Output summary of the CUED program

The CUED program is developed and maintained by:

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Date of execution: February 22, 2021

Run time: 134.3 s

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Contents

1 Electric-field pulse

The following electric driving field is employed in the simulation:

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

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

- $\hat{e}_\phi = \hat{e}_x$
- Pulse frequency: $f_0 = 90.0\,\mathrm{THz}$
- Chirp: $f_{\mathrm{chirp}} = 0.0\,\mathrm{THz}$
- Carrier-envelope phase: $\phi = 0.0$
- $\alpha = 12.5\,\mathrm{fs}$, full width at half maximum (FWHM) of the Gaussian envelope $= 41.628\,\mathrm{fs}$

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

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

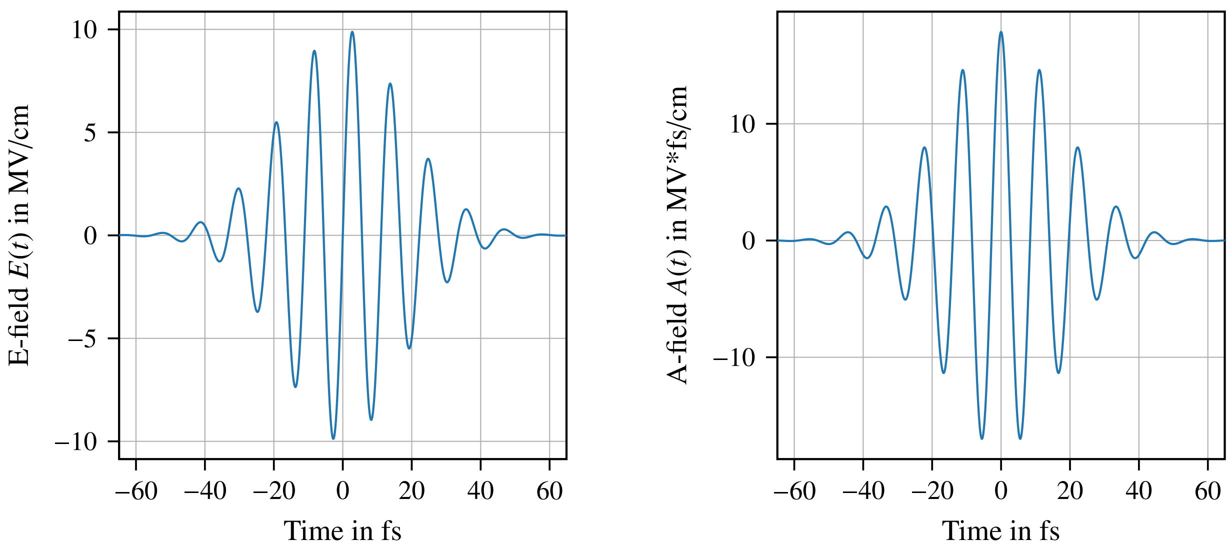

Figure 1: Left: Electric driving field $E(t)$ from Eq. (1), right: Gauge field $A(t)$ from Eq. (2).

2 Brillouin zone and k-point grid

You are using a rectangle as Brillouin zone (BZ) with a mesh size of 1200×1. 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}).

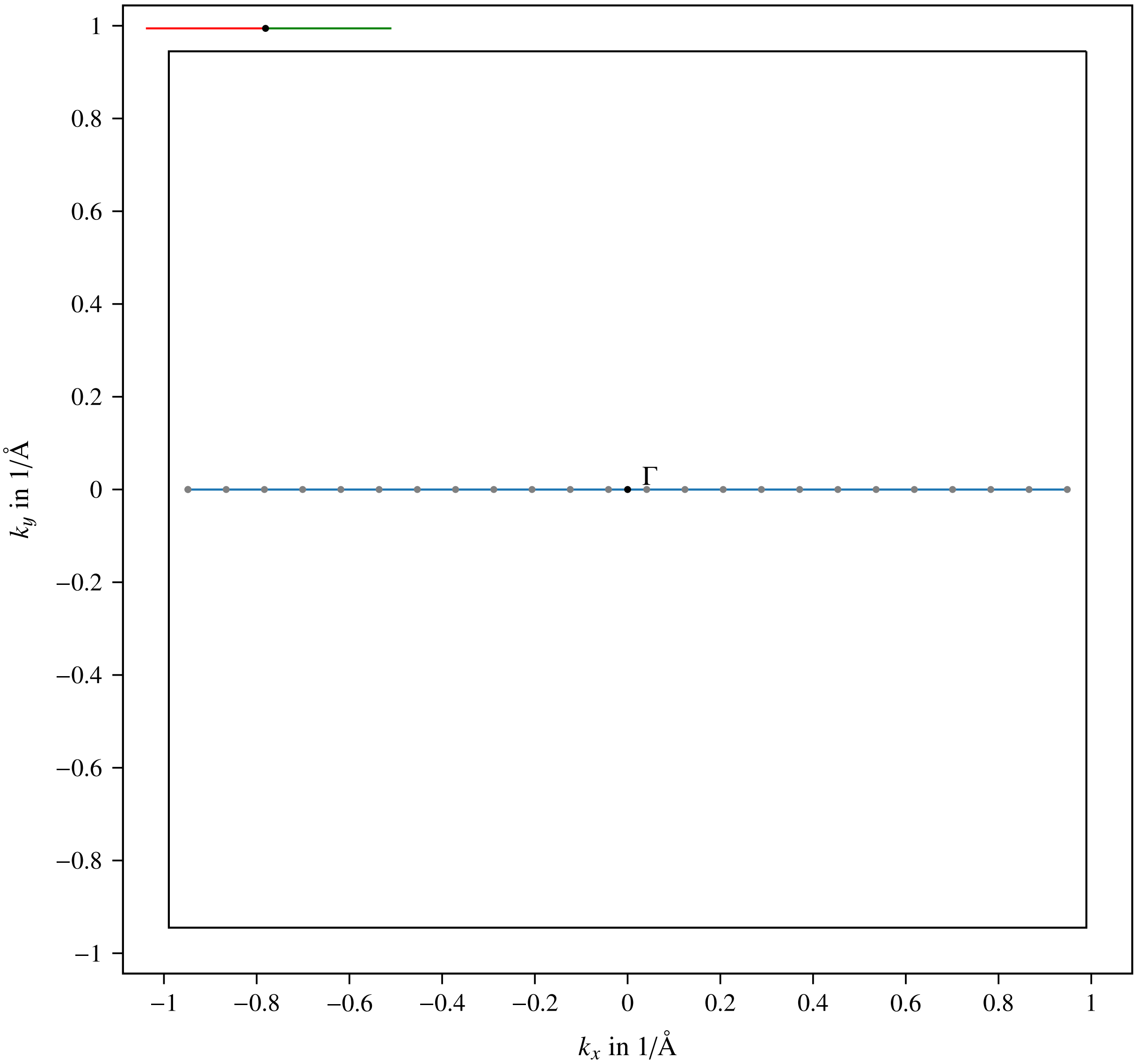

Figure 2: Brillouin zone (BZ) and 24×1 k-point mesh. The BZ is indicated by the black rectangle. Gray points indicate k-points, colored lines indicate k-points that are coupled via the term $\mathbf{E}(t) \cdot \nabla_{\mathbf{k}}$. The green and red line at the top left corner sketch $\mathbf{A}_{\text{max}}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

3 Hamiltonian, bandstructure and dipoles

This still needs to be filled; Gauge; how to print the Hamiltonian properly? (e.g. Dirac or Bi_2Te_3?) Printing of band structure for rectangle along $k_x, k_y = 0$, $k_y, k_x = 0$, for hexagon along K-Γ-M. Plotting of dipoles as in Patricks plot with 4 diagrams (dvv, dcc, Re(dvc), Im(dvc)), additionally along K-Γ-M (also absolute value of dvc).

4 Time evolution of the density matrix

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

$$\left[\frac{\partial}{\partial t} + q\mathbf{E}(t)\frac{\partial}{\partial \mathbf{k}}\right]\rho_{nn'}(\mathbf{k},t) = [i(\epsilon_{n'}(\mathbf{k}) - \epsilon_n(\mathbf{k})) - 1/T_2]\,\rho_{nn'}(\mathbf{k},t) - i\mathbf{E}(t)\sum_{\underline{n}}(\rho_{n\underline{n}}(\mathbf{k};t)\mathbf{d}_{\underline{n}n'}(\mathbf{k}) - \mathbf{d}_{n\underline{n}}(\mathbf{k})\rho_{\underline{n}n'}(\mathbf{k};t)) \tag{3}$$

with a dephasing time $T_2 = 1$ fs. TODO: Plots of initial vv and cc density matrix elements, plot of time evolution at a k-point, snapshot of density matrix at 3 time points for whole BZ.

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

$$\mathbf{j}(t) = q\sum_{nn'}\int_{\mathrm{BZ}}\frac{d\mathbf{k}}{(2\pi)^2}\,\langle u_{n\mathbf{k}}|\frac{\partial h(\mathbf{k})}{\partial \mathbf{k}}|u_{n'\mathbf{k}}\rangle\,\rho_{n'n}(\mathbf{k},t)\ . \tag{4}$$

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

$$\langle u_{n\mathbf{k}}|\frac{\partial h(\mathbf{k})}{\partial \mathbf{k}}|u_{n'\mathbf{k}}\rangle = \delta_{nn'}\partial_{\mathbf{k}}\epsilon_n(\mathbf{k}) + \frac{i}{q}\,\mathbf{d}_{nn'}(\mathbf{k})\,(\epsilon_n(\mathbf{k}) - \epsilon_{n'}(\mathbf{k}))\ . \tag{5}$$

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 $\hat{e}_{\phi+\pi/2}$:

$$j_{||}(t) = \hat{e}_\phi\ \mathbf{j}(t)\ , \qquad j_\perp(t) = \hat{e}_{\phi+\pi/2}\ \mathbf{j}(t)\ , \tag{6}$$

and we recover

$$\mathbf{j}(t) = \hat{e}_\phi\ j_{||}(t) + \hat{e}_{\phi+\pi/2}\ j_\perp(t)\ . \tag{7}$$

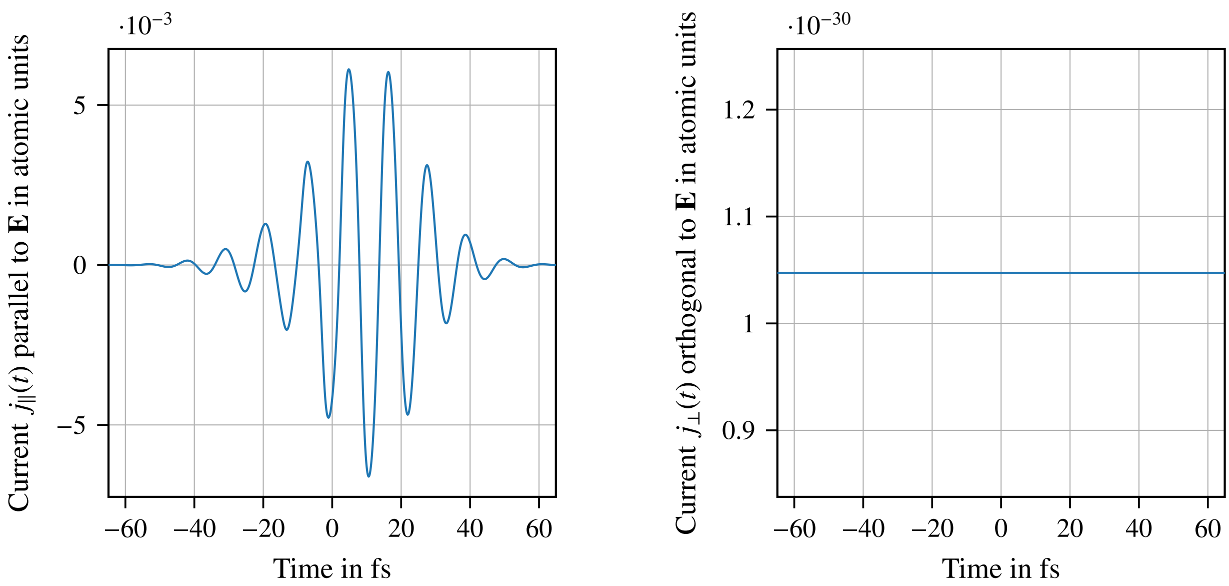

Figure 3: Components of the time-dependent current $\mathbf{j}(t)$: left: parallel to the driving field, right: orthogonal to the driving field, see Eq. (6).

6 Frequency-resolved emission spectrum

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

$$I(\omega) = \frac{\omega^2}{3c^3} |\mathbf{j}(\omega)|^2 \,, \tag{8}$$

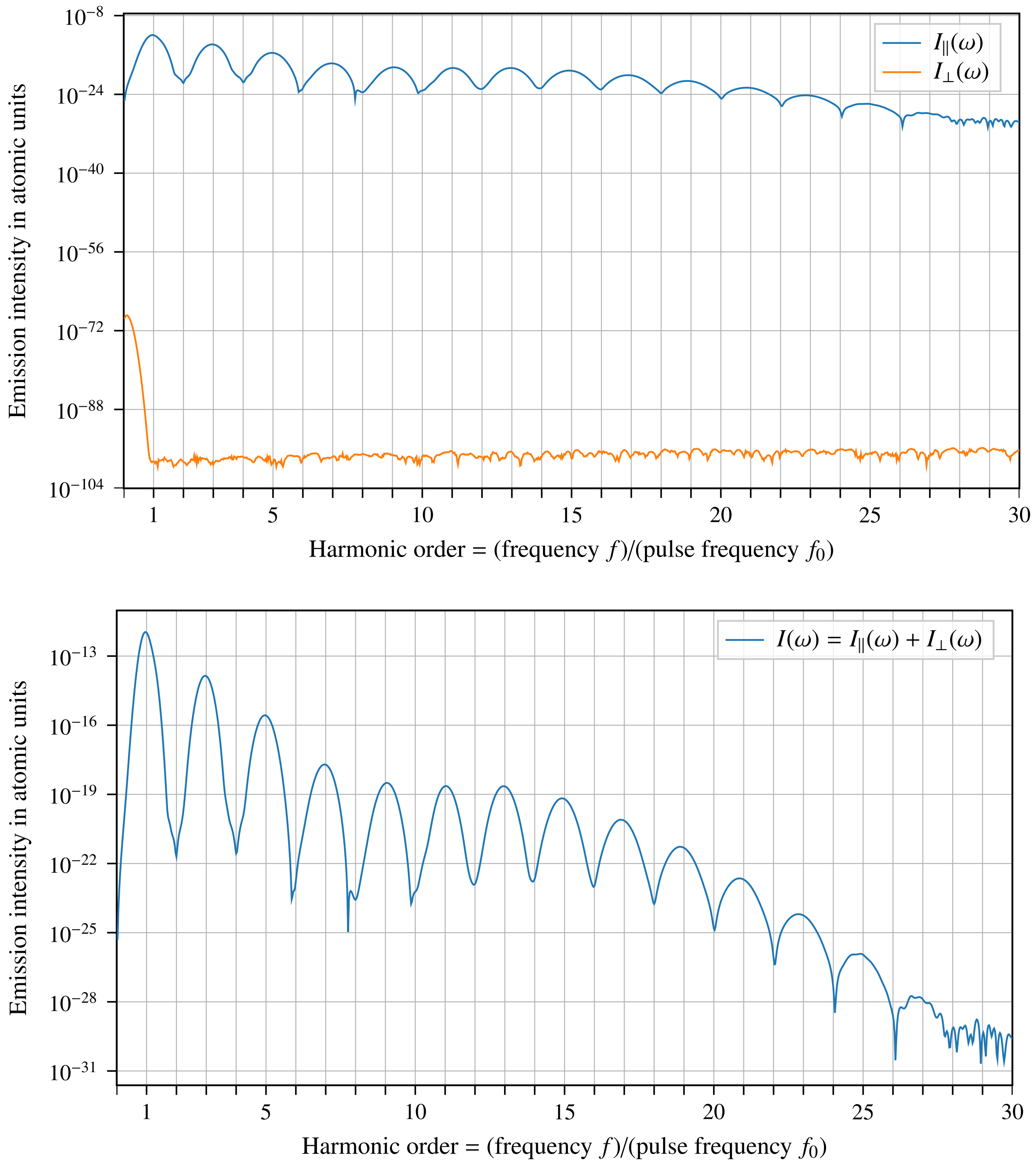

Figure 4: Emission intensity from the irradiated material computed from Eqs. (8) and (10). The frequency is given by $f = \omega/(2\pi)$.

where $\mathbf{j}(\omega)$ is the Fourier transform of $\mathbf{j}(t)$ and c is the speed of light. The emission is sketched in Fig. 4. When inserting Eq. (7) in the frequency domain, we have

$$I(\omega) = \frac{\omega^2}{3c^3}\left(|\mathbf{j}_{\|}(\omega)|^2 + |\mathbf{j}_{\perp}(\omega)|^2 \right) , \tag{9}$$

that motivates the definitions

$$I_{\|}(\omega) = \frac{\omega^2}{3c^3}\,|\mathbf{j}_{\|}(\omega)|^2 \, , \qquad I_{\perp}(\omega) = \frac{\omega^2}{3c^3}\,|\mathbf{j}_{\perp}(\omega)|^2 \, . \tag{10}$$

We recover $I(\omega) = I_{\|}(\omega) + I_{\perp}(\omega)$.

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).