

Thesis Outline

1. Introduction.

2. Pump-probe experiments and the group V semimetals.

- Optical pump-probe experiments.
- Physical processes involved.
- Crystal structure and phonons of group Vs.
- Electronic structure of the group Vs.
- Some pump-probe results for Bi and Sb.

3. Density functional perturbation theory.

- Many-body Hamiltonian.
- Density functional theory.
- Pseudopotentials.
- Plane-wave expansion of wavefunctions.
- LDA.
- Perturbation theory.
- Sternheimer equation.
- Phonon frequencies.
- Electron-phonon matrix elements.

4. Electron-phonon scattering

- Interacting Hamiltonian.
- Quantising the phonon coordinates.
- Electron-phonon matrix elements.
- Scattering rates
- Change in occupations: Quantum kinetic equations.
- Markovian approximation: Semi-classical Boltzmann-equation.
- Smearing of energy-conservation condition.
- Equilibrium relaxation times (RTA).
- Numerical implementation
- Tetrahedral linear interpolation of electron-phonon matrix elements.
- Wannier interpolation
- Maximally localised Wannier functions.
- Interpolation of electronic energies.
- Interpolation of matrix elements.

5. Ultrafast relaxation of symmetry-breaking photo-induced atomic forces by electron-phonon scattering.

- This will essentially be a copy-paste of my PRL.

6. Electron-electron scattering.

- Bare Coulomb matrix-elements with and without Born approximation.
- Screening of Coulomb interaction.
- Interband contribution to the electron dielectric function.
- Intraband contribution to the electron dielectric function.
- Dielectric function and screened W in Bi and Sb.
- Electron-electron rate equations.
- Equilibrium electron lifetime due to electron-electron interactions (RTA).
- Equilibrium lifetimes in Bi and Sb.

7. Ultrafast thermalisation of photo-excited carriers in Bi and Sb.

- Snapshots of electronic occupations versus time.
- Temperature(s) of electronic distribution versus time.
- Comparison of the effects of electron-electron and electron-phonon scattering.
- What does this tell us about the two-temperature model?
- Conclusions.

8. Conclusions

Appendix 1: Convergence of E_g force lifetime with BZ sampling.

Appendix 2: Modification of Experimental E_g force lifetimes.