The effects of various approximations on electron-electron scattering calculations in QCLs

Philip Slingerland  Christopher Baird  Robert Giles

Submillimeter-Wave Technology Laboratory
University of Massachusetts Lowell

SPIE Photonics West, 2011
Outline

Introduction
  QCL background
  Motivation

Numerical approximations
  Variable definitions
  Integral convergence

Physical Approximations
  State-blocking and screening
  Asymmetric transitions

Conclusions
Outline

Introduction
  QCL background
  Motivation

Numerical approximations
  Variable definitions
  Integral convergence

Physical Approximations
  State-blocking and screening
  Asymmetric transitions

Conclusions
QCL description

- QCL: semiconductor laser whose emission frequency can be chosen by design of epitaxial layers (thickness and alloy concentration).
- Spacing of electron energy levels and wavefunction shapes controlled by design.
- Lasing can occur by tailoring energy levels and wavefunctions.
Motivation

- Electron-electron scattering essential for carrier transport in many THz QCL designs
- Often used as means for injection and depopulation
- Inaccuracies in scattering rate calculations leads to inaccuracies in simulation results
- Despite importance, many approximations often made to reduce computational demands
Electron-electron scattering

- Electron in state \((i, k_i)\) scatters with electron in state \((j, k_j)\) into final states \((f, k_f)\) and \((g, k_g)\)

\[ i, j \rightarrow f, g \]

- Fermi’s Golden Rule

\[ W_{ijfg} = \frac{2\pi}{\hbar} |M|^2 \delta(\Delta E) \]

- Energy and momentum conserved
QCL prediction code uses self-consistent semi-classical approach.

- Schrödinger eq. for electron states.
- Poisson eq. to include electron-electron interactions.

- Transition rates found from Fermi’s Golden Rule.

- Populations found from iterative rate equations.

- Populations modify Poisson eq. and code repeats.
Outline

Introduction
- QCL background
- Motivation

Numerical approximations
- Variable definitions
- Integral convergence

Physical Approximations
- State-blocking and screening
- Asymmetric transitions

Conclusions
Electron scattering can be calculated using two different definitions:

- Exchange with non-relative wavevector definition:
  \[ q = |k_i - k_f| \]

- Exchange with relative wavevector definition:
  \[ q = \frac{|k_{ij} - k_{fg}|}{2} \]
Integral convergence

Convergence of integration types depends on step size

Both are closer to convergent value with more integration points
QCL structures

- RP structure with non-relative $k$’s
- RP structure with relative $k$’s
Outline

Introduction
  QCL background
  Motivation

Numerical approximations
  Variable definitions
  Integral convergence

Physical Approximations
  State-blocking and screening
  Asymmetric transitions

Conclusions
State-blocking

- Scattering rate reduced by effect of state-blocking:

\[ W_{i,j,f,g}(k_i) \propto \int dk_j d\theta_{ij} d\theta \frac{|A_{ijfg}(q)|^2}{q^2 \epsilon(q)^2} k_j f_j(k_j) [1 - f_f(k_f)] [1 - f_g(k_g)] \]

- Due to Pauli exclusion principle
- Dependant on final state population densities
State-blocking

- RP structure using $10^6$ points
- BTC structure using $10^6$ points
Screening

- Modification of potential due to presence of conduction electrons
  - Electrons reduce coulomb potential, reduce scattering rate
  - Population dependent
- Single subband models easy to implement, but either over or underestimate effect
- Modified single subband approach recently suggested

\[ \epsilon_{sc}(q) = 1 + \frac{e^2}{2 \epsilon q} \sum_i \Pi_{ii}(q, T) A_{iii}(q) \]
Screening

- RP structure using $10^6$ points
- BTC structure using $10^6$ points
Asymmetric transitions do not occur in symmetric quantum wells due to selection rules.

Due to asymmetry of QCL potential structure they can occur.

Asymmetric transitions have significant scattering rates.
Asymmetric scattering rates

### RP 4 → 3 transition

<table>
<thead>
<tr>
<th>Scattering Event ( (i, j \rightarrow f, g) )</th>
<th>Rate ( \times 10^9 ) 1/s</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 4, 2 \rightarrow 3, 2 = 2, 4 \rightarrow 2, 3 )</td>
<td>14.16541</td>
</tr>
<tr>
<td>( 4, 3 \rightarrow 3, 3 = 3, 4 \rightarrow 3, 3 )</td>
<td>12.00632</td>
</tr>
<tr>
<td>( 4, 5 \rightarrow 3, 5 = 5, 4 \rightarrow 5, 3 )</td>
<td>11.86801</td>
</tr>
<tr>
<td>( 4, 4 \rightarrow 3, 3 )</td>
<td>10.78851</td>
</tr>
<tr>
<td>( 4, 4 \rightarrow 3, 4 = 4, 4 \rightarrow 4, 3 )</td>
<td>9.516328</td>
</tr>
<tr>
<td>Transition rate ( 4 \rightarrow 3 )</td>
<td>82.17494</td>
</tr>
</tbody>
</table>

### BTC 11 → 10 transition

<table>
<thead>
<tr>
<th>Scattering Event ( (i, j \rightarrow f, g) )</th>
<th>Rate ( \times 10^9 ) 1/s</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 11, 12 \rightarrow 10, 12 = 12, 11 \rightarrow 12, 10 )</td>
<td>4.898878</td>
</tr>
<tr>
<td>( 11, 11 \rightarrow 10, 11 = 11, 11 \rightarrow 11, 10 )</td>
<td>3.440731</td>
</tr>
<tr>
<td>( 11, 10 \rightarrow 10, 10 = 10, 11 \rightarrow 10, 10 )</td>
<td>3.361894</td>
</tr>
<tr>
<td>( 11, 11 \rightarrow 10, 10 )</td>
<td>2.793062</td>
</tr>
<tr>
<td>( 11, 9 \rightarrow 10, 9 = 9, 11 \rightarrow 9, 10 )</td>
<td>0.841501</td>
</tr>
<tr>
<td>Transition rate ( 11 \rightarrow 10 )</td>
<td>30.11034</td>
</tr>
</tbody>
</table>
Outline

Introduction
  QCL background
  Motivation

Numerical approximations
  Variable definitions
  Integral convergence

Physical Approximations
  State-blocking and screening
  Asymmetric transitions

Conclusions
Conclusions

- Relative wavevector scattering integral preferred over non-relative form
- For error < 1%, $10^8$ integration points needed
- State-blocking can decrease scattering rate by up to 2%
- Screening reduced scattering rate by 15% in RP design and 30% in BTC design
- Asymmetric scattering events shown to be on same order as symmetric ones, therefore they must be included
Thank you

- For further discussion or comments please stop by the University of Massachusetts Lowell booth (#1027)