



Output summary of the CUED program

The CUED program is developed and maintained by:

Computational Condensed Matter Theory Group

Head: Ferdinand Evers

Institute of Theoretical Physics

University of Regensburg

Universitätsstraße 31

D - 93053 Regensburg

Germany

Date of execution: February 14, 2021

Run time: 171.4 s

With contributions from (in alphabetic order):

Jack Crewse

Patrick Grössing

Maximilian Nitsch

Adrian Seith

Jan Wilhelm

Contents

| | | |
|---|--|---|
| 1 | Electric-field pulse | 1 |
| 2 | Brillouin zone and k -point grid | 1 |
| 3 | Hamiltonian, bandstructure and dipoles | 2 |
| 4 | Time evolution of the density matrix | 2 |
| 5 | Time-dependent current | 2 |
| 6 | Frequency-resolved emission spectrum | 3 |
| 7 | References | 3 |

1 Electric-field pulse

The following electric driving field is employed in the simulation:

$$\mathbf{E}(t) = E(t) \hat{e}_\phi, \quad E(t) = E_0 \sin\left(2\pi f_0 (1 + f_{\text{chirp}}t) + \varphi\right) e^{-t^2/(2\alpha)^2}. \quad (1)$$

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

- $\hat{e}_\phi = \hat{e}_x$
- Pulse frequency: $f_0 = 25.0$ THz
- Chirp: $f_{\text{chirp}} = 0.0$ THz
- Carrier-envelope phase: $\phi = 0.0$
- $\alpha = 25.0$ fs, full width at half maximum (FWHM) of the Gaussian envelope = 83.255 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

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

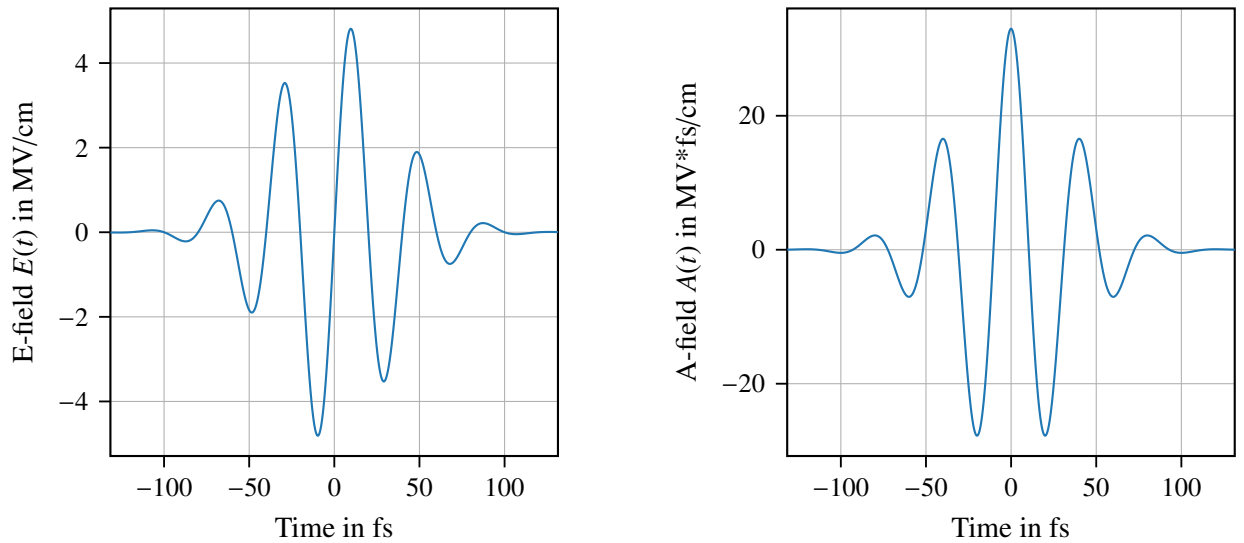


Figure 1: Left: Electric driving field $E(t)$ from Eq. (1), right: Gauge field $A(t)$ from Eq. (2).

2 Brillouin zone and k -point grid

You are using a rectangle as Brillouin zone (BZ) with a mesh size of 50×4 . The BZ and a 24×4 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 $1/\text{\AA}$.

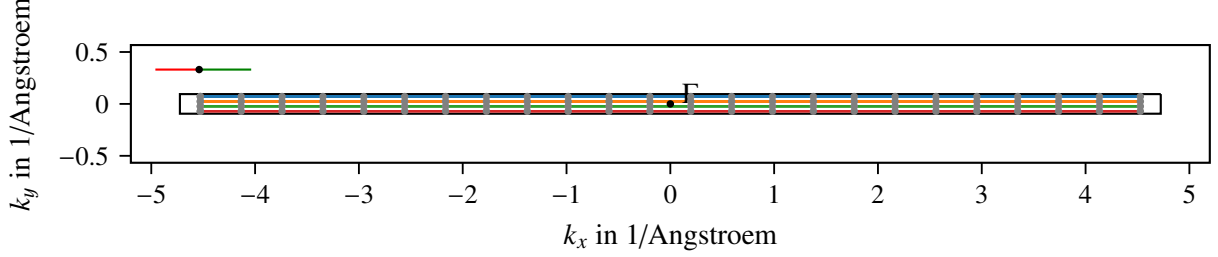


Figure 2: Brillouin zone (BZ) and 24×4 k -point mesh. The BZ is indicated by the black rectangle. Gray points indicate k -points, colored lines indicate k -points that are coupled via the term $\mathbf{E}(t) \cdot \nabla_{\mathbf{k}}$. The green and red line at the top left corner sketch $\mathbf{A}_{\max} := \hat{e}_\phi \max(-qA(t)/\hbar)$ and $\mathbf{A}_{\min} := \hat{e}_\phi \min(-qA(t)/\hbar)$ 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

We solve semiconductor Bloch equations in the length gauge, Eq. (50) in Ref. [1]:

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

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

The current is computed from Eq. (67) in Ref. [1] as

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

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

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

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

$$j_{\parallel}(t) = \hat{e}_\phi \cdot \mathbf{j}(t), \quad j_{\perp}(t) = \hat{e}_{\phi+\pi/2} \cdot \mathbf{j}(t), \quad (6)$$

and we recover

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

6 Frequency-resolved emission spectrum

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

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

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

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

that motivates the definitions

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

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

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).

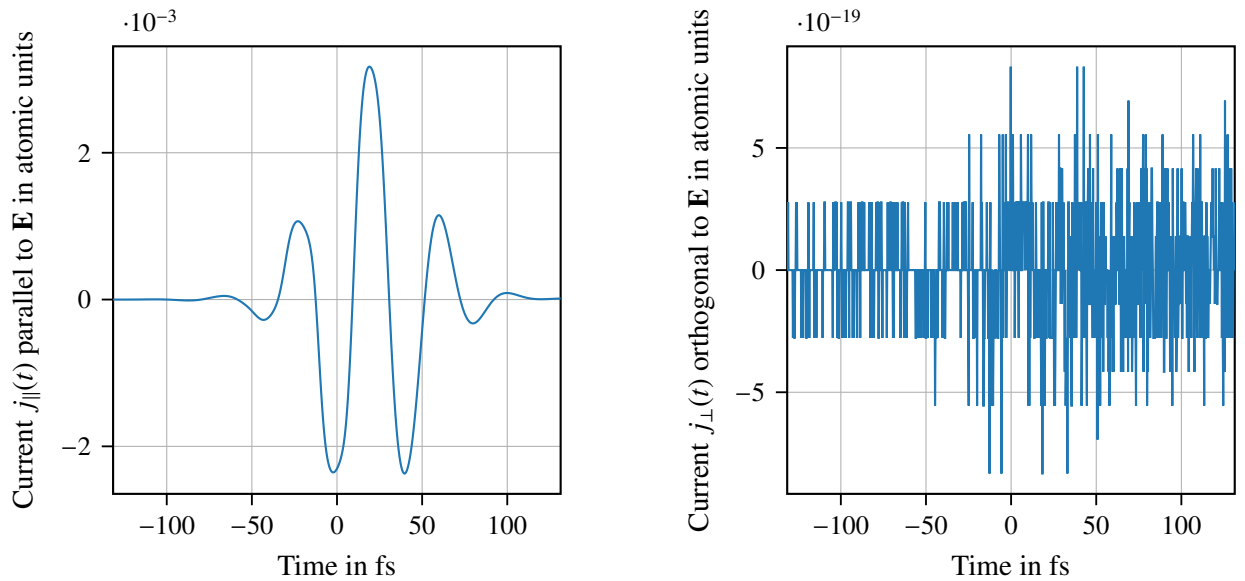


Figure 3: Components of the time-dependent current $\mathbf{j}(t)$: left: parallel to the driving field, right: orthogonal to the driving field, see Eq. (6).

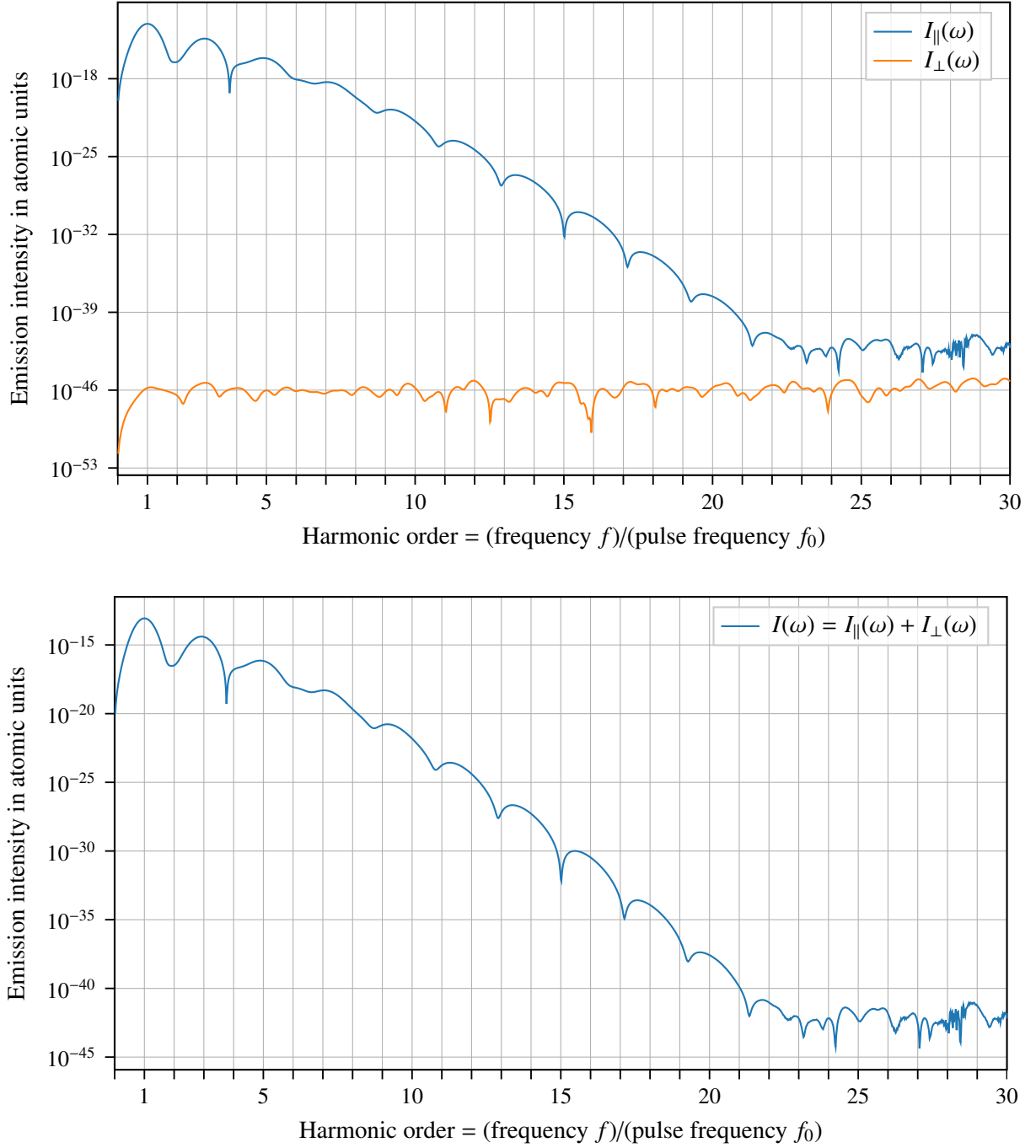


Figure 4: Emission intensity from the irradiated material computed from Eqs. (8) and (10). The frequency is given by $f = \omega/(2\pi)$.