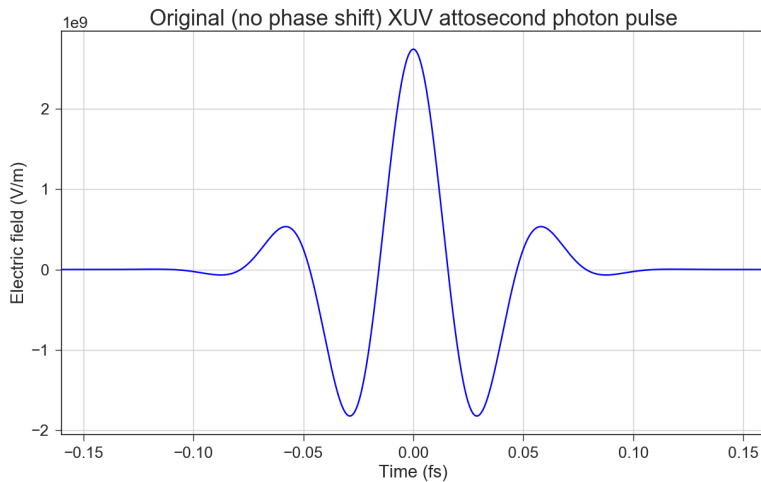.8 but with the momentum set to $1.9 \cdot 10^{-24}$ kg·m/s and a separation of 1.3 fs between each other since that is the separation between the XUV attosecond pulses. Two differences are also plotted in order to see around what point the XUV attosecond pulses should be symmetric.

4.2.1   Two attosecond pulses made of XUV photons

In figure, Fig.15, the first set of attosecond pulses made of XUV photons are plotted. It can be seen that the pulse that is 1.3 fs in front of the other pulse gets the phase shift 1.3 fs before the other pulse.

In the next figure, Fig.16, the Fourier transform of the electric field shown in Fig.15 has been calculated. That Fourier transform has then been amplified according to Eq.3 and the values from 17 are used.

In this paragraph I will clarify what has been done when plotting the following figure, Fig.16. In Fig.15 the real part of the XUV attosecond pulses is plotted using the following formula.

$$E(t) = \sqrt{\frac{2I}{c\epsilon_0}} \cdot \mathrm{Re} \left(\sum_{j=1}^{n} e^{i(\omega(t-jT)+\phi_j)} e^{-\frac{1}{2}a^2(t-jT)^2} \right) \tag{18}$$

18

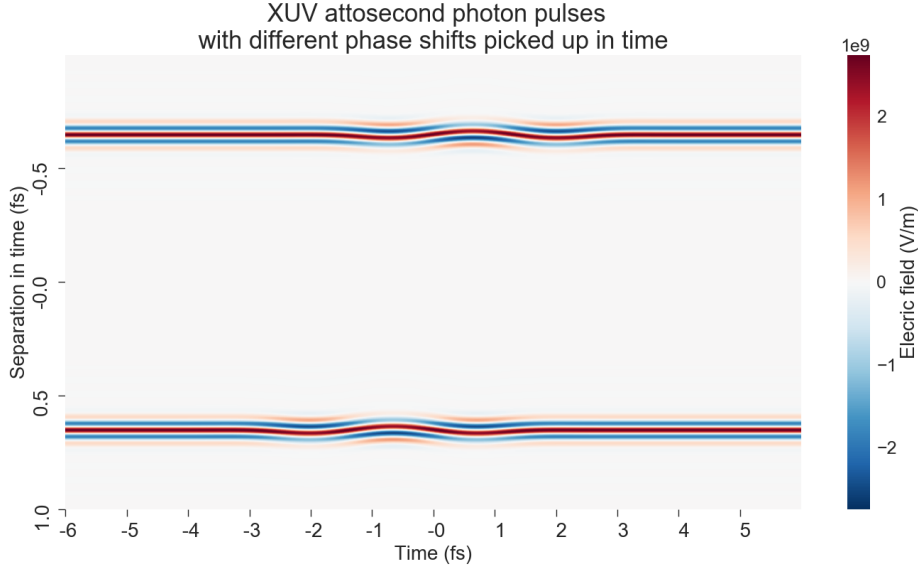Figure 15: In this figure the first set of pulses are plotted over time, their separation is viewed on the y-axis. The colours show the amplitude of the electric field that the photons represent. I have used the same values as before.

Which is the real part of Eq.5 . This equation can be Fourier transformed according to Eq.15 giving the following.

$$E_F(\nu) = \sqrt{\frac{2I}{c\epsilon_0}} \cdot \int_{-\infty}^{\infty} \mathrm{Re}\left(\sum_{j=1}^{n} e^{i(\omega(t-jT)+\phi_j)} e^{-\frac{1}{2}a^2(t-jT)^2}\right) \cdot e^{-i2\pi\nu t} dt \qquad (19)$$

Where I have used $10 \cdot \pi$ instead of ∞. In Fig.5 and Fig.6 it can be seen why this is a good approximation. The Fourier transformed electric field is now made into an intensity but Eq.19 is complex and Eq.3 is only for real values. The left part in Eq.3 can be modified as follows.

$$I = \frac{1}{2}c\epsilon_0 |E_0|^2 \qquad (20)$$

Where $|E_0|^2$ is the modulus square of the electric field. Now the electric field in Eq.19 can be put in Eq.20 as follows giving the intensity of the Fourier transformed electric field.

$$I_F(\nu) = I \cdot \left| \int_{-\infty}^{\infty} \mathrm{Re}\left(\sum_{j=1}^{n} e^{i(\omega(t-jT)+\phi_j)} e^{-\frac{1}{2}a^2(t-jT)^2}\right) \cdot e^{-i2\pi\nu t} dt \right|^2 \qquad (21)$$

Writing out the modulus square in Eq.21 gives the following expression.

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$$I_F(\nu) = I\left[\int_{-\infty}^{\infty} \mathrm{Re}\left(\sum_{j=1}^{n} e^{i(\omega(t-jT)+\phi_j)} e^{-\frac{1}{2}a^2(t-jT)^2}\right)\cos(-2\pi\nu t)dt\right]^2$$

$$+ I\left[\int_{-\infty}^{\infty} \mathrm{Re}\left(\sum_{j=1}^{n} e^{i(\omega(t-jT)+\phi_j)} e^{-\frac{1}{2}a^2(t-jT)^2}\right)\sin(-2\pi\nu t)dt\right]^2 \qquad (22)$$

Which is plotted on the right-hand side in the following figure, Fig.16.
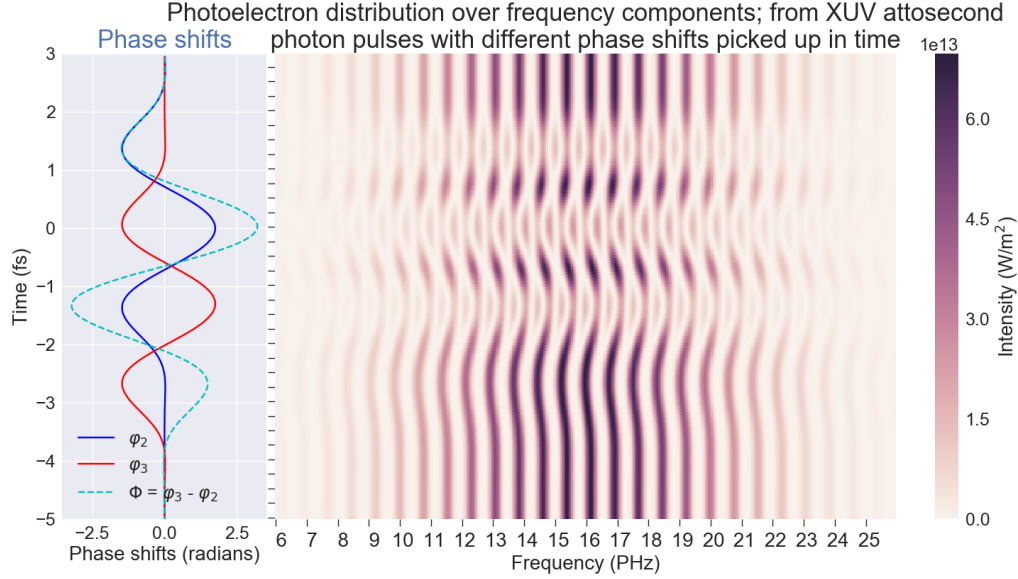

Figure 16: In this figure the phase shifts are shown to the left and the different photoelectron distributions over frequencies are shown to the right. Thus you could transform the frequencies on the x-axis to energies through multiplying by Plank's constant. Then you would have to know what ionization potential the atoms or molecules that you are photo ionizing have. Below that energy the photoelectron distribution that you have will not contribute to the photoelectron distribution of that case. That is according the formula that Einstein proposed (which is an approximation) although one can also take into account for quantum physics which makes it more complicated. For each time on the x-axis in Fig.15, here represented by the time with the phase shifts, the Fourier transformed phase shifted XUV attosecond pulses have different distributions over frequencies given to the photoelectrons. The code was running for ~ 7 minutes in order to produce this figure.

It can be seen that the photoelectron distribution do not have any symmetry in time. That is not reasonable since the phase shifts have symmetries in time, around $t = 1.3/2$ fs, and there is nothing special about $t = 1.3/2$ fs. The same photoelectron distribution should emerge although the phase shifts are symmetric around another point in time than $t = 1.3/2$ fs. Time is not what gives the photoelectron distribution it is the XUV attosecond

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pulses and there phase shift that gives the photoelectron distribution. The phase shifts are put into the attosecond pulses made of XUV photons which then also have symmetry – around an inversion axis. These pulses are then Fourier transformed and the result is not symmetric around $t = 1.3/2$ fs. The explanation is that the Fourier transform does not have any symmetry around $t = 1.3/2$ fs. It has its symmetry around $t = 0$ fs. In order to get a result that has some symmetry around $t = 1.3/2$ fs the time in the exponential part of the Fourier transform, Eq.15, has to be shifted to $t = 1.3/2$ fs. Which has been done in the following figure.
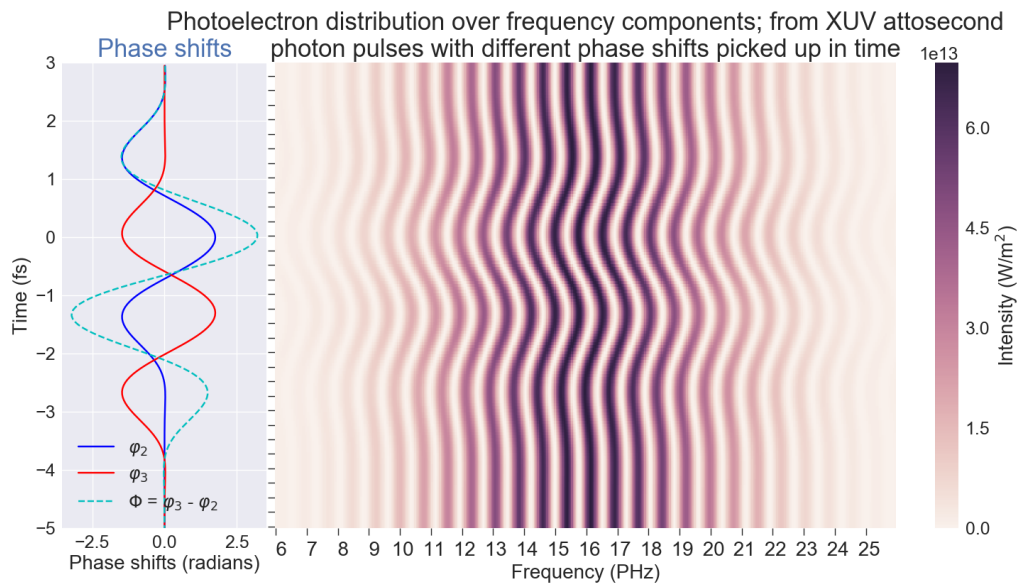
Figure 17: In this figure the phase shifts are shown to the left and the different photoelectron distributions over frequencies are shown to the right. Thus you could transform the frequencies on the x-axis to energies through multiplying by Plank's constant. Then you would have to know what ionization potential the atoms or molecules that you are photo ionizing have. Below that energy the photoelectron distribution that you have will not contribute to the photoelectron distribution of that case. That is according the formula that Einstein proposed (which is an approximation) although one can also take into account for quantum physics which makes it more complicated. For each time on the x-axis in Fig.15, here represented by the time with the phase shifts, the Fourier transformed phase shifted XUV attosecond pulses have different distributions over frequencies given to the photoelectrons. The code was running for ~14 minutes in order to produce this figure.

5 Conclusion and Outlook

In this work attosecond pulses made of XUV photons producing photoelectrons through photoionization were looked at. First different phase shifts that could be induced into an electron wave packet were looked at. These phase shifts were produced by an IR-field. One IR-field with specific values giving a pattern of phase shifts was chosen. Then two XUV photon attosecond pulses were chosen with a separation between each pulse of 1.3 fs. The attosecond pulses made of XUV photons got a phase shift shaped like the one from the chosen IR-field. The attosecond pulses made of XUV photons were placed at different positions in time with respect to the IR-field. For each position in time they got the corresponding phase shift. These phase shifted attosecond pulses made of XUV photons were then Fourier transformed into components in the Fourier plane representing the photoelectron distribution produced in photoionization.

One IR-field that gave phase shifts that were put into the XUV photon attosecond pulses was looked at in this work. In order to further look into this, more of the phase shifts plotted in section 4.1 should be used for the attosecond pulses made of XUV photons. Making a video could be a good option but having a fast computer would be recommended since it takes a while (around 15 min/figure) to get one plot of the Fourier transformed attosecond pulses made of XUV photons. Which can be seen in the section 4 Results and Discussion under each figure with a set of Fourier transformed attosecond pulses made of XUV photons.

6 Appendix; Code written in Python

6.1 Checking the integrator

```python
import matplotlib.pyplot as plt
from pylab import *
from math import *
import scipy
from scipy.integrate import quad
import seaborn as sns


# the function to be integrated:
def f(x):
    return -4.0*e**(-x**2)*x*np.cos(10*x) - 20*e**(-x**2)*np.sin(10*x)


x = arange(-3, 3, 0.0001)
Der = [ -4.0*e**(-x**2)*x*np.cos(10*x) - 20*e**(-x**2)*np.sin(10*x) for x in x]
y_sin = []
y_cos_integrated = []
for element in x:      y_sin.append( 2* (np.e**(- element**2 ))*np.cos( 10*element ) )
    y_cos_integrated.append(quad(f, -pi*10, element)[0] - sin(pi))
    print( y_sin[0] )
L = len(x)
M = []
for i in range(L):
    MT = y_cos_integrated[i] - y_sin[i]
    M.append(MT)
    print( M[0] )
sns.set_style("ticks", "xtick.major.size":7, "ytick.major.size":7)
fig = plt.figure()
axes1 = fig.add_axes( [0.08, 0.6, 0.9, 0.35] )
```

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```python
sns.set(font_scale=1.8)
axes1.plot(x, y_sin, 'r', label= 'Original function')
axes1.plot(x, y_cos_integrated, 'b', label=r'The differentiated '
          '\n'
          r'and integrated function ' )
axes1.set_ylabel('Units of electric field', size=20)
axes1.set_xlabel('Time in fs', size=20)
axes1.set_xlim(-3, 3)
axes1.set_title('Functions', size=25)
leg = axes1.legend();
axes1.legend(loc='lower left', frameon=False)
axes1.grid()

sns.set_style("ticks", "xtick.major.size":7, "ytick.major.size":7)
ax = fig.add_axes( [0.08, 0.1, 0.9, 0.32] )
ax.set_title('Difference between the two functions', size=25, fontdict=None, loc='right')
ax.set_xlim(-3, 3)
ax.plot(x, M, 'y')
ax.set_ylabel('Difference', size=20)
ax.set_xlabel('Time in fs', size=20)
ax.grid()
show()
```

6.2   Plotting of phase shifts for Fourier transform

```python
import seaborn as sns
import matplotlib.pyplot as plt
from pylab import *
from math import *
import scipy
from scipy.integrate import quad
```

```python
# the function to be integrated:
def f(x, omega, a):
    return ( - (1/omega) * (np.sin( omega*x )) * (np.e**( - (1/2)* (a**2 )* x**4 )) )


# Pre sets
Intensity = (10**(8))
e = 1.60218 * 10**(-19)
m_e = 9.10939 * 10**(-31)
h_bar = ( 6.62608*10**(-34) ) / (2*np.pi)
elc_p_mag = 1.9 * 10**(-24) # around 12 eV
PAmp = - Intensity*( e/(m_e * h_bar) ) * elc_p_mag
C = 299792458
Lambda = 8.20*10**(-7)
omega = 2*np.pi* (C/Lambda ) * 10**(-15)
omega_fs_comp = 10**(-30)
E_0 = 8.8541878176*10**( -12 )
E_mag = sqrt( 2/( E_0 * C ) )
a = 0.3


# Main
xR = arange(-6, 6, 0.02)
phi1 = []
for elmer in xR:
    Par1 = E_mag*omega_fs_comp*PAmp*quad(f , elmer, 10*np.pi, args=(omega, a) )[0]
    phi1.append( Par1 )
    print(Par1)
phi2 = []
for elmer in xR:
```

```
        Par2 = E_mag*omega_fs_comp*PAmp*quad(f , elmer + 1.3, 10*np.pi, args=(omega,
a) )[0]

        phi2.append( Par2 )

        print(Par2)

    Phi = []

    Xer = len(xR)

    for i in range(Xer):

        Phi.append( phi2[i] - phi1[i] )

        print(Phi[0])

    phi3 = []

    for elmer in xR:

        Par3 = E_mag*omega_fs_comp*PAmp*quad(f , elmer - 1.3, 10*np.pi, args=(omega,
a) )[0]

        phi3.append( Par3 )

        print(Par2)

    Phi = []

    for i in range(Xer):

        Phi.append( phi2[i] - phi1[i] )

        print(Phi[0])

    PhiPrim = []

    for i in range(Xer):

        PhiPrim.append( phi2[i] - phi3[i] )

        print(PhiPrim[0])


    fig = plt.figure()

    ax2 = fig.add_axes( [0.08, 0.1, 0.87, 0.8] )

    sns.set(font_scale=1.8)

    ax2.plot(xR, phi3, 'orange', label='$ \u03C6 _1$')

    ax2.plot(xR, phi1, 'b', label='$ \u03C6 _2$')

    ax2.plot(xR, phi2, 'r', label='$ \u03C6 _3$')
```

```
ax2.plot(xR, Phi, '–c', label='$ \u03A6 $ = $ \u03C6 _3$ - $ \u03C6 _2$')

ax2.plot(xR, PhiPrim, '–m', label='$ \u03A6 ´$ = $ \u03C6 _3 $ - $ \u03C6 _1 $')

ax2.set_ylabel(' Phase shifts in radians ', size=20)

ax2.set_xlabel('Time in fs', size=20)

ax2.set_title(' Phase shifts ', size=25)

leg = ax2.legend();

ax2.legend(loc='lower left', frameon=False)
```

6.3   Heat maps

6.3.1   Plot of phase shift dependent on momentum and time

```
import seaborn as sns

import matplotlib.pyplot as plt

from pylab import *

from math import *

import scipy

from scipy.integrate import quad


def f(x, omega, a, n):
    return ( - (1/omega) * (np.sin( omega*x )) * (np.e**( - (1/2)* (a**2 )* x**(2*n) )) )


# Pre sets

Intensity = (10**(8))

e = 1.60218 * 10**(-19)

m_e = 9.10939 * 10**(-31)

h_bar = ( 6.62608*10**(-34) ) / (2*np.pi)

elc_p_mag = 1.9 *10**(-24) # around 12 eV

PAmp = - Intensity*( e/(m_e * h_bar) ) * elc_p_mag

C = 299792458

Lambda = 2.80*10**(-7)
```

```python
omega = 2*np.pi* (C/Lambda ) * 10**(-15)
omega_fs_comp = 10**(-30)
E_0 = 8.8541878176*10**( -12 )
E_mag = sqrt( 2/( E_0 * C ) )
a = sqrt( 2)
n = 2


# Main
xR = arange(-4, 4, 0.02)
p = arange(0, 1.9, 0.02)
Z = []
for i in p:
    ZP = []
    for elmer in xR:
        ZP.append( E_mag*omega_fs_comp*PAmp*i* quad(f , elmer, 10*np.pi, args=(omega,
a, n) )[0] )
    Z.append( ZP )
    print(Z[0][0])


# Plotting
ax = sns.heatmap(Z, xticklabels=xR, yticklabels=p)
xlabels = [':3.1f'.format(x) for x in xR]
ylabels = [':3.1f'.format(y) for y in p[::-1] ]
LABELLimX = 25
LABELLimY = 15
ax.set_xticks(ax.get_xticks()[::LABELLimX])
ax.set_xticklabels(xlabels[::LABELLimX])
ax.set_yticks(ax.get_yticks()[::LABELLimY])
ax.set_yticklabels(ylabels[::LABELLimY])
plt.title('Phase shift', size=20)
```

plt.ylabel(' Momentum of electron in 10^(-24) kgm/s ', size=15)

plt.xlabel('Time in fs', size=15)

6.3.2 Plot of three attosecond pulses made of XUV photons without imports and presets

```
# the function to be integrated:
def f(x, omega, a):
    return ( - (1/omega) * (np.sin( omega*x )) * (np.e**( - (1/2)* (a**2 )* x**4 )) )


# Main
xR1 = arange(-6, 6, 0.01)
phi1 = []
for elmer in xR1:
    Par1 = E_mag*omega_fs_comp*PAmp*quad(f , elmer, 10*np.pi, args=(omega, a) )[0]
    phi1.append( Par1 )
    print(Par1)
phi2 = []
for elmer in xR1:
    Par2 = E_mag*omega_fs_comp*PAmp*quad(f , elmer + 1.3, 10*np.pi, args=(omega, a) )[0]
    phi2.append( Par2 )
    print(Par2)
phi3 = []
for elmer in xR1:
    Par3 = E_mag*omega_fs_comp*PAmp*quad(f , elmer - 1.3, 10*np.pi, args=(omega, a) )[0]
    phi3.append( Par3 )
    print(Par3)
def f(x, omega, a, fas, fasPrim):
```

```python
        return ( (np.cos( omega*(x + fas) + fasPrim )) * (np.e**( - (1/2)* (a**2 )* (x + fas)
**2 )) )
    INTENSITY = []
    OMEGA = 100
    xlen= len(xR1)
    xR2 = arange(-1.5, 1.5, 0.005)
    for i in xR2:
        INTENSITYTemp = []
        for j in range(xlen):
            p1 = phi1[j]
            p2 = phi2[j]
            p3 = phi3[j]
            # E-field
            # Inter = Intensity * E_mag*(f(i, OMEGA, 30, 0, p1) + f(i, OMEGA, 30, -1.3,
p2) + f(i, OMEGA, 30, +1.3, p3) )
            # its intensity
            Inter = (Intensity**2) * ( (f(i, OMEGA, 30, 0, p1)**2 ) + (f(i, OMEGA, 30, -1.3,
p2) **2) + (f(i, OMEGA, 30, +1.3, p3)**2) )
            INTENSITYTemp.append( Inter )
        INTENSITY.append( INTENSITYTemp )
    print(INTENSITY[0][0])


    sns.set_style("ticks", "xtick.major.size":7, "ytick.major.size":7)
    fig = plt.figure()
    axes1 = fig.add_axes( [0.1, 0.11, 0.9, 0.77] )
    sns.set(font_scale=1.8)
    # Electric field
    # axes1 = sns.heatmap(INTENSITY, xticklabels=xR1, yticklabels=xR2,
    #                     cbar_kws= 'label': 'Elecric field in V/m' )
    # Its intensity
```

```python
axes1 = sns.heatmap(INTENSITY, xticklabels=xR1, yticklabels=xR2,
                    cbar_kws= 'label': 'Intensity in W/m² ' )
xlabels = [':3.0f'.format(x) for x in xR1 ]
ylabels = [':3.1f'.format(y) for y in xR2[::-1] ]
LABELLimX = 100
LABELLimY = 100
axes1.set_xticks(axes1.get_xticks()[::LABELLimX])
axes1.set_xticklabels(xlabels[::LABELLimX], fontsize=20)
axes1.set_yticks(axes1.get_yticks()[::LABELLimY])
axes1.set_yticklabels(ylabels[::LABELLimY], fontsize=20)
axes1.set_title(r' XUV attosecond photon pulses'
                '\n'
                r' with different phase shifts picked up in time ', size=25)
axes1.set_xlabel( ' Time in fs ', size=20)
axes1.set_ylabel(' Separation in time, fs ', size=20)
```

6.3.3 Fourier transform of three attosecond pulses made of XUV photons without imports and presets

```python
# Main
xR = arange(-6, 6, 0.05)
phi1 = []
for elmer in xR[::-1] :
    Par1 = E_mag*omega_fs_comp*PAmp*quad(f , elmer, 10*np.pi, args=(omega, a) )[0]
    phi1.append( Par1 )
    print(Par1)
phi2 = []
for elmer in xR[::-1] :
    Par2 = E_mag*omega_fs_comp*PAmp*quad(f , elmer + 1.3, 10*np.pi, args=(omega, a) )[0]
    phi2.append( Par2 )
```

```python
            print(Par2)
        phi3 = []
        for elmer in xR[::-1] :
            Par3 = E_mag*omega_fs_comp*PAmp*quad(f , elmer - 1.3, 10*np.pi, args=(omega, a) )[0]
            phi3.append( Par3 )
            print(Par3)
        Phi = []
        Xer = len(xR)
        for i in range(Xer):
            Phi.append( phi2[i] - phi1[i] )
            print(Phi[0])
        PhiPrim = []
        for i in range(Xer):
            PhiPrim.append( phi2[i] - phi3[i] )
            print(PhiPrim[0])


        def f(x, omega, a, fas, fasPrim):
            # E-field
            return ( (np.cos( omega* (x + fas) + fasPrim )) * (np.e**( - (1/2)* (a**2 )* (x + fas ) **2 )) )
            # Intensity
            # return (Intensity**2) *( (np.cos( omega* (x + fas) + fasPrim )) * (np.e**( - (1/2)* (a**2 )* (x + fas ) **2 )) )
        def Foriercos(x, freq, PHI1, PHI2, PHI3, OMEGA):
            return ( ((f(x, OMEGA, 30, 0, PHI1))) + ((f(x, OMEGA, 30, -1.3, PHI2))) + ((f(x, OMEGA, 30, +1.3, PHI3))) ) * (np.cos( -2*(np.pi)*freq*x ))
        def Foriersin(x, freq, PHI1, PHI2, PHI3, OMEGA):
            return ( ((f(x, OMEGA, 30, 0, PHI1))) + ((f(x, OMEGA, 30, -1.3, PHI2))) + ((f(x, OMEGA, 30, +1.3, PHI3))) ) * (np.sin( -2*(np.pi)*freq*x ))
```

```python
INTENSITY = []
FR = arange(0, 30, 0.1)
xlen= len(xR)
for j in range(xlen):
    p1 = phi1[j]
    p2 = phi2[j]
    p3 = phi3[j]
    INTENSITYTemp = []
    for i in FR:
        INTERT = (Intensity**2) * ( ((quad(Foriercos , -10*np.pi, 10*np.pi , args=(i, p1,
p2, p3, 100) )[0])**2) + ((quad(Foriersin , -10*np.pi, 10*np.pi , args=(i, p1, p2, p3, 100)
)[0])**2) )
        INTENSITYTemp.append( INTERT )
    INTENSITY.append( INTENSITYTemp )
    print(INTENSITY[0][0])


sns.set_style("ticks", "xtick.major.size":7, "ytick.major.size":7)
fig = plt.figure()
axes1 = fig.add_axes( [0.32, 0.15, 0.65, 0.75] )
sns.set(font_scale=1.8)
axes1 = sns.heatmap(INTENSITY, xticklabels=xR, yticklabels=Phi,
                cbar_kws= 'label': 'Intensity in W/m$^2$ ' )
xlabels = [':3.0f'.format(x) for x in FR ]
ylabels = [':3.1f'.format(y) for y in Phi ]
LABELLimX = 20
LABELLimY = 5
axes1.set_xticks(axes1.get_xticks()[::LABELLimX])
axes1.set_xticklabels(xlabels[::LABELLimX], fontsize=20)
axes1.set_yticks(axes1.get_yticks()[::LABELLimY])
axes1.set_yticklabels(ylabels[::LABELLimY], fontsize=0.01)
```

axes1.set_title(r' Electron distribution over frequencies; from XUV attosecond photon pulses '

'\n'

r' with different phase shifts picked up in time ', size=25)

axes1.set_xlabel(' Frequency in PHz ', size=20)

ax = fig.add_axes([0.1, 0.15, 0.2, 0.75])

ax.set_ylim(-6, 6)

ax.plot(phi3, xR[::-1] , 'orange', label='$ \u03C6 _1$')

ax.plot(phi1, xR[::-1], 'b', label='$ \u03C6 _2$')

ax.plot(phi2, xR[::-1], 'r', label='$ \u03C6 _3$')

ax.plot(Phi, xR[::-1], '--c', label='$ \u03A6$ = $ \u03C6 _3$ - $ \u03C6 _2$')

ax.plot(PhiPrim, xR[::-1], '--m', label='$ \u03A6 ´$ = $ \u03C6 _3$ - $ \u03C6 _1$')

ax.set_xlabel(' Phase shifts in radians ', size=20)

ax.set_ylabel('Time in fs', size=20)

ax.set_title(' Phase shifts ', color='C0', size=25)

leg = ax.legend();

ax.legend(loc='lower left', frameon=False)

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