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

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ABSTRACT
Quantum cascade lasers (QCLs) employ the mid- and far-infrared intersubband radiative transitions available in semiconducting heterostructures. Through the precise design and construction of these heterostructures the laser characteristics and output frequencies can be controlled. When fabricated, QCLs offer a lightweight and portable alternative to traditional laser systems which emit in this frequency range. The successful operation of these devices strongly depends on the effects of electron transport. Electron-electron scattering is an essential mechanism involved in electron transport and approximations are often made in finding the electron-electron scattering rate in order to simplify calculations. Results will be presented characterizing various effects which are sometimes ignored in calculating electron-electron scattering rates. These effects include state-blocking, electron screening, temperature dependence, as well as the inclusion of all possible transitions that can occur in three periods of the QCL active region. These effects will be presented in the context of several QCL active region designs, including those grown and fabricated at the University of Massachusetts Lowell Photonics Center.

Keywords: quantum cascade lasers, terahertz, electron-electron scattering, device modeling

1. INTRODUCTION
The performance of terahertz quantum cascade lasers (QCL’s) has improved dramatically over recent years; however, limitations still exist in their application due to poor temperature and power performance in this frequency range. There are many mechanisms involved in the operation of QCL’s, all of which contribute in some way to these limitations. However, some mechanisms have greater importance over others. Electron-electron (e-e) scattering is a dominant means of carrier transport in QCL’s, particularly in structures which emit in the terahertz frequency (∼ 10^{12} Hz) range. However, due to the complexity of the e-e interaction, approximations are often made to ease the computational burden associated with including this scattering mechanism in a QCL simulation code. It is the purpose of this paper to examine these approximations and determine their impact on the calculation of e-e scattering rates. This will provide a guide for choosing which approximations are acceptable to retain a certain level of accuracy in the e-e scattering rates and in a QCL simulation code.

1.1 Electron-electron scattering
The derivation of scattering rate equations is well documented in the literature; however, due to the variety of definitions employed, a brief outline of the conventions used in this paper will be useful. Electron-electron scattering involves two electrons that exist in an initial state defined by the subbands i and j and the two-dimensional wavevectors \( k_i \) and \( k_j \). These electrons then scatter with one another and go into the final states f and g with the two-dimensional wavevectors \( k_f \) and \( k_g \). Using Fermi’s Golden Rule, the scattering rate for this interaction is

\[
W_{i,j \rightarrow f,g}(k_i, k_j, k_f, k_g) = \frac{2\pi}{\hbar} |M|^2 \delta(E_f(k_f) + E_g(k_g) - E_i(k_i) - E_j(k_j)).
\]

Here, \( M \) is the scattering probability amplitude or matrix element for the event:

\[
M = \langle f, k_f; g, k_g | H' | i, k_i; j, k_j \rangle \quad \text{where} \quad H' = \frac{\epsilon^2}{4\pi\epsilon} \frac{1}{|r_i - r_j|}.
\]

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In Eq. (2), $H'$ is the perturbing Hamiltonian and is simply that of the Coulomb interaction between two electrons described by the three-dimensional position vectors $\mathbf{r}_i$ and $\mathbf{r}_j$. Since the electrons are confined in the growth dimension ($z$) and unconfined in the remaining two dimensions the wavefunctions describing these states can be represented in a basis of stationary states $\zeta_i(z)$ combined with quasi-free states with momentum $\hbar \mathbf{k}_i$. A form factor is then typically defined such that

$$A_{ijfg}(q) = \int_0^{L_z} dz \int_0^{L_z} dz' \zeta_j^*(z)\zeta_j^*(z')\zeta_i(z)\zeta_i(z') e^{-i\mathbf{q} \cdot (z-z')}$$  

(3)

where the exchange vector $\mathbf{q}$ is defined using the wavevectors

$$\mathbf{q} = \mathbf{k}_i - \mathbf{k}_f$$

(4)

whose magnitude then becomes

$$q = |\mathbf{k}_i - \mathbf{k}_f| = \sqrt{k_i^2 + k_f^2 - 2k_i k_f \cos(\theta_{k_i} - \theta_{k_f})}$$

(5)

where $\theta_{k_i}$ is the angle between $\mathbf{k}_i$ and some arbitrarily chosen axis. A similar definition is made for $\theta_{k_f}$ and all other angles labelled with wavevector subscripts.

In order to account for the occupation probability of both initial and final states, the Fermi-Dirac distribution functions $f_j(k_f)$, $f_f(k_f)$, and $f_g(k_g)$ must also be included. Then the scattering rate can be summed over these distributions by integrating over $k_f$, $k_f$, and $k_g$. After doing this, applying conservation of energy and momentum, and simplifying terms, the e-e scattering rate as a function of the initial state wavevector becomes (in SI units):

$$W_{i,j \rightarrow f,g}(\mathbf{k}_i) = \frac{m^* e^4}{32 \pi^3 \hbar^3} \sum_{k_f} \int dk_f \int d\theta_{k_f} \int d\theta_{k_{f'}} \frac{k_f}{|k_s - 2k_f|} \frac{|A_{ijfg}(q)|^2}{q^2 \epsilon(q)^2} f_f(k_f)[1 - f_f(k_f)] [1 - f_g(k_g)]$$

(6)

where $k_f$ needs to be summed over two roots, $\theta_{k_{f'}}$ is the angle $\theta_{k_{f'}} - \theta_{k_i}$ and

$$k_s = k_i \cos(\theta_{k_i} - \theta_{k_f}) + k_f \cos(\theta_{k_{f'}} - \theta_{k_f}).$$

(7)

In Eq. (6), $m^*$ is the effective mass of an electron in the material system and $\epsilon(q)$ is the dielectric function.

However, Eq. (6) is not an equation that is typically implemented. Rather than use the form of the two-dimensional wavevectors in Eq. (5) a new definition is often made such that

$$q = |\mathbf{k}_{ij} - \mathbf{k}_{fg}|/2$$

(8)

where $\mathbf{k}_{ij} = \mathbf{k}_j - \mathbf{k}_i$ and $\mathbf{k}_{fg} = \mathbf{k}_g - \mathbf{k}_f$ are the so-called relative wavevectors. In this case, after applying analogous steps to arrive at Eq. (6), the e-e scattering rate can be expressed as:

$$W_{i,j \rightarrow f,g}(\mathbf{k}_i) = \frac{m^* e^4}{64 \pi^3 \hbar^3} \int dk_f \int d\theta_{k_f} \int d\theta \frac{|A_{ijfg}(q)|^2}{q^2 \epsilon(q)^2} k_f f_f(k_f)[1 - f_f(k_f)] [1 - f_g(k_g)]$$

(9)

where $\theta$ is the angle between the relative wavevectors $\mathbf{k}_{ij}$ and $\mathbf{k}_{fg}$.

The final step is to then average over the initial state wavevector and derive a mean e-e scattering rate. This is done by integrating Eqs. (6) or (9) over $\mathbf{k}_i$ with the Fermi-Dirac distribution $f_i(k_i)$, dividing by the number of states and then simplifying:

$$W_{i,j \rightarrow f,g} = \frac{\int d\mathbf{k}_i W_{i,j \rightarrow f,g}(\mathbf{k}_i) k_i f_i(k_i)}{\int d\mathbf{k}_i k_i f_i(k_i)}.$$  

(10)

Both forms were used to study e-e scattering within three structures along with the effects of various approximations as explained in Sec. 2.
1.2 Prediction code

The model employed to study the QCL structures was a semi-classical, self-consistent model\textsuperscript{5} where the Schrödinger-Poisson equation was used to determine the electron eigenstates and eigenfunctions within three periods of the active region. The eigenstates from the central period were then copied to the two adjacent periods to avoid artificial boundary effects. Waveguide properties and electron-photon scattering rates were found before the calculation of electron-phonon (e-LO) and e-e scattering rates. The e-LO and e-e rates were then used to solve iterative rate equations based on periodic boundary conditions.\textsuperscript{6} The resulting populations were then fed back into the Schrödinger-Poisson solver and the entire process repeated until convergence of the electron populations was reached. The resulting states and population densities were used in the analysis of e-e scattering.

1.3 Structures

Electron-electron scattering was studied using three different structures. The first, an infinite quantum well, was included to examine various effects in a simple system with controlled conditions. In this case, the full machinery of the prediction code was not necessary since only the eigenstates and eigenenergies, which could be found analytically, were needed to calculate e-e rates. The well was 300 \text兒子 in width and the two lowest states in the well were used to find scattering rates at various temperatures and population densities. The effects of these parameters along with approximations are discussed in Sec. 2.

A 2.9 THz bound-to-continuum (BTC) QCL\textsuperscript{7} was modeled using the full self-consistent prediction code and the resulting states and populations (shown in Fig. 1(a)) were used to analyze the effects of e-e scattering rate approximations. This structure was designed to have a large number of energetically close states due to its dependence on e-e scattering as the means for depopulation. This therefore made it a good candidate to study the effects of e-e scattering rate approximations.

A 3.9 THz resonant-phonon (RP) QCL\textsuperscript{8} with exceptional high temperature performance was modeled in the same way as the BTC structure and is shown in Fig. 1(b). Despite the depopulation scheme being based upon a phonon resonance, the role of electron-electron scattering is still important between some transitions in the RP active region. Therefore, this structure was also used as a means to study the effects of approximations on the e-e scattering rate.
1.4 Overview

In the following sections, each approximation will be described and then its effect within the infinite quantum well, BTC and RP structures will be presented. First, the relative and non-relative wavevector definitions of the scattering rate (Eqs. (6) and (9)) will each be calculated as a function of the number of integration points. Next, the impact of including state-blocking and screening will be evaluated using several vital transitions within the structures. Finally, the importance of calculating transition rates other than the symmetric type \((i, i \rightarrow f, f)\) will be discussed.

2. APPROXIMATION ANALYSIS

2.1 Convergence and integration types

In order to numerically implement the integrals in Eq. (10), the step size for each integration has to be chosen. The mean scattering rate equations consist of four nested integrals (not including the sum over states in the denominator). Therefore, if the step size along each integration axis is defined so that there are 100 points, then the total number of integration points used to find the scattering rate is \(100^4 = 10^8\). Deciding whether to use more or less points is a compromise between speed and accuracy and requires some consideration.

As more points are used, the e-e rate eventually converges to some value. However, if this convergence can be reached more quickly, then fewer integration points are necessary to achieve a certain level of accuracy. The behavior of the integrals in Eq. (10) was studied as a function of the number of integration points to see whether the non-relative wavevector or the relative wavevector form reached convergence with fewer points. This was done for the infinite quantum well, the BTC structure and the RP structure.

The scattering rate as a function of the number of integration points is shown in Fig. 2 for the infinite quantum well at one particular temperature and population density. The non-relative form seems to have converged before the relative form; however, this was not always the case at different temperatures and populations. The situation was equally complex in the modeled QCL structures making it difficult to reach a conclusion as to the superiority of one form over another in terms of convergence speed.

In order to make a general statement about the relative performance of the integration types, the percent error was averaged from each scattering rate at a particular temperature. This error was determined from the scattering rate calculated using \(2.56 \times 10^{10}\) integration points. The average percent error created from simulation results of the BTC design is shown in Fig. 3(a) and (b) as a function of the number of integration points. Despite the averaging, neither form consistently converged faster than the other. This is also the case in the RP design as shown in Fig. 4(a) and (b). However, both Figs. 3 and 4 have lower percent error at higher numbers of integration points and indicate that in order to guarantee a percent error of less than 1% at all temperatures, \(10^8\) points (or 100 points per integration axis) must be used.

2.2 State-blocking and screening

When two electrons scatter with one another, they can only go into final states which are not already occupied due to Pauli’s exclusion principle. This effect is commonly referred to as state-blocking and is accounted for in Eqs. (6) and (9) by the inclusion of the Fermi-Dirac distribution functions \(f_f(k_f)\) and \(f_g(k_g)\). However, at low enough carrier densities, the effect of state-blocking can be neglected. Considering the densities encountered in a typical QCL \((10^{13} \text{ to } 10^{15} \text{ m}^{-2})\), this approximation is questionable. Additionally, the scattering rate without state-blocking is

\[
W_{i,j \rightarrow f,g}(k_i) = \frac{m^*e^4}{64\pi^3\hbar^3} \int dk_j \int d\theta_{ij} \int d\theta_{ij} |A_{ijfg}(q)|^2 f_j(k_j) \tag{11}
\]

which is an attractive form since it does not contain \(k_f\) or \(k_g\) and therefore does not require any conversion from relative wavevectors.

Another effect dependent on the electron population density is screening. It is treated in many texts, but no consensus exists yet on an optimal implementation in QCL prediction software. The full form of the 2D polarization function is the modified Lindhard formula in the random phase approximation (RPA):

\[
\Pi_{mn}(q, \omega) = \lim_{\delta \to 0} \sum_k \frac{f_m(k + q) - f_n(k)}{E_{m, k+q} - E_{m, k} - \hbar \omega - i\delta}. \tag{12}
\]
Figure 2: Convergence of the scattering rate as more integration points are used for the infinite quantum well at a temperature of 300 K and a subband population density of $10^{15} \, (1/m^2)$. The form using the non-relative wavevector definition and the form using the relative wavevector definition are compared. All integrals were performed with state-blocking and screening included.

Figure 3: Convergence of scattering rates within the bound-to-continuum structure as more points are used in the integrals at different temperatures. The percent error is averaged over all symmetric transitions at each temperature and all integrals are performed with state-blocking and screening included.
This is used to modify the Coulomb potential in a tensor equation of the form

\[
V_{ijfg}^{\text{sc}} = V_{ijfg} + \sum_{mn} V_{ijmn} \Pi_{mn} V_{ijfg}^{\text{sc}}
\]  

(13)

where \( V_{ijfg}^{\text{sc}} \) is the screened form of the bare Coulomb interaction \( V_{ijfg} \). Due to computational demands, it is extremely difficult to implement this in a QCL prediction code, especially in structures which contain a large number of electron states.

In order to reduce complexity a single subband model is often used, with two variations. Either the ground state (i.e. the subband with the highest population density) is used to determine the effect of screening for all subbands, or only the initial subband in each scattering event is used to calculate this effect.\(^4\, 13\) Both of these approaches have been shown to be flawed.\(^4\, 14\, 15\) However, a modified single subband model has been proposed\(^15\) and has been used in this work to determine the effect of screening on e-e scattering. It includes a temperature dependent polarization function\(^16\) of the form

\[
\Pi_{ii}(q, T) = \frac{m^*}{2\pi\hbar^2} \left[ 1 + \tanh \left( \frac{E_F}{2kT} \right) \right] \left[ 1 - \Theta(q - 2k_F) \sqrt{1 - \left( \frac{2k_F}{q} \right)^2} \right]
\]  

(14)

where \( \Theta \) is a step function, \( E_F \) is the quasi-Fermi energy for subband \( i \), \( k \) is Boltzman’s constant, \( T \) is the electron temperature in subband \( i \) and \( k_F \) is a wavevector defined as

\[
k_F = \sqrt{\frac{2\pi N_i}{g}}
\]  

(15)

where \( N_i \) is the population density for subband \( i \) and \( g \) is a degeneracy factor dependent on the active region material. This function is summed over all subbands in one period of the active region along with the intrasubband form factor \( A_{iii}(q) \) and then replaces the dielectric function \( \epsilon(q) \) in Eqs. (6) or (9) so that

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

(16)
Figure 5: The $W_{1,1\rightarrow 0,0}$ scattering rates in the infinite quantum well as a function of temperature and population density. The legend indicates which approximations were used in each plot: state-blocking included (SB on), state-blocking not included (SB off), screening included (SC on) and screening not included (SC off). For all points, $10^6$ integration points were used in the relative wavevector form of e-e scattering.

(a) $N_i = N_f = 10^{14} \text{ (1/m}^2\text{)}$

(b) $T = 100 \text{ K}$

The effect of both screening and state-blocking were studied using the three structures from Sec. 2.1. For the infinite quantum well, the lowest two states were once again used to find the scattering rate $W_{1,1\rightarrow 0,0}$. As shown in Fig. 5, this rate was studied as a function of 2D population density $N_i$ as well as temperature $T$. As more carriers were present in the well, a reduction of the scattering rates due to screening and state-blocking became more noticeable, where screening had the most pronounced impact with an increase in $N_i$.

The 2.9 THz BTC device, as shown in Fig. 1(a), was studied in a similar manner. Two transitions were singled out to demonstrate the reduction in scattering rates due to these effects. First, the primary transition responsible for depopulation, from the lower laser level (subband 16) to the next lowest state (subband 15), was plotted as a function of the initial and final population densities ($N_i$ and $N_f$, respectively) as well as temperature (Fig. 6). Due to the large number of states within each period of the active region screening had a noticeable impact and reduced the rates by 10 to 15 percent. State-blocking reduced the rates by only 1 to 2 percent. Another transition (subband 13 to subband 12) was plotted in Fig. 7. This exhibited similar behavior as the depopulation transition in terms of state-blocking; however, screening reduced the rate by as much as 30 percent.

Finally, the 3.9 THz RP structure, as shown in Fig. 1(b), was studied. In this case, since the depopulation scheme is based on a phonon resonance, there are fewer transitions which have an obvious dependence on the e-e scattering rate. However, a vital injection transition was studied (from subband 6 to subband 5) in Fig. 8. Screening was once again significant, reducing the rates by 5 to 10 percent. State-blocking was only noticeable at higher carrier densities and only reduced the rates by 1 to 2 percent.

2.3 Symmetric and asymmetric transitions

In order to find a transition rate $W_{ij}$ from subband $i$ to subband $j$ all scattering events that can contribute to that transition must be considered. Using a simple two-level system as an example, a $2 \rightarrow 1$ transition rate is the result of the symmetric scattering event $2,2 \rightarrow 1,1$ as well as the asymmetric scattering events $2,1 \rightarrow 1,1$ and $1,2 \rightarrow 1,1$. The situation is considerably more complicated in a QCL structure where many more states exist within the active region.

For the infinite quantum well, asymmetric scattering cannot occur, due to the quantum selection rules for a transition in a symmetric quantum well. However, due to the asymmetry of the potential structure in any
Figure 6: The $W_{16,16 \rightarrow 15,15}$ scattering rates in the bound-to-continuum structure as a function of electron temperature and the initial and final 2D subband population densities. For all points, $10^6$ integration points were used in the relative wavevector form of e-e scattering.

Figure 7: The $W_{13,13 \rightarrow 12,12}$ scattering rates in the bound-to-continuum structure as a function of electron temperature and the initial and final 2D subband population densities. For all points, $10^6$ integration points were used in the relative wavevector form of e-e scattering.
type of QCL, asymmetric transitions can occur. This opens up a myriad of possible scattering events which can contribute to a total transition rate \( W_{ij} \). In order to simplify this somewhat, only scattering events resulting from four adjacent subbands were considered for each transition.

As a representative example for the BTC design, the scattering events which contributed to the upper-state injection transition rate \( W_{11,10} \) are listed in Table 1. The symmetric scattering event \( 11,11 \rightarrow 10,10 \) is seen to have only the fifth highest rate of the scattering events included. Scattering events of the type \( 11,m \rightarrow 10,m \) and \( m,11 \rightarrow m,10 \), where \( m \) is one of the four adjacent subbands, are seen to contribute significantly to the transition rate \( W_{11,10} \). When all possible scattering events among the four adjacent subbands are summed, a total transition rate of \( 3.01 \times 10^{10} \) (1/s) is found. This is a factor of five times greater than the transition rate found from just symmetric scattering events. Therefore, it is essential that scattering events of this type along with the symmetric one be considered when determining transition rates which will eventually be used in the rate equations.

The same was also true in the RP structure as shown in Table 2, where the symmetric transition rate \( (4,4 \rightarrow 3,3) \) is only the fourth highest rate among those listed. This transition is also responsible for injection into the upper lasing state (subband 3). When all possible scattering events are summed, a total transition rate of \( 8.22 \times 10^{10} \) (1/s) is found. This is a factor of four times greater than the symmetric transition rate. This result is verified by comparison to results of published Monte Carlo simulations.\(^6\) Once again, the influence of these additional scattering events must be considered to improve the accuracy of transition rates.

### 3. CONCLUSION

The convergence of both the non-relative and relative wavevector forms of the scattering rates (Eqs. (6) and (9)) were shown to improve with an increase in the number of integration points. From this, it was concluded that if an error of less than 1 percent is needed, then \( 10^8 \) integration points (or 100 points per integration axis) are necessary to calculate a scattering rate. Within the QCL structures, the scattering rate was shown to be significantly affected by screening with scattering rates reduced by up thirty percent in the BTC structure and ten percent in the RP structure. In both structures state-blocking was shown to only reduce scattering rates by one to two percent. Finally, the importance of including both symmetric and asymmetric scattering events when finding a transition rate was demonstrated. Asymmetric scattering events were shown to increase the transition rate by a factor of five in the \( 11,11 \rightarrow 10,10 \) BTC transition and by factor of four in the \( 4,4 \rightarrow 3,3 \) RP transition.
Table 1: The e-e scattering rates in the bound-to-continuum structure for all possible transitions which significantly contribute to $W_{11,10}$ at a temperature of 40 K. The e-e rates were calculated using the relative wavevector form with $10^6$ integration points and with state-blocking and screening included.

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<th>scattering event $(i,j \rightarrow f,g)$</th>
<th>rate ($\times 10^9$ 1/s)</th>
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<tr>
<td>11, 12 $\rightarrow$ 10, 12 = 12, 11 $\rightarrow$ 12, 10</td>
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Table 2: The e-e scattering rates in the resonant phonon structure for all possible transitions which significantly contribute to $W_{4,3}$ at a temperature of 80 K. The e-e rates were calculated using the relative wavevector form with $10^6$ integration points and with state-blocking and screening included.

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