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Quantum Cascade Laser Theory Code Overview

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Initialization Modules:

- Bundle all displays, data structures, and run inputs.
- Error check user inputs.
- Load/save file.
- Load material layer properties.
- Initialize data structures.
- Find bulk Fermi energy and donor ionization density.
- Create waveguide look-up table.

Find Space Charge:

- The first time being run, use a simple exponential model so that electrons bunch up before the injection barrier.
- The second time being run, use the simple exponential model times the sum of the wavefunctions.
- In all subsequent runs, calculate the space charge as the level populations times the sum of the wavefunctions.

Poisson Equation:

- Solve the Poisson equation as a function of the space charge, while matching boundary values.

Schrödinger Equation:

- Solve the one-electron Schrödinger equation. The potential is the conduction band edge plus the built-in potential from the Poisson eq.
- Normalize all wavefunctions.

Copy Wavefunctions:

- Throw away all wavefunctions with center-of-masses in the outer periods and copy all middle-period wavefunctions to the outer periods.

Form Factors:

- Precalculate scattering form factors to create look-up tables, including antisymmetric possibilities.

Waveguide Look-ups:

- Look-up all waveguide effects at the frequency of each transition using the tables precalculated at the beginning of code.

Individual Fermi Levels:

- Based on the current iteration's electron populations and electron temperatures, calculate the corresponding individual Fermi levels.

Phonon Rates:

- Calculate LO phonon rates.

Electron-Electron Rates:

- Precalculate electron-electron screening to create a screening constant look-up table.
- Calculate symmetric and anti-symmetric rates.

Photon Rates:

- Calculate the line-broadened one-mode spontaneous photon emission rate for every possible transition for use in the rate equations.

Rate Equations:

- Self-consistently solve the all-level electron rate equations, enforcing periodic boundary conditions, and with the photon population dependence included.
- Self-consistently solve the photon populations rate equations for all possible transitions.

Final Equations

- Calculate the total output laser power for each transition from the photon populations.
- Identify the lasing transition as the one with highest output power.
- Report the lasing frequency, wavelength, etc.

