CUED

Computing Ultrafast Electron Dynamics

Output summary of the CUED program

The CUED program is developed and maintained by:

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Run time: 83.9 s

Number of used processors: 1

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Contents

1 Electric-field pulse

The following electric driving field is employed in the simulation:

$$\mathbf{E}(t) = E(t)\,\hat{e}_\phi\,, \qquad E(t) = E_0\,\sin\Big(2\pi f_0\,(1 + f_{\text{chirp}}t)\,t + \varphi\Big)\,e^{-t^2/\sigma^2}\,. \tag{1}$$

The pulse is sketched in Fig. 1. The following parameters are used in the simulation:

- Amplitude: $E_0 = 10.0\,\text{MV/cm}$
- $\hat{e}_\phi = \hat{e}_x$
- Pulse frequency: $f_0 = 90.0\,\text{THz}$
- Chirp: $f_{\text{chirp}} = 0.0\,\text{THz}$
- Carrier-envelope phase: $\phi = 0.0$
- $\sigma = 25.0\,\text{fs}$, full width at half maximum (FWHM) of the Gaussian envelope = 41.628 fs

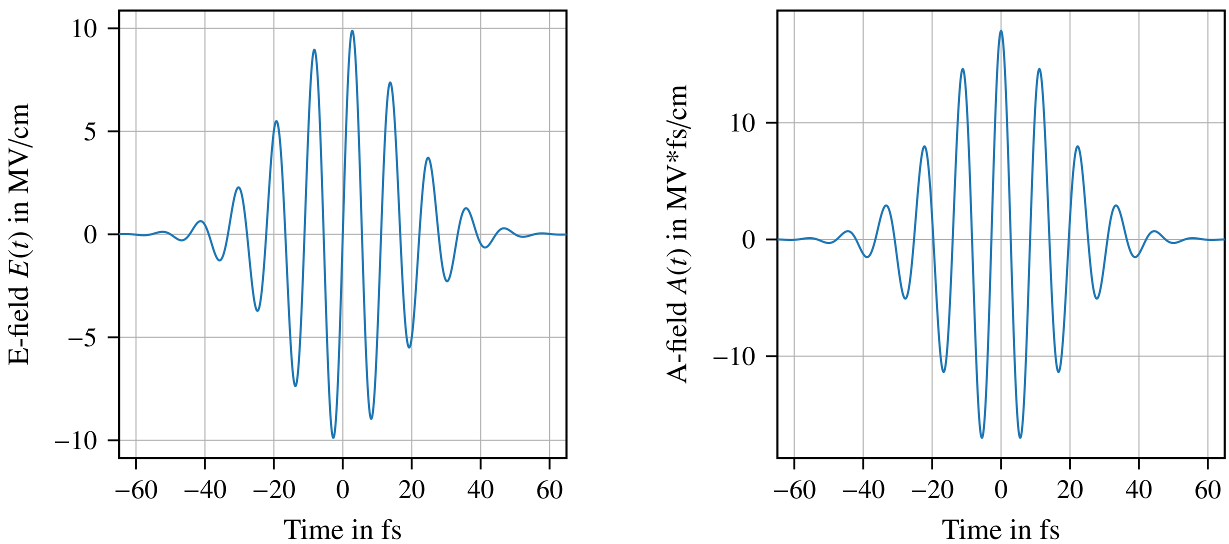

Figure 1: Left: Electric driving field $E(t)$ from Eq. (1), right: Gauge field $A(t)$ from Eq. (2).

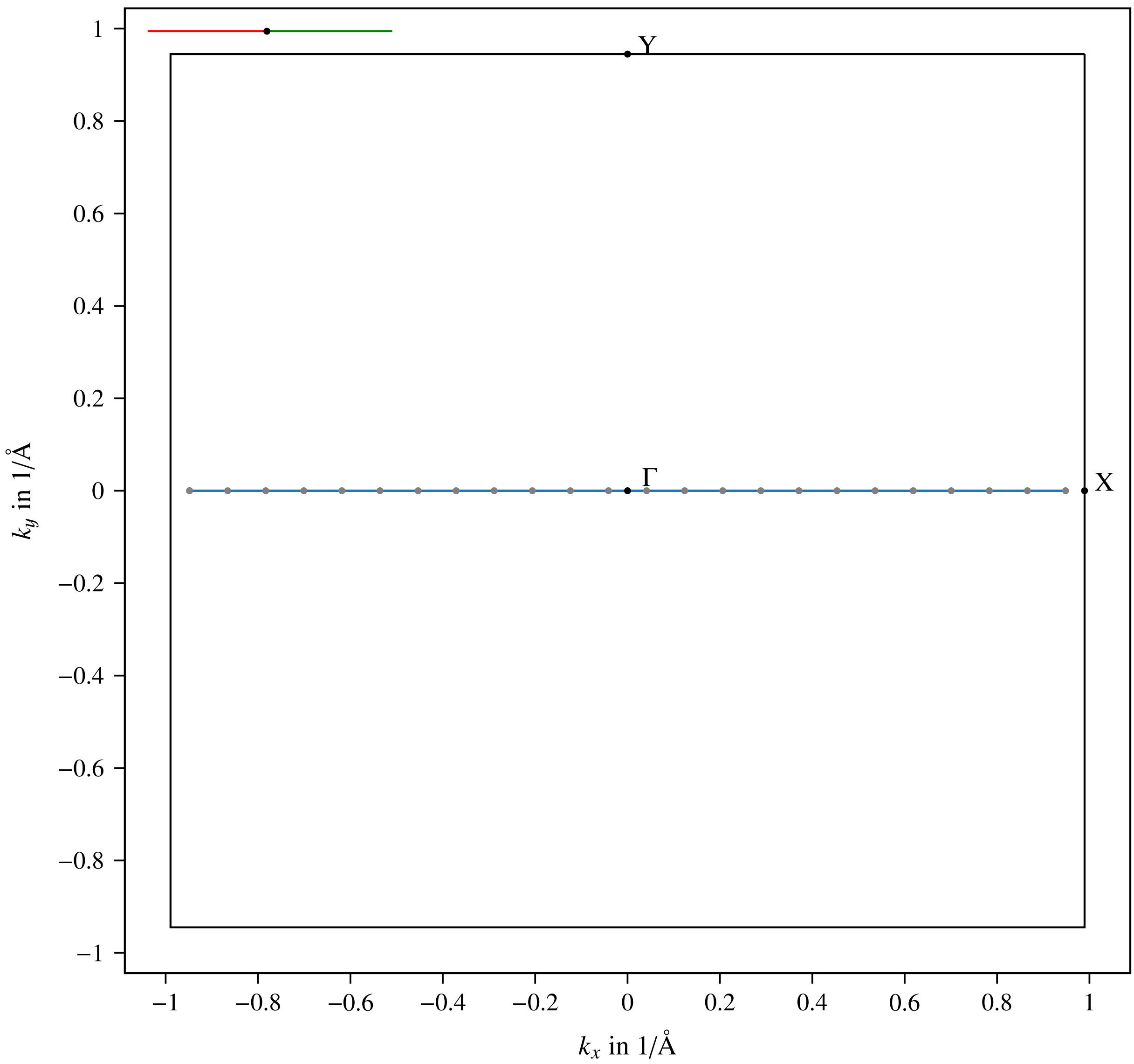

Figure 2: Brillouin zone (BZ) and 24×1 k-point mesh. The BZ is indicated by the black rectangle. Gray points indicate k-points, colored lines indicate k-points that are coupled via the term $\mathbf{E}(t) \cdot \nabla_{\mathbf{k}}$. The green and red line at the top left corner sketch $\mathbf{A}_{\mathrm{max}} := \hat{e}_\phi \max(-qA(t)/\hbar)$ and $\mathbf{A}_{\mathrm{min}} := \hat{e}_\phi \min(-qA(t)/\hbar)$ indicating the extremal excursion of electrons in the BZ.

The gauge field $\mathbf{A}(t) = A(t)\,\hat{e}_\phi$ follows from $\dot{\mathbf{A}}(t) = -\mathbf{E}(t)$. We compute $A(t)$ for the sketch in Fig. 1 as

$$\dot{A}(t) = -E(t) \qquad \Rightarrow \qquad A(t) = -\int_{-\infty}^{t} E(t')\,dt' \ . \tag{2}$$

2 Brillouin zone and k-point grid

A rectangle as Brillouin zone (BZ) with a mesh size of 1200×1 is used. The BZ and a 24×1 k-point mesh is sketched in Fig. 2. Please note that in the params.py file, the BZ size (in case of a rectangular BZ) and the lattice parameter a (in case of a hexagonal BZ) are both given in atomic units, while the output here is in 1/Å (note: 1 atomic length unit = $1a_0$ = 0.529 Å, a_0: Bohr radius, 1 atomic inverse length unit = 1/(0.529 Å) = 1.890 Å^{-1}).

3 Hamiltonian, bandstructure and dipoles

The n-band Hamiltonian $h(\mathbf{k})$ is an $n \times n$ matrix that is given as an input. Diagonalizing $h(\mathbf{k})$ yields the band structure and the eigenvectors $|u_{n\mathbf{k}}\rangle$,

$$h(\mathbf{k})\,|u_{n\mathbf{k}}\rangle = \epsilon_n(\mathbf{k})\,|u_{n\mathbf{k}}\rangle\,. \tag{3}$$

Dipoles are computed from

$$\mathbf{d}_{nn'}(\mathbf{k}) = iq\,\langle u_{n\mathbf{k}}|\,\partial_{\mathbf{k}}\,|u_{n'\mathbf{k}}\rangle\,, \tag{4}$$

where $q=-e$ is the electron charge. The band structure and the dipoles are sketched in Fig. 3.

4 Time evolution of the density matrix

In case you choose the length gauge (`gauge = 'length'`, that is also the default) and $1/T_1 = 0$, we solve semiconductor Bloch equations in the length gauge, Eq. (50) in Ref. [1]:

$$\left[\frac{\partial}{\partial t} + q\mathbf{E}(t)\frac{\partial}{\partial \mathbf{k}}\right]\rho_{nn'}(\mathbf{k},t) = \left[i(\epsilon_{n'}(\mathbf{k}) - \epsilon_n(\mathbf{k})) - 1/T_2\right]\rho_{nn'}(\mathbf{k},t) - i\mathbf{E}(t)\sum_{\underline{n}}(\rho_{n\underline{n}}(\mathbf{k};t)\mathbf{d}_{\underline{n}n'}(\mathbf{k}) - \mathbf{d}_{n\underline{n}}(\mathbf{k})\rho_{\underline{n}n'}(\mathbf{k};t)) \tag{5}$$

with a dephasing time $T_2 = 1$ fs.

5 Time-dependent current

In case you choose the length gauge (`gauge = 'length'`, that is also the default), the current is computed from Eq. (67) in Ref. [1] as

$$\mathbf{j}(t) = q\sum_{nn'}\int_{\mathrm{BZ}}\frac{d\mathbf{k}}{(2\pi)^2}\,\langle u_{n\mathbf{k}}|\frac{\partial h(\mathbf{k})}{\partial \mathbf{k}}|u_{n'\mathbf{k}}\rangle\,\rho_{n'n}(\mathbf{k},t)\,. \tag{6}$$

The matrix element $\langle u_{n\mathbf{k}}|(\partial_{\mathbf{k}}h(\mathbf{k}))|u_{n'\mathbf{k}}\rangle$ can be computed from Eq. (68) in Ref. [1] as

$$\langle u_{n\mathbf{k}}|\frac{\partial h(\mathbf{k})}{\partial \mathbf{k}}|u_{n'\mathbf{k}}\rangle = \delta_{nn'}\partial_{\mathbf{k}}\epsilon_n(\mathbf{k}) + \frac{i}{q}\,\mathbf{d}_{nn'}(\mathbf{k})\,(\epsilon_n(\mathbf{k}) - \epsilon_{n'}(\mathbf{k}))\,. \tag{7}$$

In our case, the current is a two-dimensional vector. For generating meaningful plots, we project the current onto the axis $\hat{e}_\phi$ of the incoming E-field and its orthogonal direction $\hat{e}_{\phi+\pi/2}$:

$$j_{||}(t) = \hat{e}_\phi\,\mathbf{j}(t)\,, \qquad j_\perp(t) = \hat{e}_{\phi+\pi/2}\,\mathbf{j}(t)\,, \tag{8}$$

and we recover

$$\mathbf{j}(t) = \hat{e}_\phi\,j_{||}(t) + \hat{e}_{\phi+\pi/2}\,j_\perp(t)\,. \tag{9}$$

6 Frequency-resolved emission spectrum

Experiments measure the frequency resolved emission intensity I, which is computed by Eq. (53) in Ref. [1]

$$I(\omega) = \frac{\omega^2}{3c^3}\,|\mathbf{j}(\omega)|^2\,, \tag{10}$$

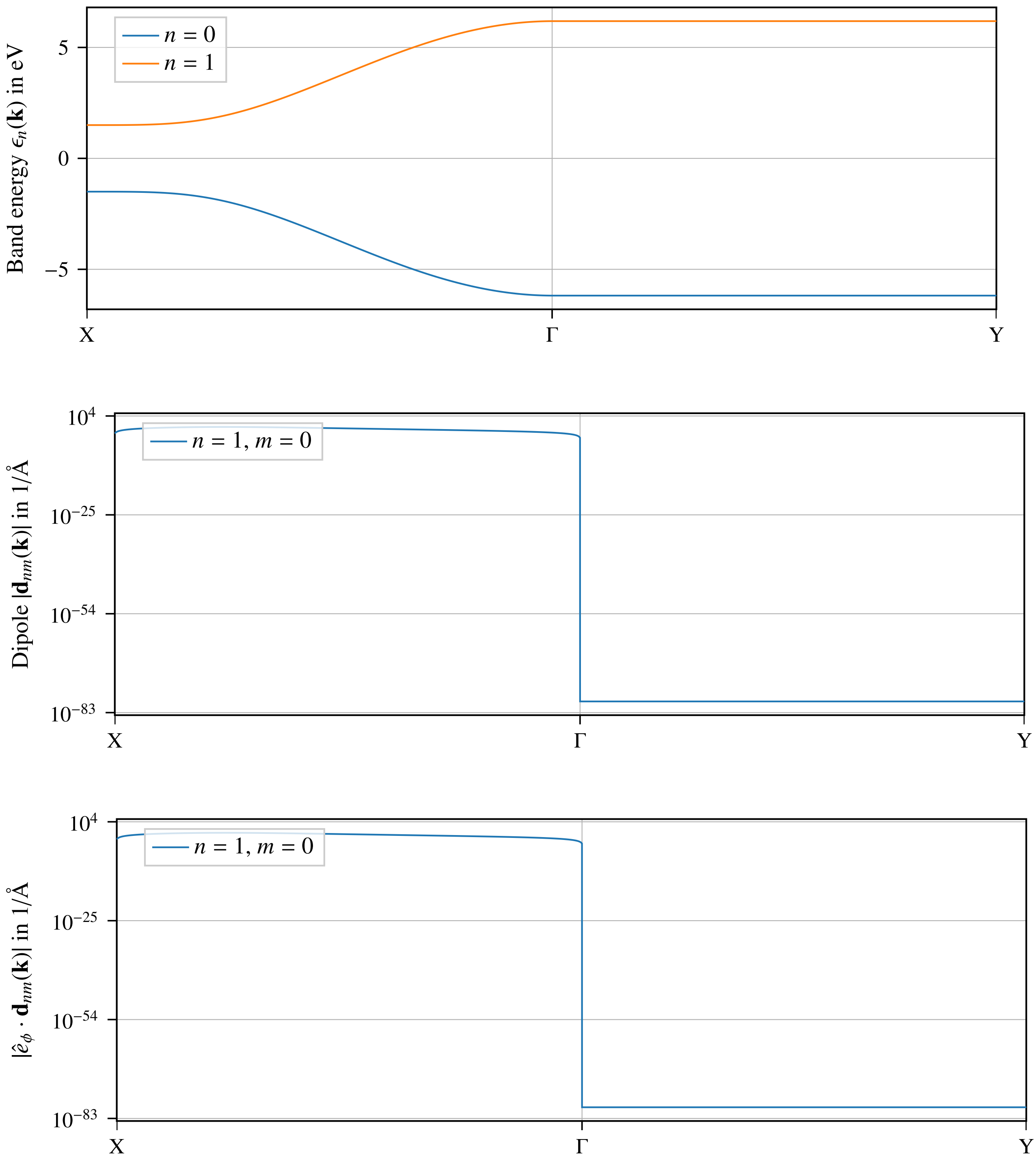

Figure 3: Band structure $\epsilon_n(\mathbf{k})$ as computed from the Hamiltonian $h(\mathbf{k})$, see Eq. (3).

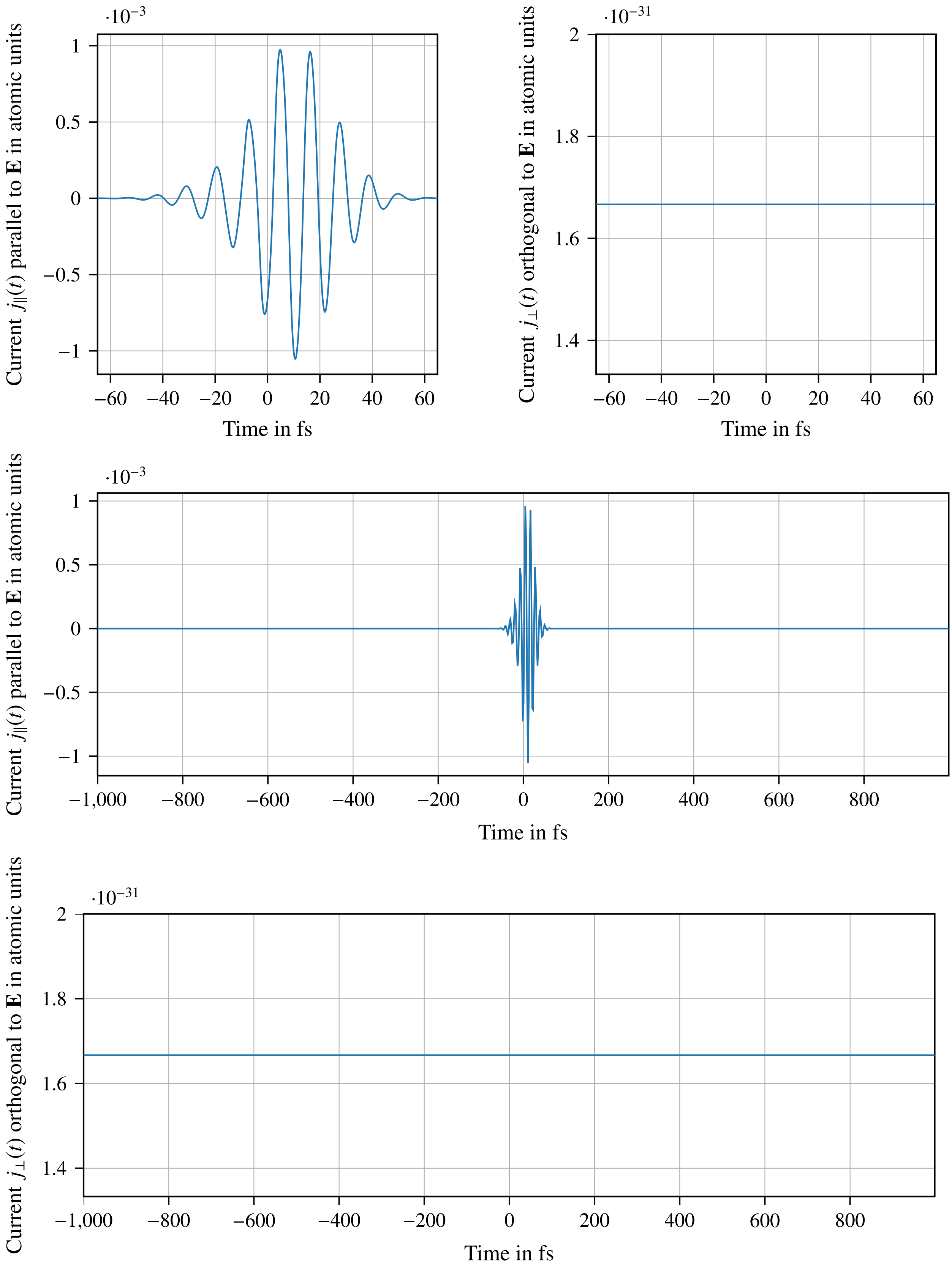

Figure 4: Components of the time-dependent current $\mathbf{j}(t)$: top left: parallel to the driving field, top right: orthogonal to the driving field, see Eq. (8). Middle and bottom: Current over the whole time window of the simulation.

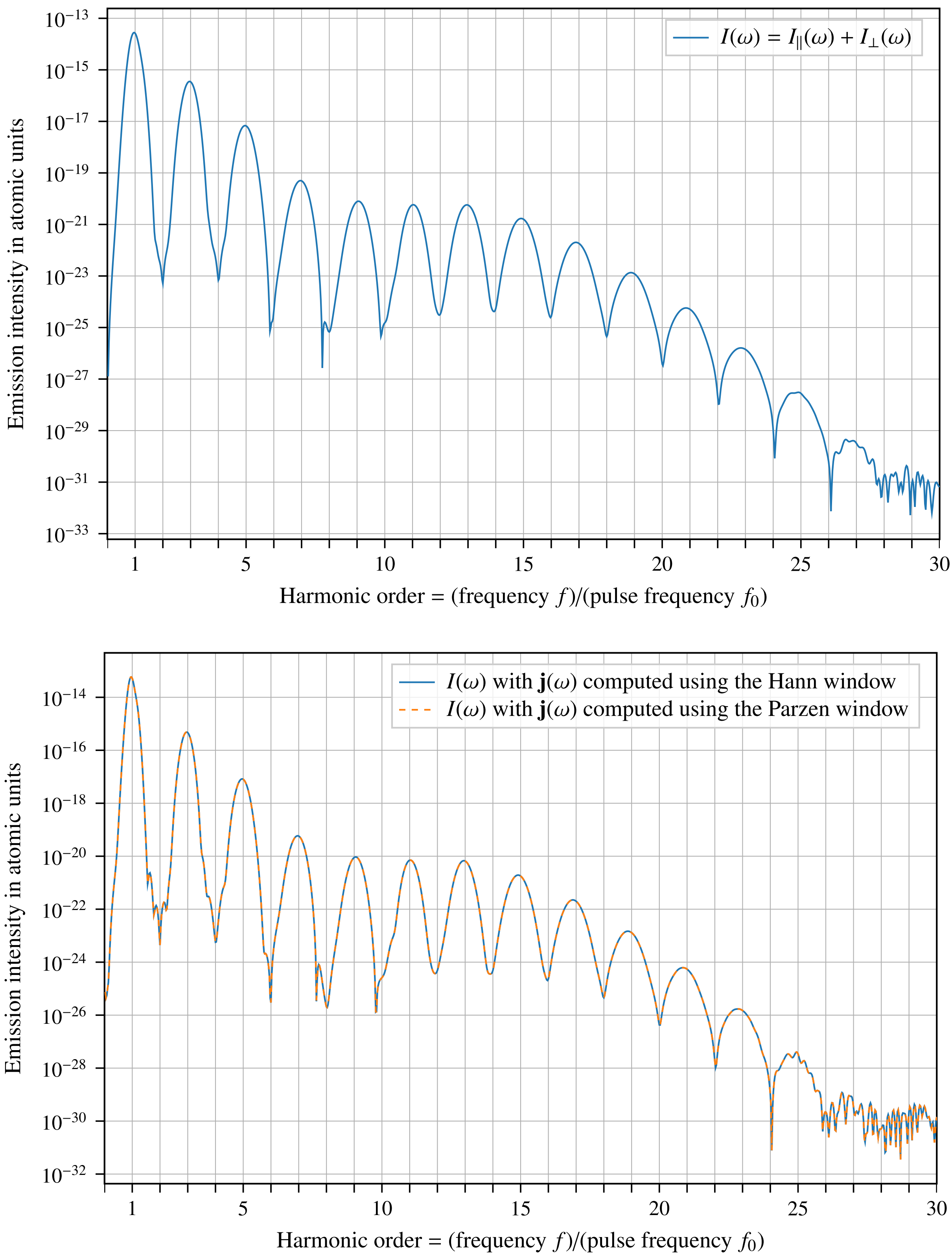

Figure 5: Total emission intensity from the irradiated material computed from Eq. (10). In the lower graph, the emission computed from $\mathbf{j}_w(\omega)$ is sketched where the Hann and the Parzen window have been used as window $w(t)$. This is a check: If both Fourier transforms coincide, the Fourier transform is converged with respect to the time window $[-t_0, t_0]$. If the Fourier transforms with Hann and Parzen window differ, increase t_0. The frequency is given by $f = \omega/(2\pi)$.

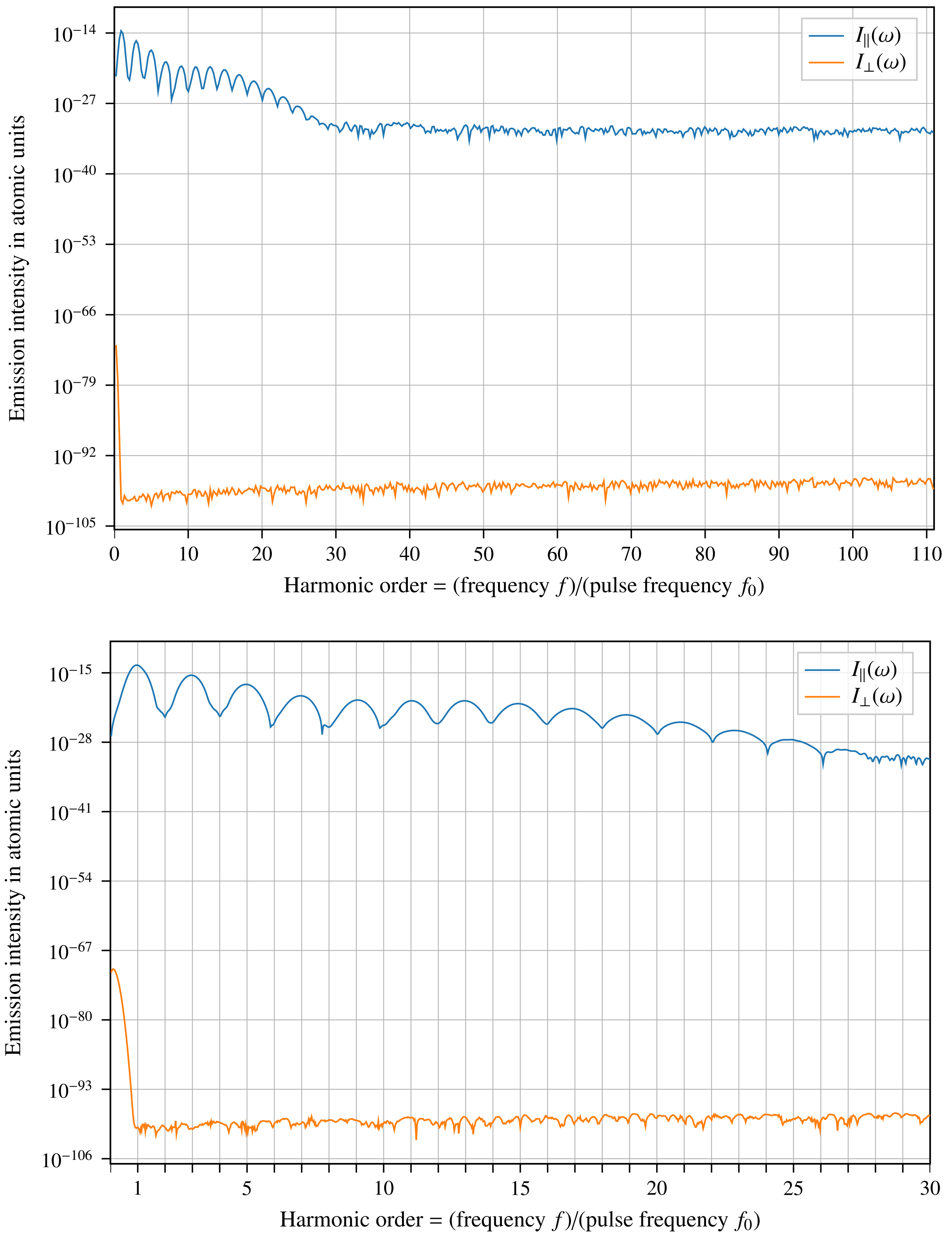

Figure 6: Emission intensity of the polarization parallel and orthogonal to the incoming electric field from the irradiated material computed from Eq. (13). The data is displayed using two different frequency scales. The frequency is given by $f = \omega/(2\pi)$.

where c is the speed of light and $\mathbf{j}(\omega)$ is the Fourier transform of the current $\mathbf{j}(t)$. Since the current $\mathbf{j}(t)$ is not periodic in time, short-time Fourier transform (STFT) is used with a window function $w(t)$,

$$\mathbf{j}(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-t_0}^{t_0} w(t)\, \mathbf{j}(t)\, e^{-i\omega t} \,. \tag{11}$$

As window, a Hann, Parzen and Gaussian window are available in the code. The emission is sketched in Fig. 5 including a test of the window function. When inserting Eq. (9) in the frequency domain, we have

$$I(\omega) = \frac{\omega^2}{3c^3} \left(|\,\mathbf{j}_{||}(\omega)|^2 + |\,\mathbf{j}_{\perp}(\omega)|^2 \right) , \tag{12}$$

that motivates the definitions

$$I_{||}(\omega) = \frac{\omega^2}{3c^3} |\mathbf{j}_{||}(\omega)|^2 \,, \qquad I_{\perp}(\omega) = \frac{\omega^2}{3c^3} |\mathbf{j}_{\perp}(\omega)|^2 \,. \tag{13}$$

We recover $I(\omega) = I_{||}(\omega) + I_{\perp}(\omega)$. The emission intensity of parallel and orthogonal polarized light is sketched in Fig. 6.

7 References

When using the CUED software package, please reference to CUED by citing the following publication:

[1] J. Wilhelm, P. Grössing, A. Seith, J. Crewse, M. Nitsch, L. Weigl, C. Schmid, and F. Evers, *Semiconductor-Bloch Formalism: Derivation and Application to High-Harmonic Generation from Dirac Fermions*, Phys. Rev. B **x**, y (2021).