FRIEDRICH-SCHILLER-UNIVERSITÄT JENA
PHYSIKALISCH-ASTRONOMISCHE-FAKULTÄT

FRIEDRICH-SCHILLER-
UNIVERSITÄT
JENA

DR. MATTHIAS KÜBEL

Strong Field Laser Physics

All Exercises

Summer term 2021

Name: MARTIN BEYER

Contents

1 Electron trajectories

1.1 Motion of an electron in an oscillating electric field

In the lecture, we discussed Newtons equations of motion for an electron in an oscillating electric field, $E(t) = E_0 \cos(\omega t)$, ($E_0 = const., \omega = const.$), in atomic units

$$\frac{\partial p}{\partial t} = -E_0 \cos(\omega t). \tag{1.1}$$

Verify the analytical results for $x(t)$ and $v(t)$ derived in the lecture by numerically integrating Newton's equation of motion for two different values for ωt_0, assuming that $x(t_0) = 0, v(t_0) = 0$. In your simulation, propagate the electron for a few cycles.

Plot the numerical and analytical results in the same diagram. Find the oscillation amplitude, oscillation velocity and ponderomotive energy. Compare the numerical results to the formulas derived in the lecture.

Plot a few example trajectories, starting at different phases ωt_0 of the laser field and describe your observations.

Solution: We can start this problem by creating a simple integrator which uses a *Euler forward* technique to integrate the equation of motion and calculate the electron trajectory. For that we initialize a time, position and velocity array, define a time step dt and specify the electric field.

```
def integrate(tstart, E, dt, x, v):
    for i in range(round(tstart), len(x)-1):
        v[i+1] = v[i]-E[i]*dt
        x[i+1] = x[i]+v[i]*dt
```

The electric field amplitude and the time were chosen accordingly to the figure in the script as $E_0 = 0{,}01$ a.u. and $t \in [0, 400]$a.u..

First the electron motion was calculated for the rest position ($x_0 = 0, v_0 = 0$) at the phase $\omega t_0 = 0$. The results are displayed in figure 1. The integrated function was also compared to the analytical result of the electron motion which was

$$x(t) = \frac{E_0}{\omega^2}\cos(\omega t) - \frac{E_0}{\omega^2}, \quad v(t) = -\frac{E_0}{\omega}\sin(\omega t). \tag{1.2}$$

The corresponding curve is also displayed in figure 1. We observe that both lines look very similar. This is due to the choice of a reasonably small time step d$t = 0.01$ where the *Euler forward* is sufficiently accurate.

The red curve of figure 1 shows the electron trajectory for a rest postion at a phase position $\omega t_0 = 2.97$. The physical interpretation of this is, that the electron was placed in the field which can be achieved by tunneling.

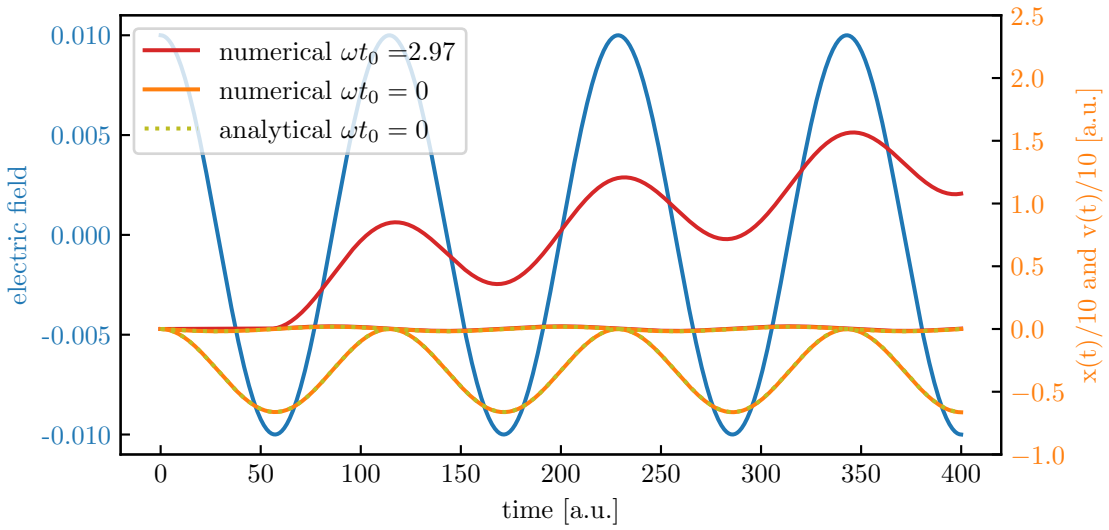

Fig. 1: Oscillating electric field with angular frequency $\frac{2\pi \cdot 3.5}{400}$ a.u. and electron trajectories for different initial phase positions.

Now we want to find the oscillation amplitude, -velocity and ponderomotive energy. The oscillation amplitude can be estimated by finding the maximum and minimum x-position of our electron and recognizing the amplitude as the half of the peak-peak value `amplitude =(max(x)-min(x))/2)`. The analytical amplitude can be calculated easily as

$$\text{analytical} \qquad \frac{E_0}{\omega^2} = 0.01\left(\frac{2\pi \cdot 3.5}{400}\right)^{-2} = 3.318 \tag{1.3}$$

$$\text{numerical} \qquad \frac{E_0}{\omega^2} = 3.308. \tag{1.4}$$

The osscillation velocity can be estimaed in the same way using the v-values of the electron. Here we obtain

$$\text{analytical} \qquad \frac{E_0}{\omega} = 0.01\left(\frac{2\pi \cdot 3.5}{400}\right)^{-1} = 0.181891364 \tag{1.5}$$

$$\text{numerical} \qquad \frac{E_0}{\omega} = 0.181891365. \tag{1.6}$$

Both values are very similar. Finally we calculate the ponderomotive energy as the time averaged kinetic energy of the electron. For that we have to integrate the velocity over one oscillation cycle and divide by the oscillation period

$$U_P = \left\langle \frac{1}{2}\dot{x}^2 \right\rangle = \frac{1}{T}\int_0^T \frac{1}{2}\dot{x}^2 \,\mathrm{d}t = \frac{1}{4}\frac{E_0^2}{\omega^2}. \tag{1.7}$$

We can calculate this numerically using the trapezian integration technique in the following way:

```
period = int(2*np.pi/(w*dt))  # calculates array position of period end
kinetic_energy = 0.5*v[0:period]*v[0:period]
integral=np.trapz(kinetic_energy, x=None, dx=dt)/(2*np.pi/w).
```

The results are the following

$$\text{analytical} \qquad \frac{E_0^2}{4\omega^2} = 0.008271118 \tag{1.8}$$

$$\text{numerical} \qquad \frac{E_0^2}{4\omega^2} = 0.008271117. \tag{1.9}$$

In the last part we plot some mor example trajectories starting at different phases. The results are shown in figure 2.

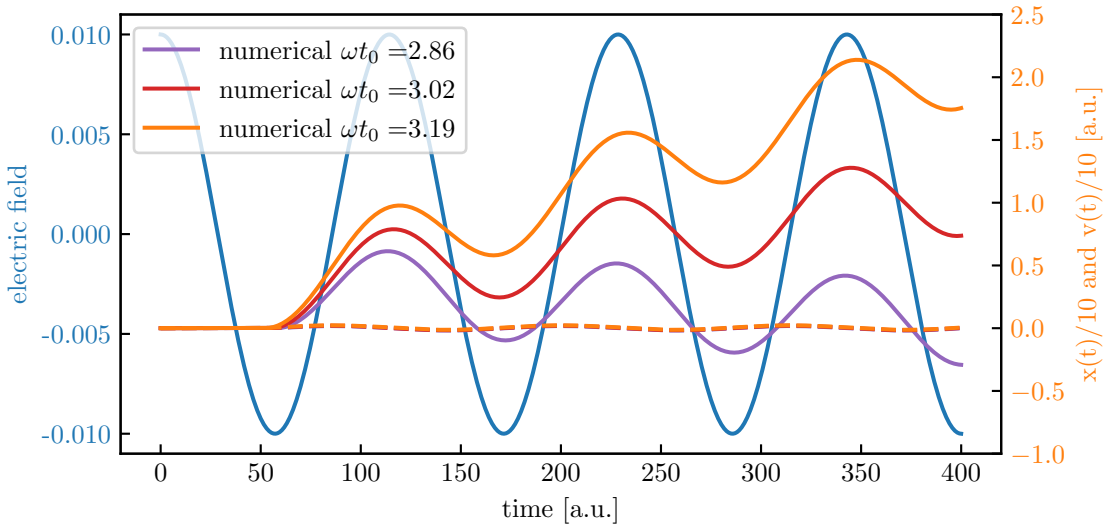

Fig. 2: Oscillating electric field with angular frequency $\frac{2\pi \cdot 3.5}{400}$ a.u. and electron trajectories for three different initial phase positions.

We observe that only small changes in the initial phase position of the oscillation cycle lead to vastly different electron trajectories.

1.2 Electron motion in a pulsed field:

Experiments in strong-field laser physics are carried out using pulsed lasers. Define the elctric field of a femtosecond laser pulse, using the function

$$E(t) = E_0(t)\cos(\omega t) \tag{1.10}$$

where the envelope function $E_0(t)$ has a femtosecond duration, e. g. a Gaussian with a full width at half maximum (FWHM) of 10 optical cycles, or a similar $\sin^2$ *envelope.*

Now explore the behaviour of the electron velocity for trajecties starting at different times in the laser pulse. Describe what happens to a free electron, i.e., one that is created before the laser pulse? Make a plot of final energy vs. initial time. Under what conditions is the maximum energy obtained?

Solution: First we translate the provided Matlab-script into Python code and run the program. The result is a laser pulse with a $\cos^2$-shaped envelope function. Figure 3 displays the electric field (red) and the corresponding envelope (black).

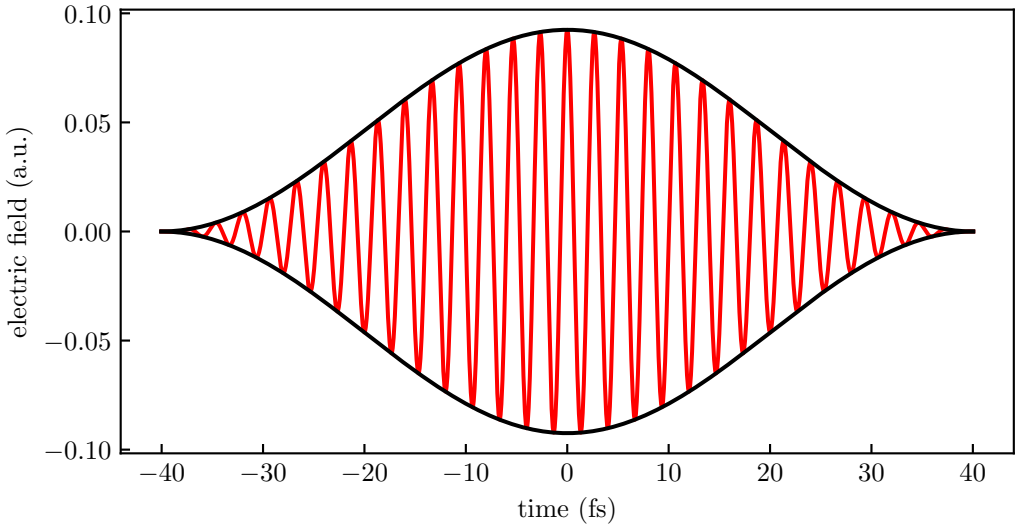

Fig. 3: Electric field of the femtosecond laser pulse and its envelope function $\cos^2$.

Now we want to look at the behaviour of the electron velocity and trajectory for different times in the laser pulse. We achieve that by using the Euler forward integration from Task 1 and start at different positions in time. The result is shown in figure 4.

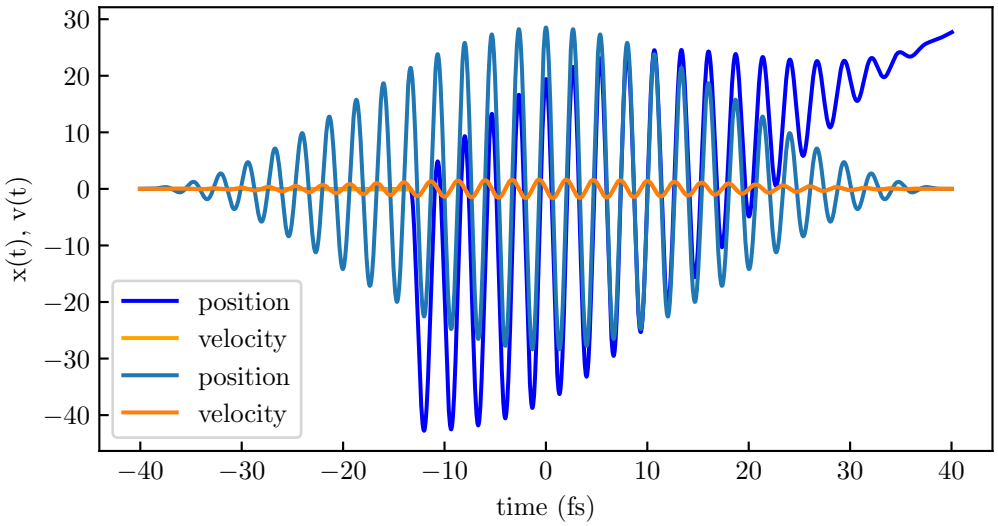

Fig. 4: Electron trajectory (blue) and velocity (orange) for two different starting times.

First the electron was inserted at the beginning of the laser pulse. We can see that the electron follows the electric field directly by comparing its trajectory to the field in figure **??**. After the laser pulse has passed, the velocity goes back to zero and the electron is at rest again in the origin. Therefore we can conclude that for an electron that was created before

the laser pulse, we cannot transfer energy to the electron. This is also known as the LAWSON-WOODWARD theorem and applies to plane waves.

However, if we insert the electron after some part of the laser pulse has already passed, the electron trajectory can be vastly different. We observe, that the electron drifts away from the origin and has a net velocity after the laser pulse is completely gone. We can further investigate this effect by calculating the final energy vs. initial time. For that we took the velocity of the electron at the end of the laser pulse and calculated its kinetic energy. This is plotted in figure 5.

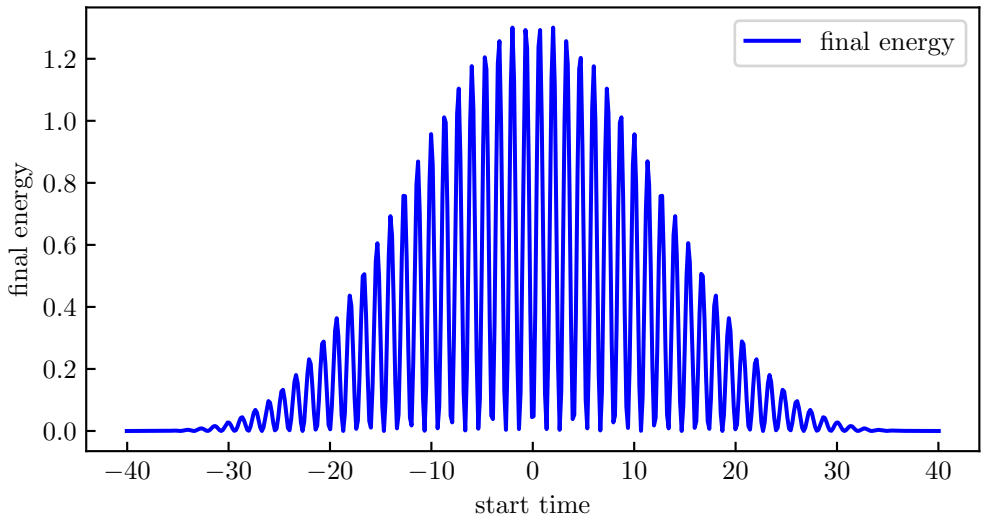

Fig. 5: Final energy of the electron for different initial times in the laser pulse.

The determination of the final energy was implemented rather simply in the following way:

```
points=500
start_time = np.linspace(0,Nt,points)
energy = np.zeros_like(start_time)
n=0

for i in start_time:
    x3 = np.zeros(len(t))
    v3 = np.zeros(len(t))
    integrate(i, E, dt, x3, v3)
    energy[n]=0.5*v3[-1]**2
    n += 1
```

We can see that the final energy peaks when the electron is inserted in the peak of the pulse. However, we also observe that the final energy does not rise continuously but rather oscillates quickly. It is presumed that the electron does not gain net energy when it is inserted at times where the field amplitude is zero.

2 Tunnel rate and simple man's model

2.1 Tunneling rate, single and multiple ionization

The instantaneous tunneling rate, calculated in three dimensions is given by

$$w = \left(\frac{3\mathscr{E}n^{*3}}{\pi Z^3}\right)^{1/2} \frac{Z^2}{4\pi n^{*3}} \left(\frac{2e}{n^*}\right)^{2n^*} \frac{(2l+1)(l+|m|)!}{2^{|m|}(|m|)!(l-|m|)!} \left(\frac{2Z^3}{\mathscr{E}n^{*3}}\right)^{2n^*-|m|-1} \exp\left(-\frac{2Z^3}{3n^{*3}\mathscr{E}}\right). \tag{2.1}$$

These rates can be used to calculate the ionization yield in a time window $[t_0, t_0 + \mathrm{d}t]$*, for which one has to solve a set of rate equations*

$$\frac{\mathrm{d}N_0}{\mathrm{d}t} = -N_0 T_0, \qquad \frac{\mathrm{d}N_1}{\mathrm{d}t} = N_0 T_0 - N_1 T_1, \qquad \frac{\mathrm{d}N_2}{\mathrm{d}t} = N_1 T_1 - N_2 T_2. \tag{2.2}$$

Solve the set of rate equations numerically for Xe (up to charge state Xe_6^+*). The relevant atomic parameters are contained in the function* set_atomic_parameters*. Use, for example, the following laser parameters to define a field:*

$$\tau = 10\,\mathrm{fs}, \quad \lambda = 800\,\mathrm{nm}, \quad I = 8\cdot 10^{14}\,\frac{\mathrm{W}}{\mathrm{cm}^2}. \tag{2.3}$$

Begin with a completely neutral target, $N_0(t=0) = 1, N_i(t=0) = 0\,\forall\, i > 0$*.*

a) *Plot the population of each charge state as a function of time.*

b) *Calculate the yield of each charge state at the end of the pulse,* $Y_j = N_j(\infty)$ *for various intensities* I *ranging from* $4\cdot 10^{12}$ *to* $8\cdot 10^{14}\,\frac{\mathrm{W}}{\mathrm{cm}^2}$*. Plot the resulting intensity dependent-yield curves, i. e.* $Y_j(I)$ *for all calculated charge states.*

c) *Perform the focal volume averaging in two dimensions by weighing the intensity-dependent results*

$$\overline{Y}(I_n) = I_n \sum_{i=1}^{n} \frac{Y(I_i)}{I_i}. \tag{2.4}$$

Plot the intensity dependent yield curves after focal volume averaging on a log-log scale. How do they compare to the results without focal volume averaging?

d) *How do the curves (with focal volume averaging) change if you allow for an additional term leading to the production of charge states* $n > 2$ *that depends on the tunneling rate for* $n-2$*, i. e.*

$$\begin{aligned}
\frac{\mathrm{d}N_0}{\mathrm{d}t} &= -(1-\alpha)N_0 T_0 - \alpha N_0 T_0 \\
\frac{\mathrm{d}N_1}{\mathrm{d}t} &= (1-\alpha)N_0 T_0 - (1-\alpha)N_1 T_1 \\
\frac{\mathrm{d}N_2}{\mathrm{d}t} &= (1-\alpha)N_1 T_1 - (1-\alpha)N_2 T_2 + \alpha N_0 T_0
\end{aligned} \tag{2.5}$$

with, e. g. $\alpha = 0.01$*? What characteristic effect is mimicked by this modification?*

a.) Solution: In order to retrieve the population of each charge state we need to solve equation (2.2) for all six charge states. For that we define a new function *integrate_Rate_equation* which already includes the α from the last task.

```
def integrate_Rate_equation(a,T,t):    # a = alpha, T = tunnel rate
  dt = t[1]-t[0]
  N = np.zeros((max_charge,len(t)))
  N[0,0] = 1                           # initial condition
  for i in range(len(t)-1):            # iterate over time
    for j in range(max_charge): # iterate over ionization states
      if(j==0):
      N[j,i+1] = N[j,i]-N[j,i]*T[j,i]*dt
      if(j==1):
      N[j,i+1] = N[j,i]+((1-a)*N[j-1,i]*T[j-1,i]-(1-a)*N[j,i]*T[j,i])*dt
      if(j==len(Z)):              # the last state is not further ionized
      N[j,i+1] = N[j,i]+(a*N[j-2,i]*T[j-2,i]+(1-a)*N[j-1,i]*T[j-1,i])*dt
      else:
      N[j,i+1] = N[j,i]+(a*N[j-2,i]*T[j-2,i]+(1-a)*N[j-1,i]*T[j-1,i]-(1-
                                              a)*N[j,i]*T[j,i])*dt
return N
```

This function requires the transition trate for each ionization process. This can be obtained by calculating the instantaneous tunneling rate given in (2.1). However, we have different tunneling rates for the various l and m. This is shown in figure 6.

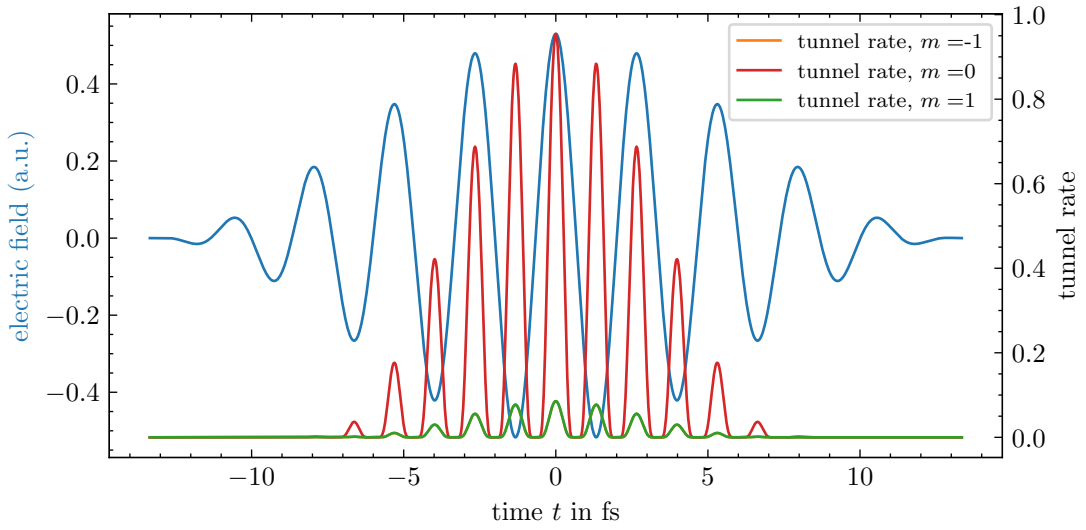

Fig. 6: Tunneling rates for the ground state of Xenon into the first ionized state for different m. We observe that the tunnel rate drops to zero when the E-field vanishes.

Since for Xenon $l = 1$ we have $m = -1, 0, 1$, therefore we must average over three tunneling rates. The averaged tunneling rates for all ionization states are depicted in figure 7.

Now we perform the integration visualize the population for every ionization state in a single plot. We can also compare the differences for different α values in figure 8.

By looking again at figure 7 we can explain the sudden jumps of population in figure 8. When the tunneling rate is high we observe a fast rise in the population state, where as for low

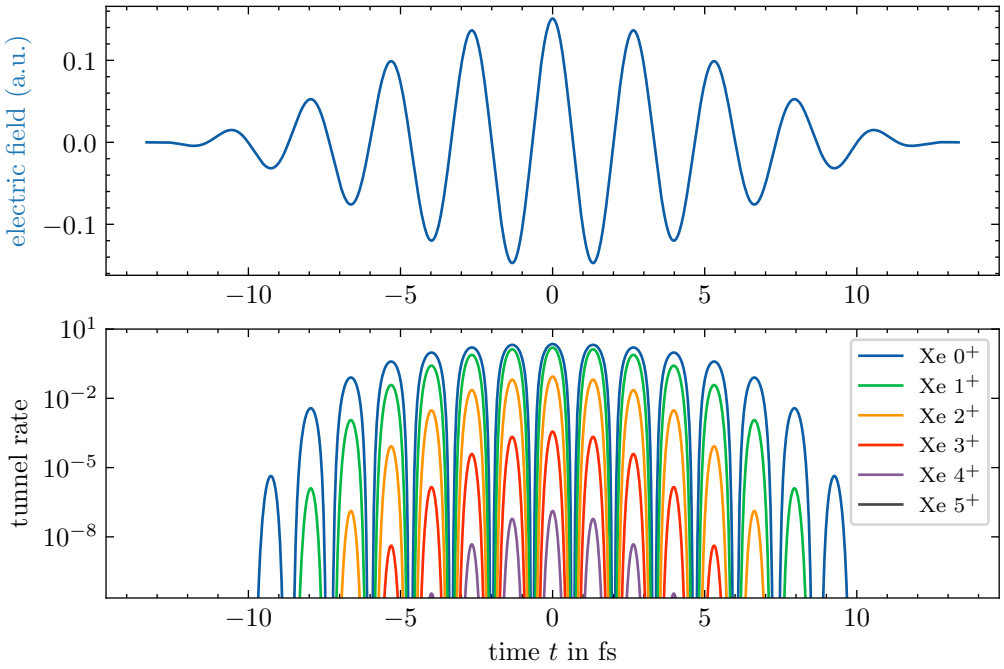

Fig. 7: Electric field and averaged tunneling rates for different ionization states. We can see that the tunneling rate drops significantly for higher ionization states.

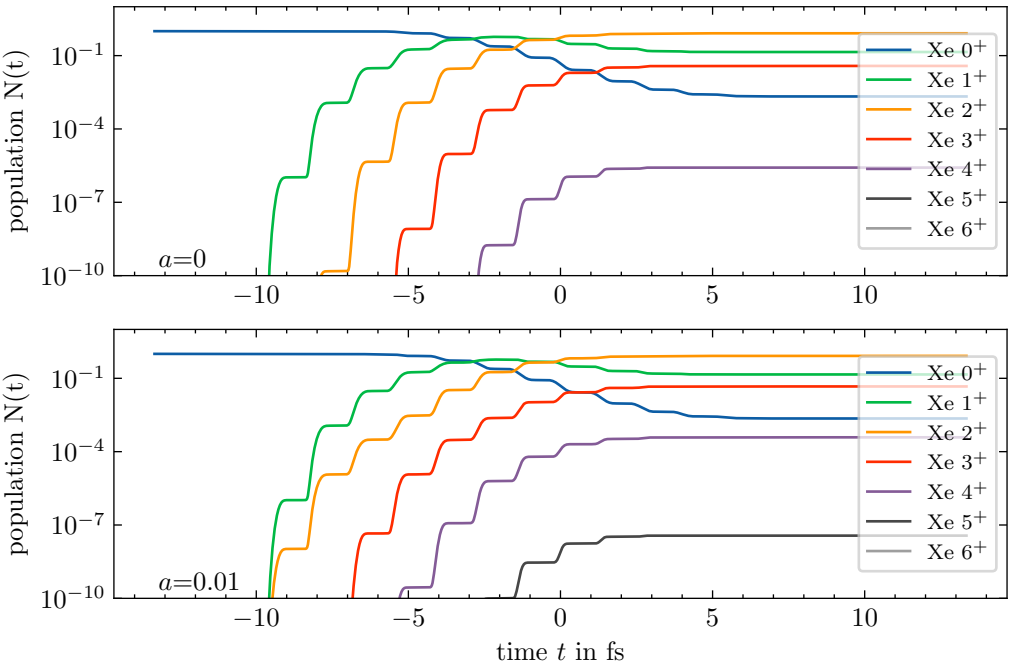

Fig. 8: Numerical integration of the rate equations for $\alpha = 0$ and $\alpha = 0.01$. We can see that for double ionization ($\alpha = 0.01$) the higher ionization states or more populated by several orders of magnitude, whereas the qualitative course of the charge states remains the same.

tunneling rates the population remains constant. After $t = 0$ there is no population left in the ground state and first excited state and the other population levels will go into equilibrium, since their tunneling rate is too low for further population changes.

b.) Solution: Now we want to calculate the yield of each charge state at the end of the pulse. Here we simply repeat the integration from a.) for various intensities and write the last value for every ionization state into a new array. Now we can plot the final population (yield) as a function of intensity. The results are displayed in figure 9.

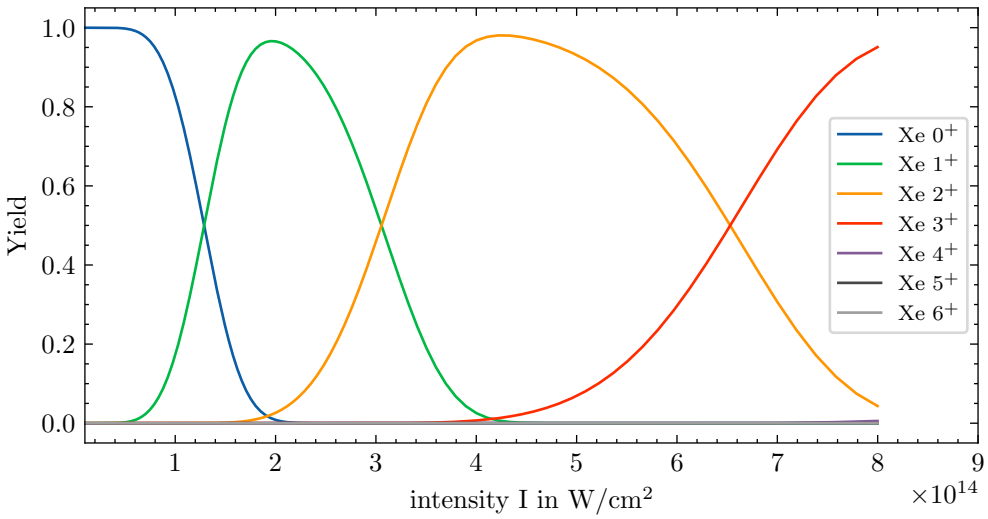

Fig. 9: Yield of each ionization state as a function of intensity for $\alpha = 0$ (no double ionization). We can see that an increase of intensity leads to stepwise ionization of the Xenon atoms.

c.) Solution: We can try to implement the focal volume averaging via a simple algorithm:

```
for n in range(len(I)):
    for i in range(n+1):
        Y_dash[:,n] += Y[:,i]/I[i]
    Y_dash[:,n] *= I[n]
```

We plot the new yield in a double logarithmic scale and compare this to the original yield (c. f. figure 9). We can see, that the yield for higher intensities stays high instead of dropping back down. This can be explained by considering the whole intensity profile of the tightly focused laser beam. There will be always a suitable frequency to generate more population in e. g. the first excited state. The graph is displayed in figure 10

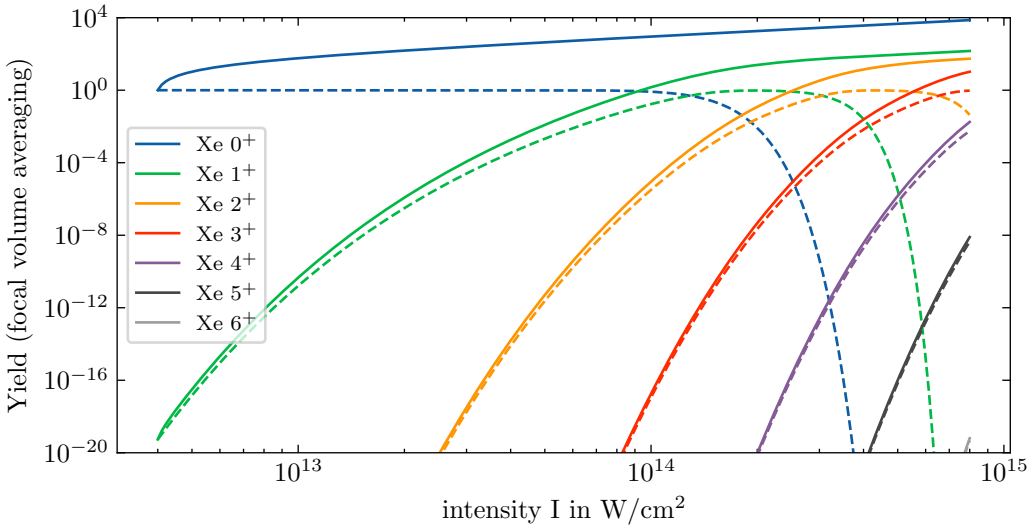

Fig. 10: Yield of each ionization state as a function of intensity with (solid line) and without (dashed line) focal volume averaging for $\alpha = 0$ (no double ionization). We can see that an increase of intensity leads to stepwise ionization of the Xenon atoms.

d.) Solution: Now we also change the strength of double ionization by adjusting the parameter α. The results are displayed in figure 11. We can see that for $\alpha > 0$ when non-sequential ionization takes place the yield of the e. g. second ionization state is magnitudes larger for lower intensities and already starts before the yield of the single ionized population is saturated.

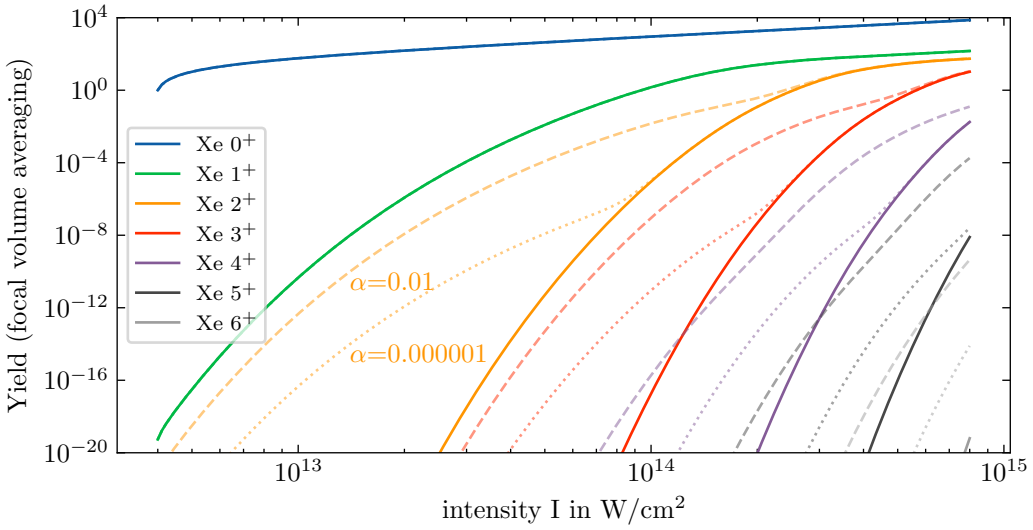

Fig. 11: Yield of each ionization state as a function of intensity for various α values. The dashed lines are the plots for $\alpha = 0.01$, whereas the dotted lines $\alpha = 0.000001$.

Reducing the alpha to significantly lower values still shows the same behaviour although it is relatively weakend. We observe that for higher intensities the curves merge with the case without non-sequential ionization.

2.2 Simple man's model: Direct electrons

The simple man's model describes a "cooking recipe" for calculating photoelectron spectra from strongfield inoization.

Implement the SMM and calculate spectra of photoelectrons for a reasonable combination of laser parameters and atom of your choice with and without focal volume averaging. Plot the kinetic energy distributions of the photoelectrons and compeare the results with and without focal colume averaging.

Solution: We use the same laser parameters as before ($\lambda = 800\,\text{nm}, \tau = 10\,\text{fs}, I = 8\cdot 10^{14}\,\frac{\text{W}}{\text{cm}^2}$) for this calculation and try to calculate the electron spectrum of Xenon. For that we again calculate the Transition rate and integrate the rate equations numerically. We now follow the simple mans model. In order to get the ionization yield per time step we subtract the take the difference of populations for every time step and ionization state.

Now we calculate the drift energy. We can use the result from the lecture

$$v_{\text{drift}}(t) = -A(t) \quad \text{with} \quad A(t) = -\frac{\partial E}{\partial t} \tag{2.6}$$

that the drift velocity can be expressed by the vector potential. In order to avoid integrating the electric field numerically for many time steps we calculate the vector potential analytically using Mathematica. The electric field used for the simulation is given as

$$E(t) = E_0 \cos(\omega t) \cos^2\left(\frac{t}{\tau}\right). \tag{2.7}$$

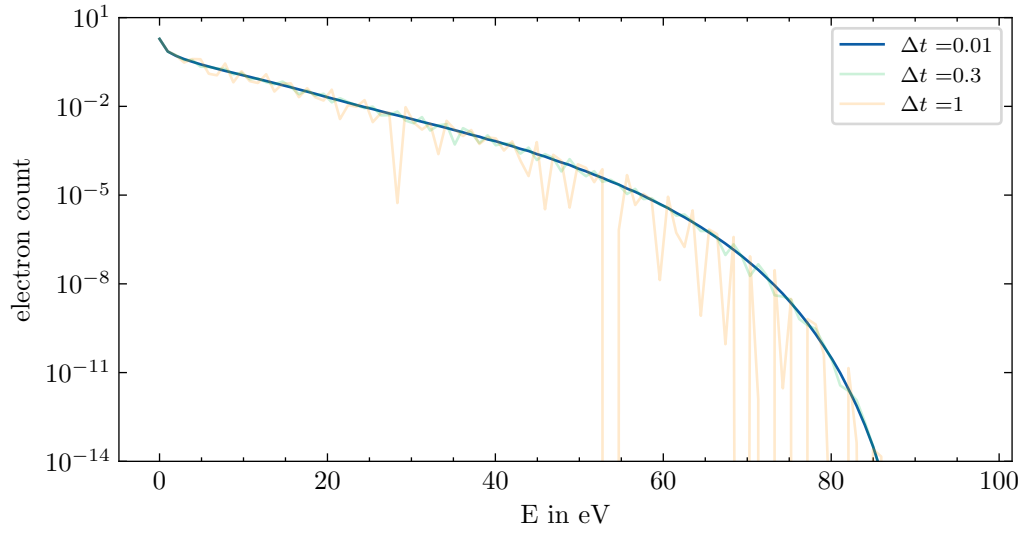

Fig. 12: Spectrum of emitted electrons for no non-sequential ionization. The calculation was performed for different integration step sizes Δt in the integration process.

The integration yields

$$A(t) = -\int E(t)\,\mathrm{d}t = -\frac{1}{4}E_0\left(\frac{2\sin(\omega t)}{\omega} + \frac{\tau\sin\left(\frac{t(\omega\tau-2)}{t}\right)}{\omega\tau-2} + \frac{\tau\sin\left(\frac{t(\omega\tau+2)}{t}\right)}{\omega\tau+2}\right) + C. \tag{2.8}$$

We can use this function to calculate the drift velocity and thus drift energy for every time step. Now we discretise the drift energy into 100 intervals and count the number of electrons in each energy interval. The resulting graph is shown in figure 12.

We observe that for the standard time step $\Delta t = 1$ there are energy intervals with no electrons corresponding to that energy. Therefore we further reduce the stepsize to obtain a smooth curve of data points. The course of this spectrum fits really well with the energy spectrum shown in the lecture.

Now we also try to implement the focal volume averaging. Here we calculate the electron spectrum for different intensities ranging from $4 \cdot 10^{12}$ to $8 \cdot 10^{14}$ $\frac{\mathrm{W}}{\mathrm{cm}^2}$. Then we weigh each spectrum with the corresponding intensity and add them up for the averaged value. Then we can compare the result to the spectrum without focal volume averaging. We normalize both spectra and set their maximum to one for a better comparison. The graph is displayed in figure 13.

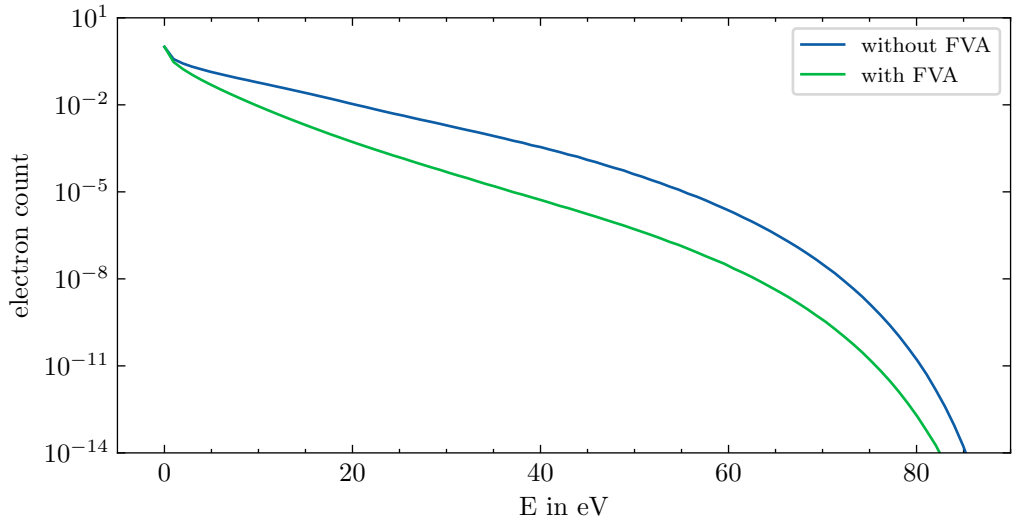

Fig. 13: Spectrum of emitted electrons for no non-sequential ionization with focal volume averaging (green) and without c. f. figure 12 (blue).

3 Tunnel rate and simple man's model

3.1 CEP effects in direct electrons 1

Consider a few cycle pulse

$$\mathscr{E} = \mathscr{E}_0(t)\cos\left(\omega t + \phi\right) \tag{3.1}$$

where the FWHM duration of $\mathscr{E}_0(t)$ is comparable to a laser cycle, e. e. 5 fs in case of a $\lambda = 800\,\text{nm}$ field ($T = 2{,}6\,\text{fs}$). Now, the carrier envelope phase ϕ becomes an important parameter. Using the code developed in Task 4.2, calculate the directional photoelectron spectra, i. e. those of electrons emitted to the left and right, as a function of CEP. Perfomr the calculations for an atom and laser parameters of your choice.

Plot the CEP-dependent asymmetry $A(\phi) = \frac{R-L}{R+L}$, where R and L are the number of electrons emitted to the right or left, respectively, as a function of CEP and drift momentum component along the laser polarization. At what pulse shapes (CEP values) are the maximum (minimum) symmetries obtained? How does the asymmetry depend on the drift momentum? What happens to the symmetry if you double (halve) the pulse duration?

Solution:

We start with our laser pulse which has a $\cos^2$ shaped envelope with a 5 fs FWHM duration, a wavelength of 800 nm (e. g. Ti:Sa), an intensity of $8 \cdot 10^{14}\,\frac{\text{W}}{\text{cm}^2}$. We want to investigate Xenon atoms. First we plot the electric field for different CEP values as shown in figure 14.

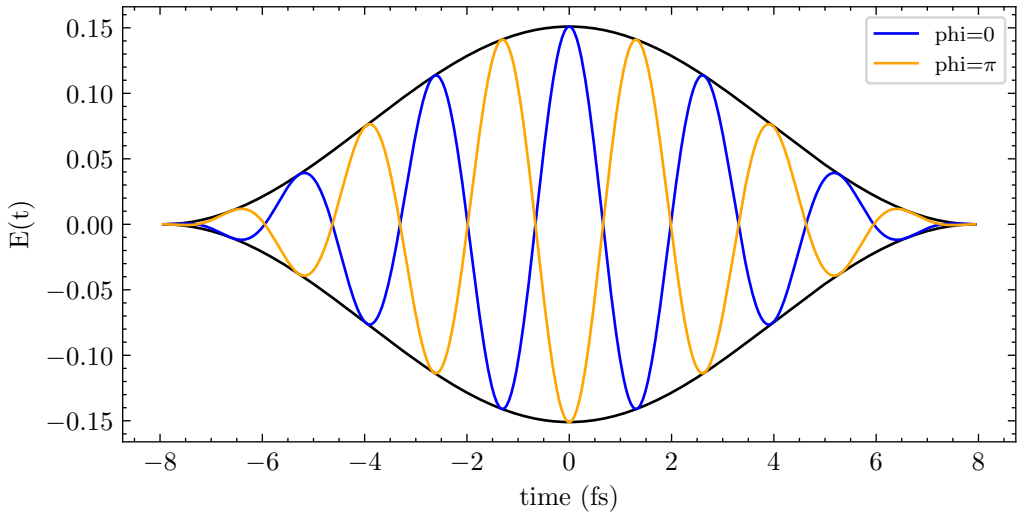

Fig. 14: Electric field for CEP = 0 (blue) and CEP = π (orange) for a 5 fs laser pulse.

We now modify our code differ between electrons with a positive drift velocity and negative drift velocity. We both count the electron yield for right emission (positive velocity) and left emission (negative velocity) and create a spectrum as in task 4.2. We calculated the spectra for seven different values of the CEP (figure 15).

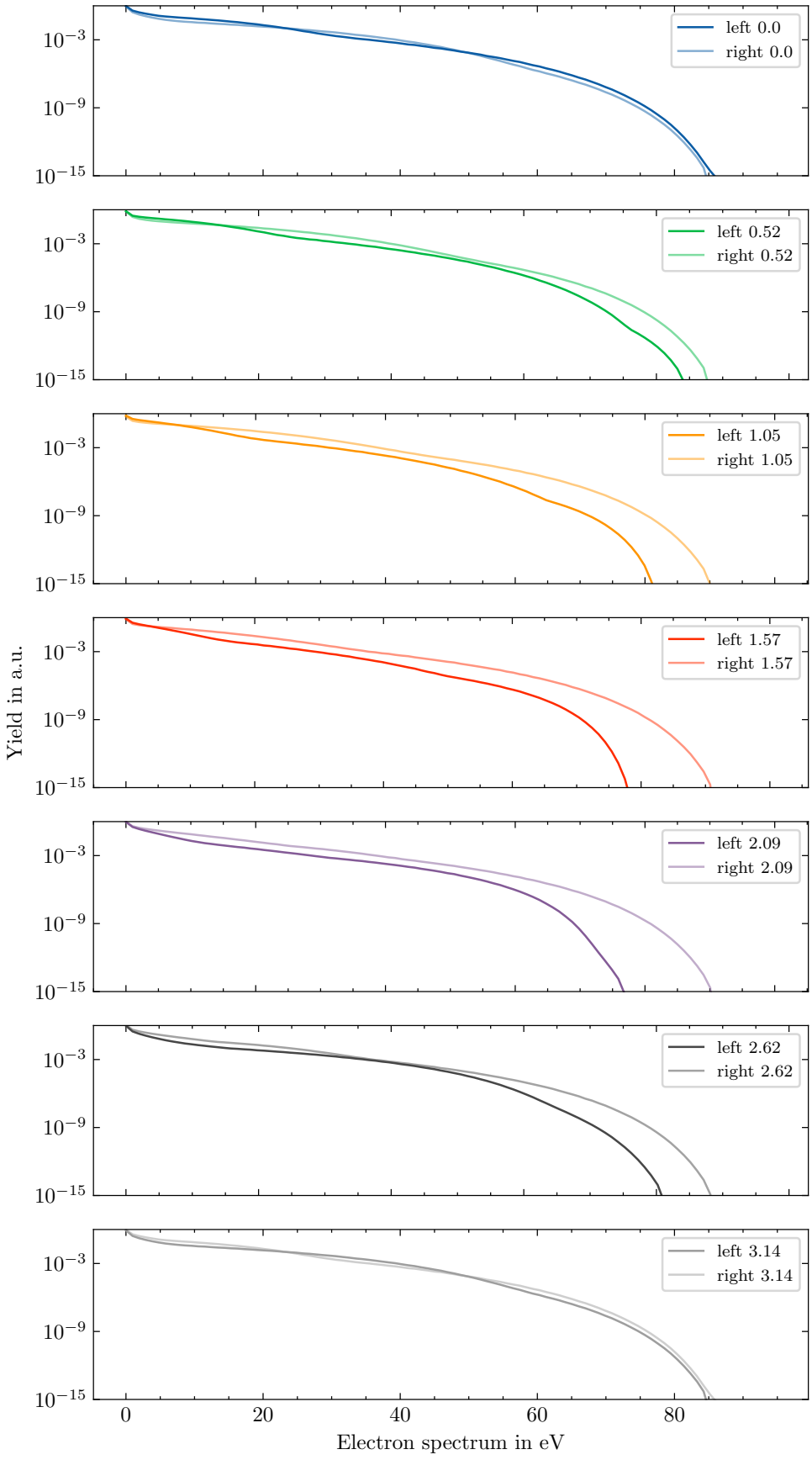

Fig. 15: Spectra of the emitted electrons for left and right emission and different values of the CEP ranging from 0 to π. We note that for CEP = π the number of electrons emitted to the left and right is reversed to the case of CEP = 0.

Now we continuously vary the carrier-envelope-phase and just calculate the total number of electrons emitted to the left and right by just summing up Spectra. We choose 100 values for the CEP ranging from 0 to 2π. For the 5 fs pulse we obtain a graph displayed in figure 17.

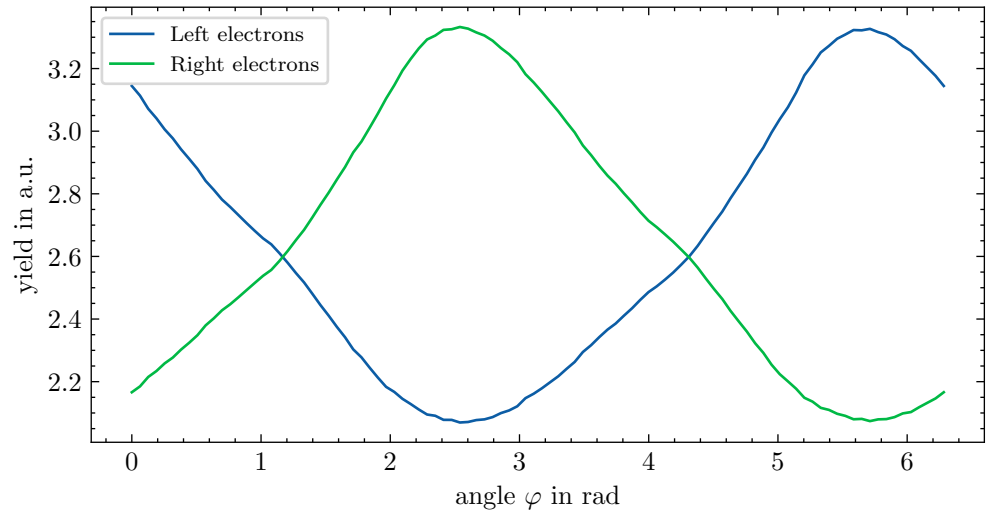

Fig. 16: Total number of electrons emitted to the left and right as a function of the carrier-envelope-phase.

Now we can also calculate the asymmetry $A(\phi) = \frac{R-L}{R+L}$. The respective graph is shown in figure 18.

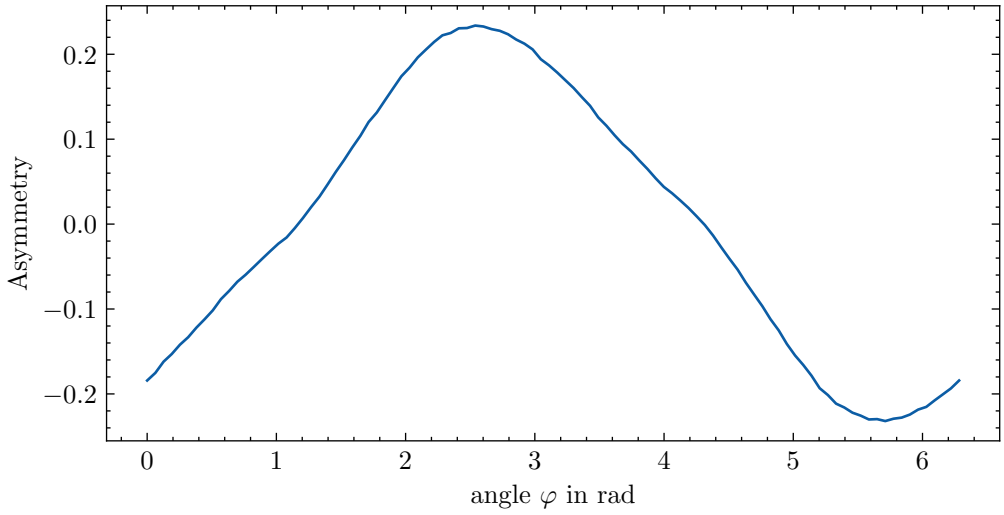

Fig. 17: Asymmetry as a function of the carrier-envelope-phase for a 5 fs pulse. We find the maximum value for the asymmetry at CEP = 1.66π and the minimum value at CEP = 0.63π.

Now we can also investigate what happens if we double or halve the pulse duration. Figure 18 shows the respective curves. One observes, that the asymmetry gets larger for smaller pulse durations. This may be explained by the vastly unsymmetric shape of the pulse in the few cycle case where the pulse is only two optical cycles 5 fs $\approx 2T$ long. For larger pulse duration the pulse gets more symmetrical which leads to a reduced asymmetry in the electron momentum distribution.

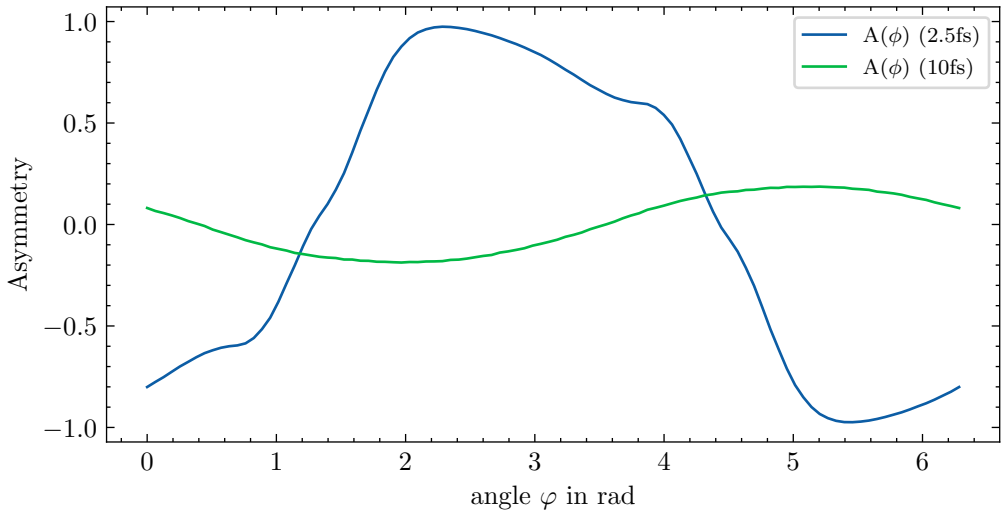

Fig. 18: Asymmetry as a function of the carrier-envelope-phase for a 2,5 fs pulse and a 10 fs pulse. For longer pulses the asymmetry becomes smaller. Note the different scaling in comparison to figure 17.

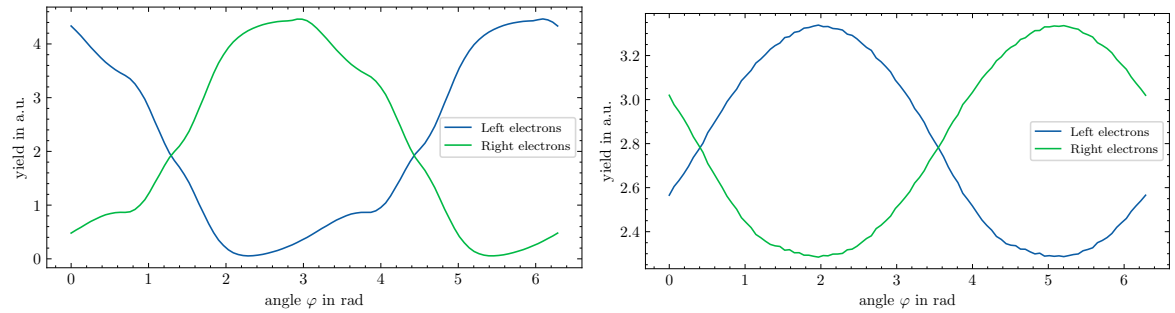

Fig. 19: Total number of electrons emitted to the left and right as a function of the carrier-envelope-phase for two different pulse lengths (left) 2,5 fs and (right) 10 fs.

3.2 Simple man's model: Direct electrons

Using (near) circular polarization $(0.9 < \varepsilon < 1)$ *allows fo an intriguing experiment known as attoclock. Extend your code to two dimensions and calculate the photoelectron momentum distribution for a circularly polarized few-cycle pulse.*

Perform the calculations for He ionized by a 4-fs laser pulse at 800 nm and $3 \cdot 10^{14} \frac{W}{cm^2}$ *peak intensity. Present results for a large value of ellipticity* ($\varepsilon = \frac{\mathscr{E}_y}{\mathscr{E}_x} = 0.95$)*. Plot the final momentum distribution in two dimensions, along with the electric field and compeare the two. Include focal volume averaging in order to obtain a distribution with a reasonable width. Interpret your result.*

Make a plot in which you relate the direction of the electric field vector (angle) at the time of tunneling to the direction of electron emission (angle of final momentum). What happens if you artificially introduce an ionization delay, i. e. assume that the electron spends some time (e. g. 100 as) in the tunnel before it is accelerated by the laser field? What is the effect of the CEP in this case?

Solution:

We first adapt our program to work in two dimension to allow circular polarization. For that we simply Calculate a second electric field which has a phase difference of $\Delta\varphi = \pi/2$ with respect to the other and modify its amplitude to account for the ellipticity. This looks like this:

```
[t,Ex]=get_field_time_sin2(Lambda, tau, intensity*ellipsy**2, cep, dt)
[t,Ey]=get_field_time_sin2(Lambda, tau, intensity, cep+np.pi/2, dt)
```

Now we calculate the transition rate for Helium using the intensity $I = \sqrt{E_x^2 + E_y^2}$ and determine the respective drift velocities $v_{x,\text{drift}}$ and $v_{y,\text{drift}}$. We now drop the analytical calculation of the drift velocity and implement a much faster method of integrating the electric field using the power of *numpy*:

```
for j in range(len(t)):
  vxdrift[j] = -np.sum(Ex[j:len(t)])*dt
  vydrift[j] = -np.sum(Ey[j:len(t)])*dt
```

Now we create a grid of 200×200 velocities ranging from the minimum to maximum drift velocity. Similar to the approach for the energy spectrum of the electrons we assign every grid point a number of emitted electrons by comparing the drift velocity at time t to the yield in the time interval $[t, t + \mathrm{d}t]$. The resulting graph is shown in figure 20 (left).

We can repeat the calculations with intensities in a logarithmic range between $3 \cdot 10^{11} \frac{\mathrm{W}}{\mathrm{cm}^2}$ and $3 \cdot 10^{14} \frac{\mathrm{W}}{\mathrm{cm}^2}$ weighed with their respective intensity and sum up the results to obtain a plot in the case of focal volume averaging. This is displayed on the right side of 20.

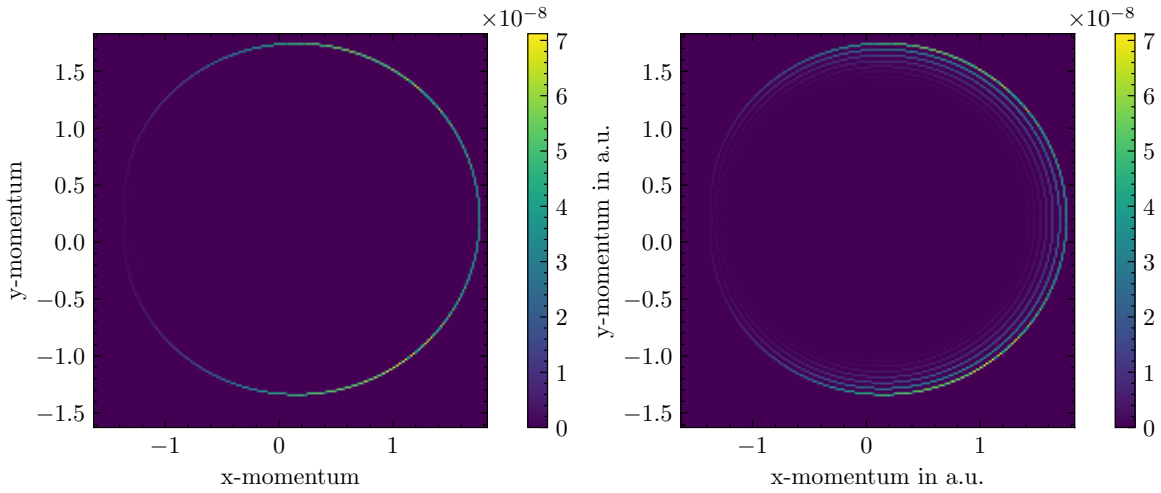

Fig. 20: 2D momentum distribution of the electrons without (left) and with focal volume averaging (right) for a carrier-envelope-phase of 0 and a pulse duration of 10 fs. We observe that the electrons are mainly moving in positive x-direction. This is explained by the higher electron yield in forward direction (c. f. 19 right) at CEP = 0. The y-distribution is nearly symmetric, however the center of the circle does not correspond to the origin.

We also want to display the electric field amplitude in two dimensions for all times. This is done in figure 21.

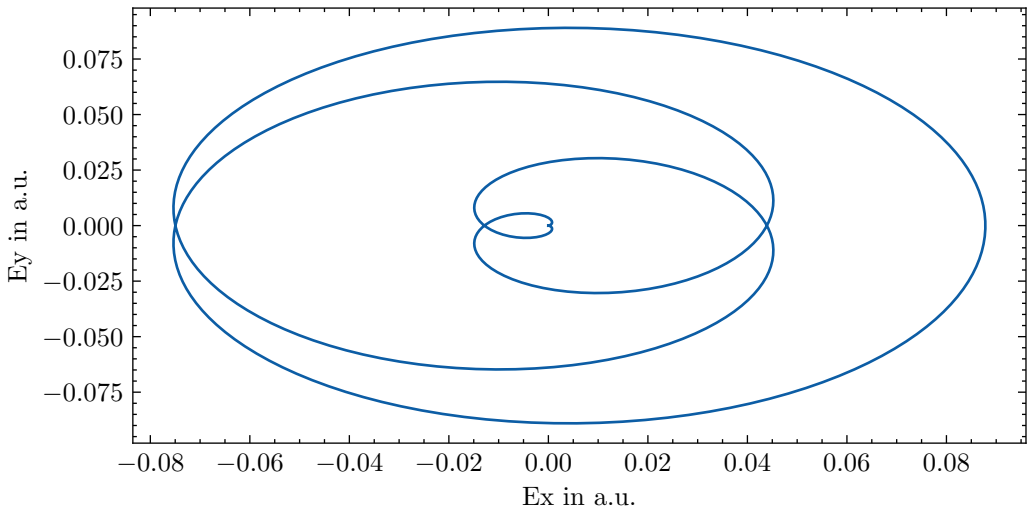

Fig. 21: 2D plot of the electric field for all times.

We observe that the electric field in y-direction is symmetric which is in agreement with the symmetric momentum distribution in y-direction. The electric field in x-direction is not symmetric which leads to a asymmetric behaviour in the momentum distribution in figure 20.

Now we want to relate the direction of the electric field vector at the tunnel time to the direction of electron emission. For both the electric field vector and the velocity we calculate the angle with respect to the y-axis in the following way:

```python
def angle_to_y_axis(x, y):
    v2 = np.array([vxdrift,vydrift])
    v2_u = v2/np.linalg.norm(v2)
    v1_u = np.array([0,1]) # y-axis
    if x >= 0:
        v1_u = np.array([0,1])
        return np.arccos(np.dot(v1_u, v2_u))
    if x < 0:
        v1_u = np.array([0,-1])
        return np.arccos(np.dot(v1_u, v2_u)) + np.pi
```

Using this function we can plot the angle of electron momentum and electric field as a function of time. This is shown in figure 22. We observe that the emission angle at first coincides with the electric field angle but drifts out of phase over time. We can now introduce an ionization delay of 100 as = 4 a.u. which leads to a small shift of the emission angles of the momentum.

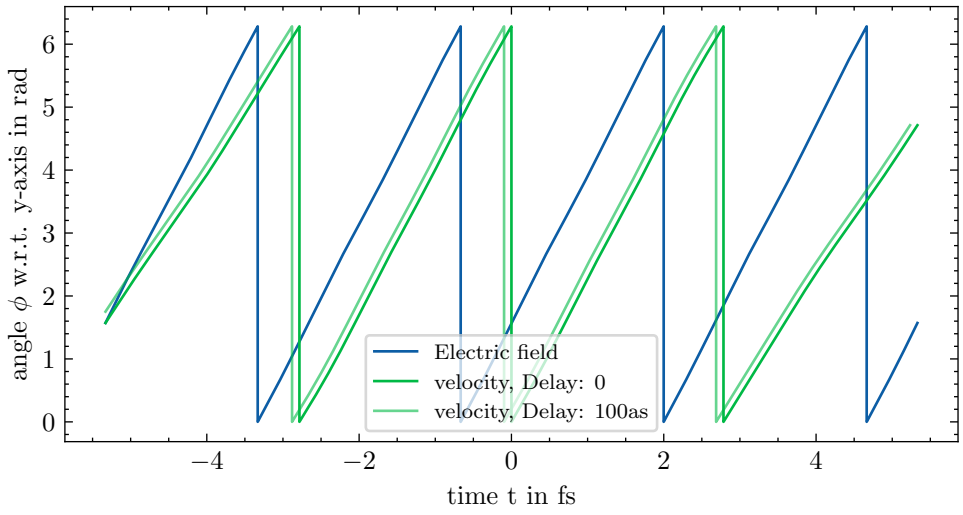

Fig. 22: Angle of electric field and drift momentum of the electrons for different times of tunneling.

Changing the CEP in this case leads to no qualitative change in the emission angles. It only shifts the values along the "y-axis". For a better visualization we can apply a phase unwrap to the date in figure 22 which is shown in figure 22.

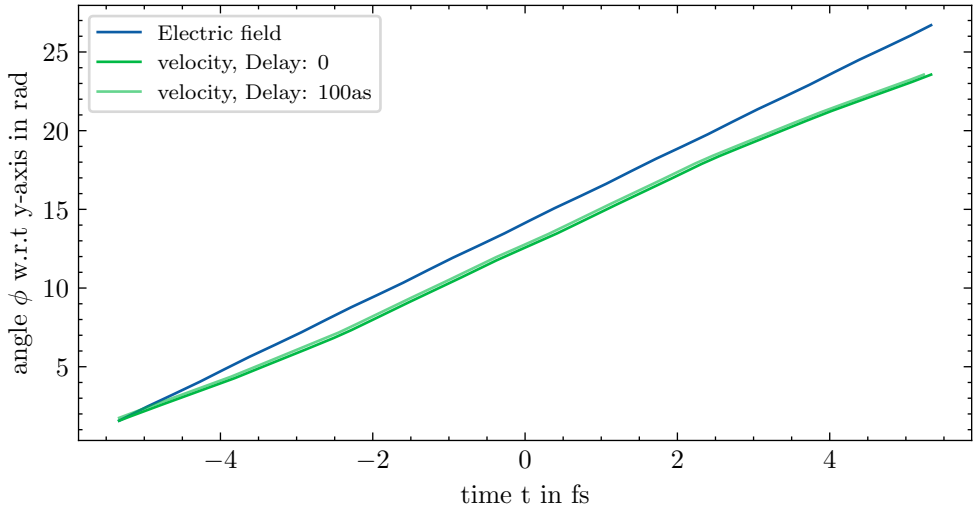

Fig. 23: Unwrapped angle of electric field and drift momentum of the electrons for different times of tunneling.

4 Recollisions

4.1 Return energy and return time

In a linearly polarized laser field, electrons emitted after the field has passed its peak value can recollide with the parent ion, roughly a 3/4 *of an optical cycle later. This idea links laser-matter interactions with collision physics and is responsible for characteristic effects, including HHG, high-order ATI (above threshold ionization) and NSDI (non-sequential double ionization).*

Define the electric field of a linearly polarized femtosecond laser pulse and calculate numerically the recollision time and energy of recolliding electrons (in units of the ponderomotive potential U_P), as a function of the ionization time. Plot the relationship between travel time (i. e. the time difference between tunneling and recollision) and return energy. What is the consequence of the relationship between the return energy and the return time for the XUV radiation generated by HHG? (bonus)

Solution:

As in the previous exercises, we start with our laser pulse which has a $\cos^2$ shaped envelope with a 10 fs FWHM duration, a wavelength of 800 nm (e. g. Ti:Sa), an intensity of $3 \cdot 10^{14} \frac{\mathrm{W}}{\mathrm{cm}^2}$. Now we can simply solve the equation of motion for the electron for all tunneling times in the laser cycle. We can determine the recollision time by looking, when a sign change of the electron position x occurs. This can be implemented numerically by taking the sign of the array of positions, shifting it by one place and subtracting it from the original one. A sign change can then be identified by looking at the maximum (of the absolute value) of the resulting array:

```
for i in range(len(t)):
  x,v = integrate(i, E, dt)

  signchange = abs(np.roll(np.sign(x), 1) - np.sign(x)) # shift sign
                                                        array by 1 step
  signchange[0] = 0 # set first index to zero (sign change between
                                                        first and last element)
  index = np.argmax(signchange) # find position of sign change
  if np.max(signchange) == 0:   # if no sign change occurs, set t1=t
      index = i
  t1[i] = t[index]
```

We can then then plot the time difference of ionization and recollision for every point in time. This is shown in figure 24.

We can see that the return time changes periodically with a frequency of the laser field. Several high spikes occur for larger times which seem a bit mysterious. They all indicate a recollision of the electrons when the laser pulse has passed. We assume that these are numerical artifacts and the highest possible return time is about 100 a.u..

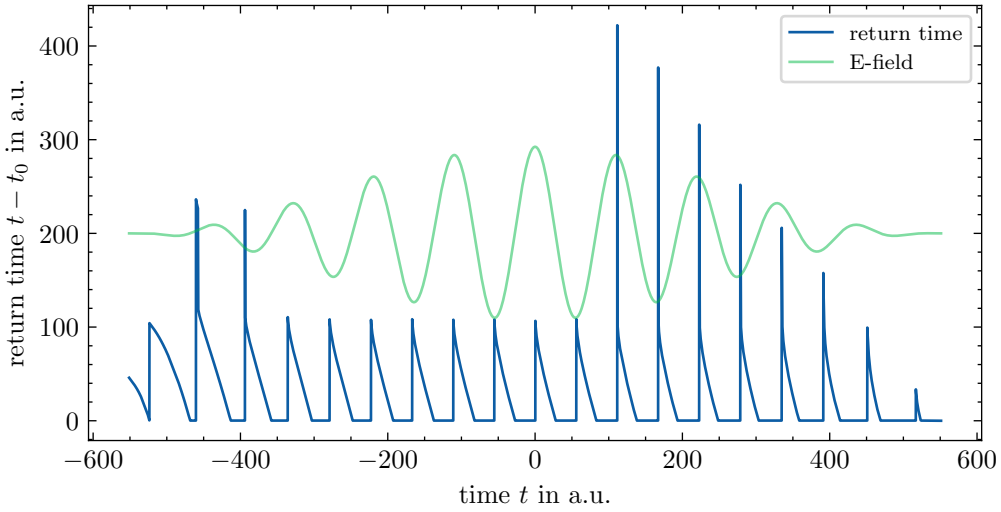

Fig. 24: Recollision times of the electrons as a function of the ionization time t shown in blue. The electric field is also displayed qualitatively. We observe that a maximum of travelling time ($(t_1 - t) \approx 110$ a.u.) occurs when the amplitude of the electric field is at its maximum. This maximum travelling time corresponds to one optical cycle.

We can also calculate the return energy by using equation (5.7) from the script

$$E_1 = \frac{m}{2} v^2 = \frac{e^2}{2m} (A(t_0) - A(t_1))^2. \tag{4.1}$$

If we want to express the return energy in units of the ponderomotive potential we can use the relation $A_0^2 = 4U_P$ (in atomic units).

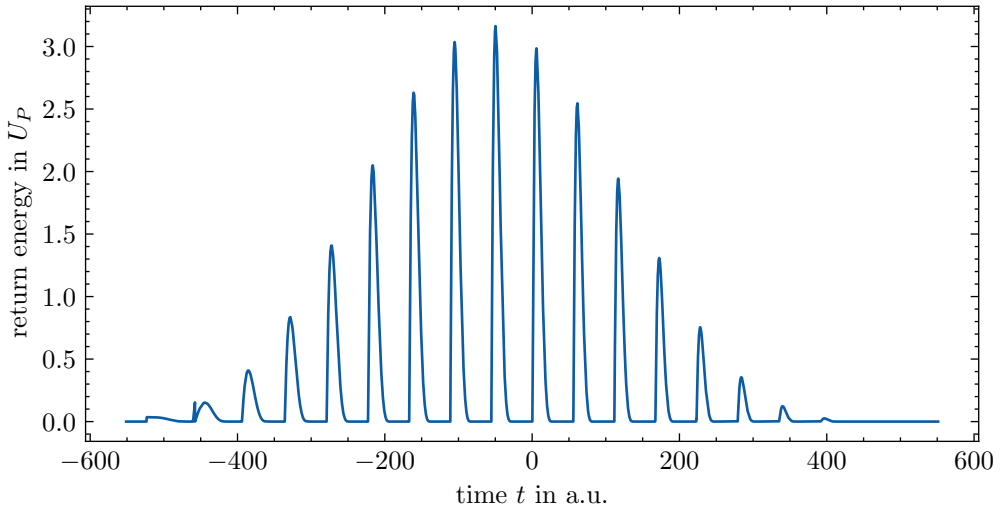

Fig. 25: Energy of the recolliding electrons in unit of the ponderomotive potential. We observe the limits $E < 3.17U_P$ that were derived in the lecture (chapter 5.3). More precisely the maximum of the return energy is $3.163U_P$.

The vector potential can be obtained by performing the integral

$$A(t_0) = -\int_{t_0}^{\infty} E(t')\,\mathrm{d}t'\,. \tag{4.2}$$

The resulting energy is displayed in figure 25. However, we still need to clarify how we obtained the ponderomotive potential U_P for our laser parameters. For that we used equation (1.30) from the script

$$U_P = 0.09337\, I \cdot \lambda^2 = 18\,\mathrm{eV} \tag{4.3}$$

where I is given in units $\frac{\mathrm{W}}{\mathrm{cm}^2}$ and λ in µm.

We can also show the relationship between the return energy and the return time in a nice looking plot (figure 26).

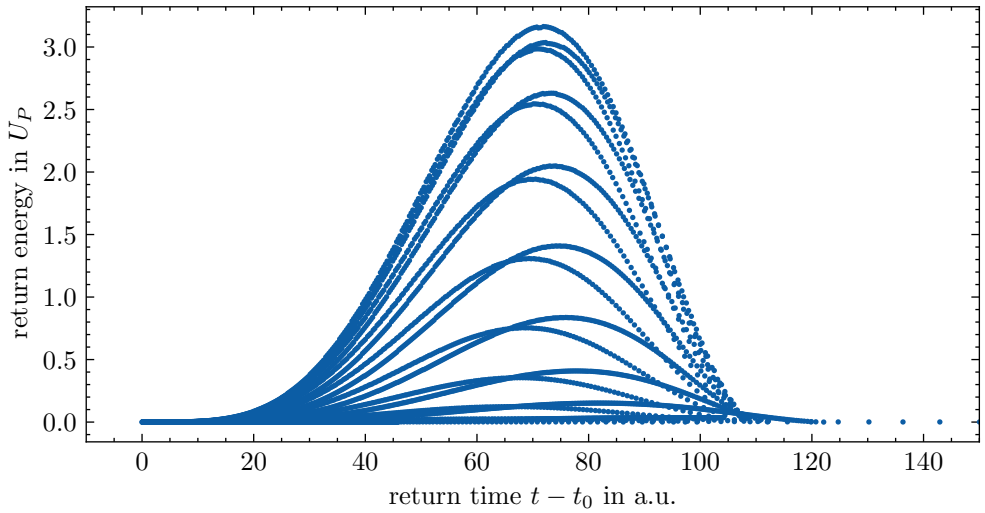

Fig. 26: Relationship between return energy (in units of U_P) and return time $t_1 - t$. We can see that medium return times correspond to the highest energies.

4.2 Backscattered electrons

The electron can also scatter elastically. Making use of the calculations developed in 4.1, extend your 1D simulations to accommodate back-scattering. For back-scattering, assume that the electron is reflected upon recollision, i. e. $v(t_1 + \mathrm{d}t) = -v(t_1)$*, where* t_1 *is the recollision time.*

Calculate photoelectron spectra (in 1D) that contain contributions from both direct and rescattered electrons, where you assume that 1 % of recolliding electrons back-scatter. Use laser parameters of your choice. Plot the resulting photoelectron spectrum on a logarithmic scale. Find the cut-off energies of direct and backscattered electrons and compare to your expectations.

As in problem 3.1, plot the CEP-dependent asymmetry $A(E,\varphi) = \frac{R-L}{R+L}$*, where* R *and* L *are the number of electrons emitted to the right or left, respectively, as a function of CEP and kinetic energy. Describe the characteristic signature of back-scattered electrons in the CEP-dependent asymmetry. How can this be utilized to measure the (relative) CEP?*

Solution:

We use the same laser parameters as before ($I = 3{\cdot}10^{14}\,\frac{\mathrm{W}}{\mathrm{cm}^2}$, $\tau = 10\,\mathrm{fs}$, $\lambda = 800\,\mathrm{nm}$) for this task. The ionizing atom was chosen to be Xenon. We now modify the scheme for the calculation of electron spectra to account for backscattering. We add an additional condition, that the drift velocity of electrons returning to the atom is determined by

$$m v_{\mathrm{drift}} = 2A(t_1) - A(t_0) \tag{4.4}$$

(in atomic units). Then we assume that only 1 % of these electrons rescatter, while the rest recombines with the atom and is lost. Then we sort the electrons whether they are emitted to the left or right and present the results in figures 27 and 28.

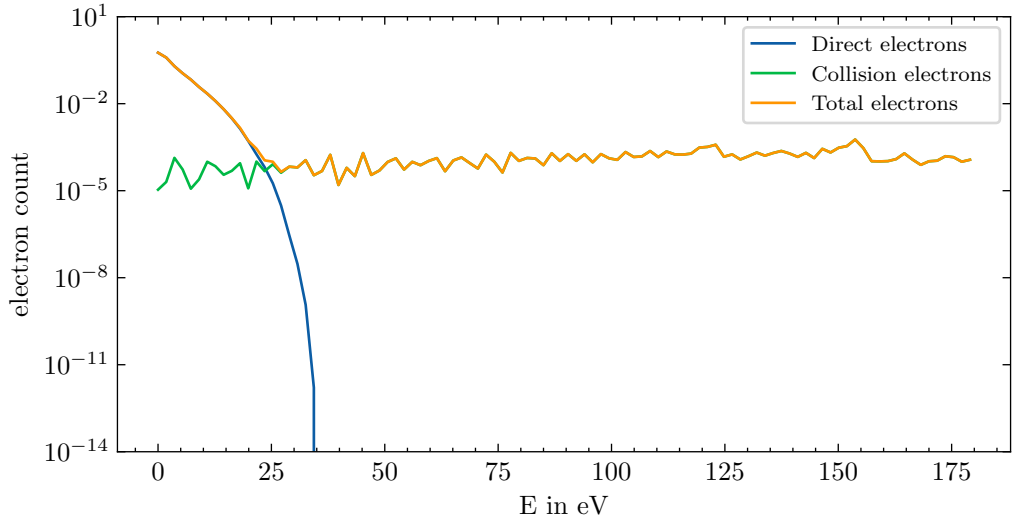

Fig. 27: Photoelectron spectra separated into two parts containing both direct and rescattered electrons.

For direct electrons we observe the same behaviour as in section where we applied the simple mans model to calculate photoelectron spectra. The cut-off of the direct electrons occurs at 35 eV. The cut-off energy of backscattered (collision) electrons is determined by the ponderomotive potential. It appears at $E_{\max} = 180\,\text{eV} = 11.25U_P$. This value seems rather odd because the derived maximum in the lecture states, that $E_{\max}$ should be around $10U_P$. We also plotted the spectrum for left and right emitted photons as shown in figure 28.

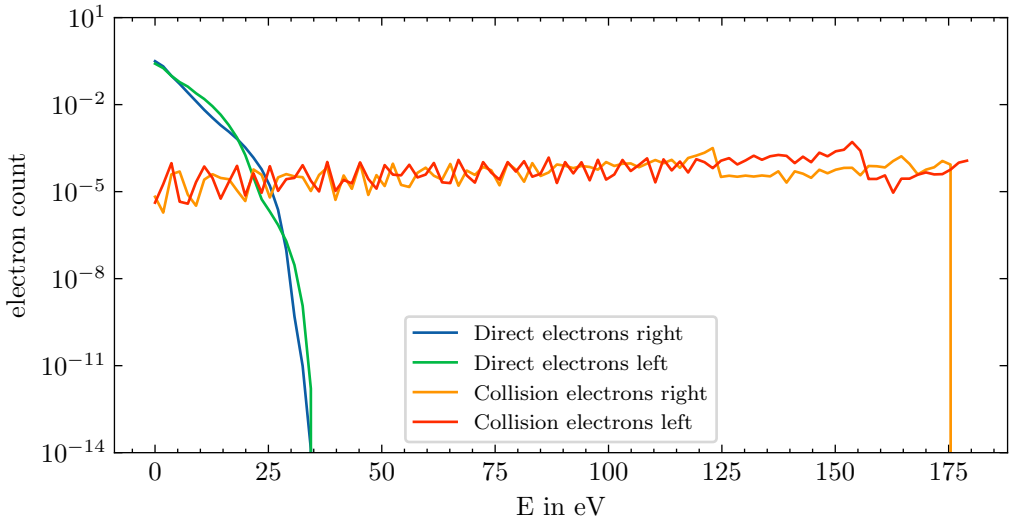

Fig. 28: Photoelectron spectra separated into two parts containing both direct and rescattered electrons. Now we also look at the different emission directions of the electrons, left and right, respectively.

Now we can also perfom the calculations for various values of the CEP. We choose an interval of $[0, 2\pi]$ with 150 sample points. The total emitted photelectrons and the respective asymmetry are displayed in figure 29.

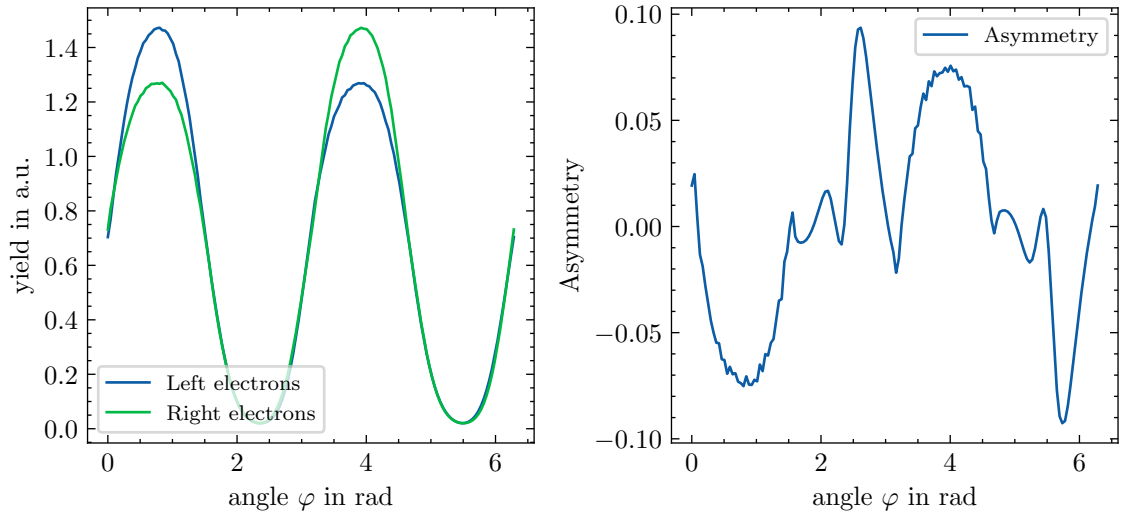

Fig. 29: Left: Total number of electrons emitted to the left and right as a function of CEP.
Right: Calculated asymmetry $A(\varphi) = (R - L)/(R + L)$.

Now we can also take a look at the Asymmetry also as a function of final kinetic energy. For

that we make a two dimensional plot and indicate the asymmetry with colours. First we can display the electrons emitted to the left and right (figure 30).

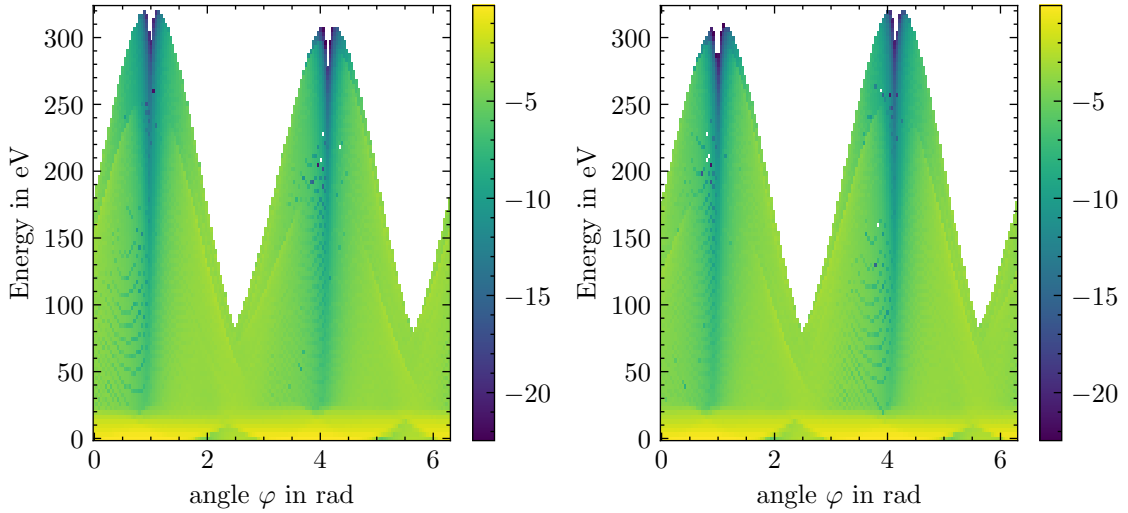

Fig. 30: Left (left figure) and right (right figure) emitted electrons as a function of CEP and final kinetic energy. The colours are rescaled on a logarithmic ($\log_{10}$) scale.

Finally we can also plot the resulting asymmetry as a function of Energy and CEP (figure 31). The maximum final kinetic energy is about $E_{\max} = 320\,\text{eV} = 20U_P$ which is twice of what we would expect based on the lecture. I am not sure what could have caused this discrepancy since the energy in figure 25 was calculated correctly.

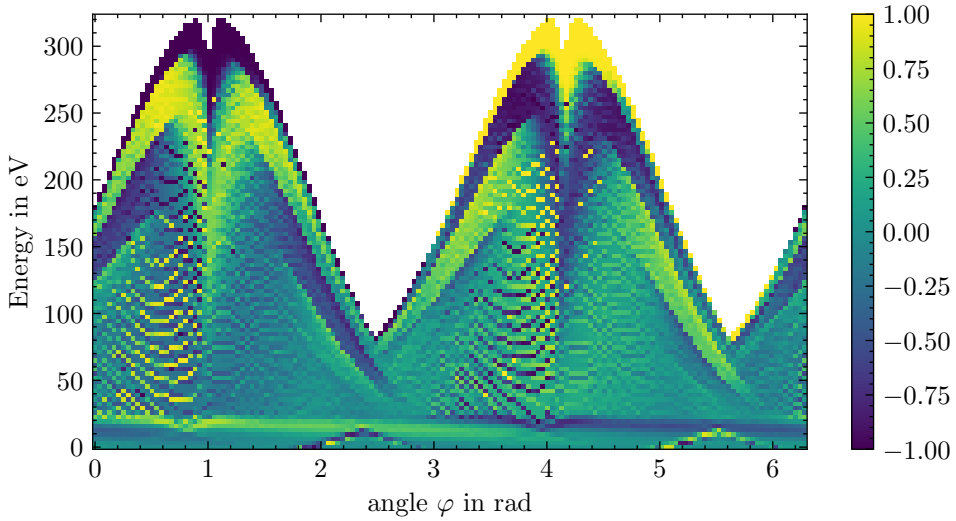

Fig. 31: Calculated asymmetry as a function of final kinetic energy and CEP. The white areas correspond to energies, where no electrons are emitted and the Asymmetry is undefined. We observe that the maximum kinetic energy strongly depends on the carrier envelope phase (which I do not really understand).

Now we want to discuss how we can utilize the results to measure the relative CEP of our laser pulse. For that we take a look back to figure 28 where we plotted the different emission directions of rescattered electrons. For larger energies we see two asymmetry for left and

right photoelectrons which differ in sign. Looking at figure 31 we should expect that these regions would appear and be shifted in phase. Now we could plot the asymmetry for both regions in a 2D plot to obtain a Lissajous figure. With that we could potentially obtain the carrier envelope phase shift.

5 Interference effects

5.1 ATI peaks and intracycle interference

The above threshold ionization peaks can be understood as constructive interferences of electron trajectories launched at times $(t_0, t_0+T, t_0+2T, \ldots)$*. In order calculate the photoelectron yield arising from all interfering trajectories, we consider not only the ionization rate* $R(t_0)$ *but also the classical action*

$$S(t_0) = \int_{t_0}^{\infty} \mathscr{L}[x_{t_0}(t)]\,\mathrm{d}t\,, \tag{5.1}$$

where $\mathscr{L}[x_{t_0}(t)]$ *is the Lagrange function of a trajectory* $x_{t_0}(t)$ *that describes the motion of an electron tunneling at time* t_0*. The yield for electrons with drift momentum* p *is given by the coherent sum over all contributing trajectories that result in drift momentum* p

$$Y(p) = \Big| \sum_{-A(t_0)=p} \sqrt{R(t_0)} \exp\left(\mathrm{i}\frac{S(t_0)}{\hbar}\right)\Big|^2. \tag{5.2}$$

Extend your code to calculate the classical action for direct electrons. Utilize the action to calculate a photoelectron spectrum of direct electrons that contains interference effects. Plot the electron spectrum for laser parameters of your choice. Specify the parameters.

Did you discover the ATI peaks? What happens if you vary the laser wavelength or the intensity?

Solution:

We start again by first stating all relevant laser parameters that were used for the numerical simulation. We use a wavelength of $\lambda = 800\,\mathrm{nm}$ with our laser pulse which has a $\cos^2$ shaped envelope with a 10 fs FWHM duration and an intensity of $10^{14}\,\frac{\mathrm{W}}{\mathrm{cm}^2}$ [1]. The atom of choice was Xenon.

We start with the definition of the Lagrange function that was given in the lecture as

$$\begin{aligned}\mathscr{L} &= \frac{1}{2}mv^2 + e\mathscr{E}x \\ &= \frac{1}{2}[A(t) - A(t_0)]^2 + \mathscr{E}(t)\left[A(t_0)(t-t_0) - \int_{t_0}^{t} A(t)\,\mathrm{d}t\right].\end{aligned} \tag{5.3}$$

With the second expression we only need to calculate the vector potential once in order to calculate the Lagrange function for all ionization times. This can be implemented in the following way

[1] We take a lower intensity than before in order to prevent saturation effects.

```
def action(A, E, t, t0): # script page 102
    dt = t[1] - t[0]
    A0 = A[t == t0]
    L = np.zeros_like(t)
    t0_index = np.argmin(abs(t-t0))
    for i in range(t0_index, len(t)):
        L[i] = 0.5*(A[i]-A0)**2 + E[i]*(A0*(t[i]-t0)- np.sum(A[
                                                t0_index:i])*dt)

    return np.sum(L)*dt
```

The calculation of the action is rather involved and takes a lot of time, because for every ionization time t_0 one must calculate $\mathscr{L}[x_{t_0}(t)]$ for all $t > t_0$ and sum them up to obtain the action. Therefore in the numerical simulation I could only analyze short pulses with a low sample size (2000) in order to have reasonable computation times.

We can now calculate the action for all ionization times t_0 and get a result that is displayed in figure 32

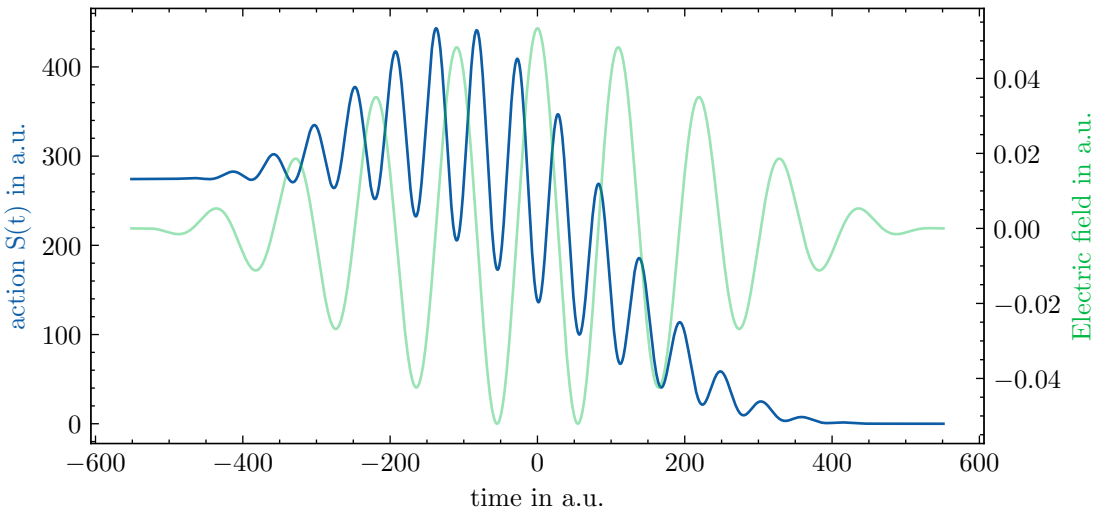

Fig. 32: Classical action of the ionized electrons for different ioniziation times t_0 (blue) for a 10 fs pulse at 800 nm. The electric field amplitude is also plotted in green. We observe that the action oscillates in a periodic fashion with twice the freqeuncy of the laser pulse. We observe local minima in the action, when the electric field has a maximum or minimum. For larger times the action goes to zero as expected.

Now we can obtain the electron spectrum in a similar way as we already did in the previous exercises. The only difference is that the yield is given by (5.2). Again we calculate the drift velocity of electrons and sum up all terms with drift energy $E \in [E_{\text{drift}}, E_{\text{drift}} + \mathrm{d}E]$.

```
def calc_spectrum(S, Nspec, Lambda, intensity):
    [t,E] = get_field_time_sin2(Lambda, tau, intensity, cep, dt)
    T = tunnel.calculateTransitionRate(t,E,1, Z, Ip)
    R = np.sum(T, axis=0)
    vdrift = np.zeros_like(t)
```

```
    for j in range(len(t)):
        vdrift[j] = -np.sum(E[j:])*dt

    Edrift = 0.5*vdrift**2
    Emin = np.min(Edrift)
    Emax = np.max(Edrift)

    Energy = np.linspace(Emin, Emax, Nspec)
    Spectrum = np.zeros_like(Energy, dtype=complex)
    Yield = np.sqrt(R)*np.exp(1j*S)

    for i in range(len(Edrift)):
            j = round((Edrift[i]-Emin)/(Emax-Emin)*(Nspec-1))
            Spectrum[j] += Yield[i]

    return Energy*27.2, np.abs(Spectrum)**2
```

Since we used Xenon as the ionizing atom, we had several ionization states. For the transition rate R we summed up all tunnel rates T of the different ionization states. The spectrum was divided into 500 grid points. The resulting spectrum as function of Energy is displayed in figure 33.

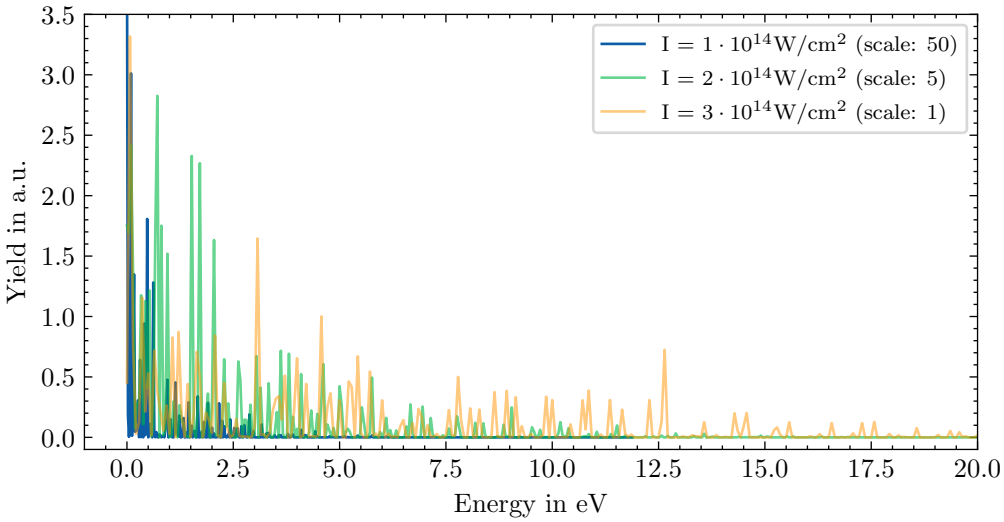

Fig. 33: Electron spectra (of direct electrons) for different laser intensities at 800 nm. For better visulization, the scales were adjusted for the first two spectra. We observe that for lower intensities the total yield is much lower but shifted towards lower energies. For the given wavelength the distance of the ATI peaks should be 1,55 eV.

We can see that the appearing peaks in the spectrum are not equidistant. However, the main peaks of the spectrum are indeed one photon energy (1,55 eV) apart which indicates, that these are indeed ATI peaks. We do not observe channel closing at higher intensities. This may be explained by the fact that we used femtosecond pulses for the calculations. According to equation (6.3) in the script the gained electron energy (for fs-pulses) is given by

$$E_m = m\hbar\omega - E_{\mathrm{IP}} - U_{\mathrm{P}}. \tag{5.4}$$

Since the ponderomotive potential U_P depends on the intensity, the position of the peaks in the energy spectrum is different for the various intensities shown in figure 33. Then it is difficult to identify peaks that correspond to the same order of multiphoton interaction.

Now we also vary the laser wavelength and use a laser intensity of $2 \cdot 10^{14} \frac{\mathrm{W}}{\mathrm{cm}^2}$. This yields spectra displayed in figure 34. We would expect that for longer wavelengths the observed ATI

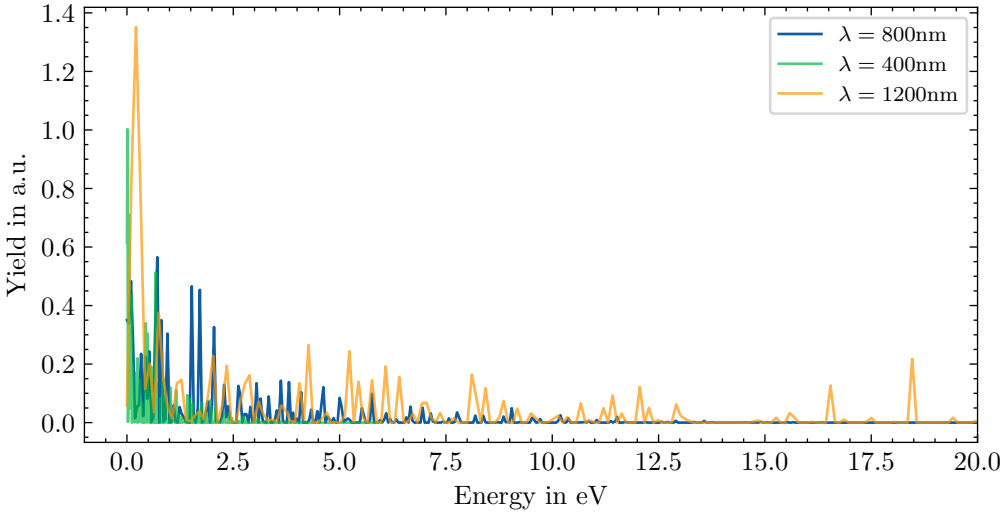

Fig. 34: Electron spectra (of direct electrons) for different laser wavelengths at $2 \cdot 10^{14} \frac{\mathrm{W}}{\mathrm{cm}^2}$. For higher wavelengths the maximum gained energy is higher.

peaks would be getting closer since the photon energy is lower. For some unknown reason we do not observe this effect.