Quantum Cascade Laser Theory
Photon Scattering

Dr. Christopher S. Baird, University of Massachusetts Lowell

1.0 Introduction

Electrons in a QCL can transition between quantum states through photon scattering. Photon scattering rates are used in the rate equations to determine electron and photon populations, and in the end, the laser power. Photon scattering events include spontaneous photon emission, stimulated photon emission, and stimulated photon absorption.

The code is most complete if there are no assumptions made in advance as to which transition is the laser transition. This means that the code calculates the photon scattering rate for all possible transitions. In the end, the laser transition is identified as the one with the most laser power emitted, which is essentially the one with the highest photon population. The photon population of each transition is a function of electron population inversion and the photon scattering rate.

2.0 General Derivation

Fermi's Golden Rule describes the transition rate $W_{i\rightarrow f}$ from an initial quantum state i in the z dimension, initial free state with wave vector $\mathbf{k}_i$ in the x-y dimension, and initial photon state $n_{\mathbf{q},\sigma}$ with polarization index σ, to a final quantum state f in the z dimension, final free state with wave vector $\mathbf{k}_f$ in the x-y dimension, and final photon state $m_{\mathbf{q},\sigma}$:

$$W_{i\rightarrow f}^{\text{ems,abs}}(\mathbf{q},\mathbf{k}_i,\mathbf{k}_f)=\frac{2\pi}{\hbar}|<f,\mathbf{k}_f,m_{\mathbf{q},\sigma}|H'|i,\mathbf{k}_i,n_{\mathbf{q},\sigma}>|^2\delta\left(E_f(\boldsymbol{k}_f)-E_i(\mathbf{k}_i)\pm E_{\mathbf{q}}\right)$$

The delta term is a statement of the conservation of energy. If a photon is emitted, then $E_{before}=E_{after}$, which means $E_i=E_f+E_{\mathbf{q}}$, and finally $E_f-E_i+E_{\mathbf{q}}=0$. If a photon is absorbed, then $E_{before}=E_{after}$, which means $E_i+E_{\mathbf{q}}=E_f$, and finally $E_f-E_i-E_{\mathbf{q}}=0$.

The interaction Hamiltonian in SI units between an electron and a photon is given by:

$$H'=-\frac{e}{m^*}\mathbf{A}\cdot\mathbf{P}$$

where **A** is the electromagnetic vector potential operator describing the photons interacting with the electron, and **P** is the momentum

operator of the electron. The effective mass is taken from the well material since this is where the electron spends most of its time.

In SI units, The Lorentz-Gauge vector potential for an harmonic interaction with a quantized EM field at a single wave vector **q** is a sum of creation and annihilation operators:

$$\mathbf{A}=\sum_{\sigma=1}^{2}\sqrt{\frac{\hbar}{2\epsilon V q c/n}}\left[a_{\mathbf{q},\sigma}\boldsymbol{\epsilon}_{\mathbf{q},\boldsymbol{\sigma}}e^{i\mathbf{q}\cdot\mathbf{r}}+a^{\dagger}_{\mathbf{q},\sigma}\boldsymbol{\epsilon}_{\mathbf{q},\boldsymbol{\sigma}}e^{-i\mathbf{q}\cdot\mathbf{r}}\right]$$

where V is the cavity volume, ε is the dielectric constant, $\boldsymbol{\varepsilon}$ is the polarization vector and **q** is the wave vector of the photon.

Now substitute this expanded Hamiltonian in Fermi's Golden Rule:

$$W^{\text{ems,abs}}_{i\to f}(\mathbf{q},\mathbf{k}_i,\mathbf{k}_f)=\frac{2\pi}{\hbar}\left|<f,\mathbf{k}_f,m_{\mathbf{q},\sigma}\left|\left[-\frac{e}{m^*}\left[\sum_{\sigma=1}^{2}\sqrt{\frac{\hbar}{2\epsilon V q c/n}}\left[a_{\mathbf{q},\sigma}\boldsymbol{\epsilon}_{\mathbf{q},\boldsymbol{\sigma}}e^{i\mathbf{q}\cdot\mathbf{r}}+a^{\dagger}_{\mathbf{q},\sigma}\boldsymbol{\epsilon}_{\mathbf{q},\boldsymbol{\sigma}}e^{-i\mathbf{q}\cdot\mathbf{r}}\right]\right]\cdot\mathbf{P}\right]\right|i,\mathbf{k}_i,n_{\mathbf{q},\sigma}>\right|^2\delta(E_f(\boldsymbol{k}_f)-E_i(\mathbf{k}_i)\pm E_{\mathbf{q}})$$

$$W^{\text{ems,abs}}_{i\to f}(\mathbf{q},\mathbf{k}_i,\mathbf{k}_f)=\frac{2\pi}{\hbar}\frac{e^2}{(m^*)^2}\frac{\hbar}{2\epsilon V q c/n}\delta(E_f(\boldsymbol{k}_f)-E_i(\mathbf{k}_i)\pm E_{\mathbf{q}})\left|<f,\mathbf{k}_f,m_{\mathbf{q},\sigma}\left|\left[\sum_{\sigma=1}^{2}\left[a_{\mathbf{q},\sigma}\boldsymbol{\epsilon}_{\mathbf{q},\boldsymbol{\sigma}}e^{i\mathbf{q}\cdot\mathbf{r}}+a^{\dagger}_{\mathbf{q},\sigma}\boldsymbol{\epsilon}_{\mathbf{q},\boldsymbol{\sigma}}e^{-i\mathbf{q}\cdot\mathbf{r}}\right]\right]\cdot\mathbf{P}\right|i,\mathbf{k}_i,n_{\mathbf{q},\sigma}>\right|^2$$

$$W^{\text{ems,abs}}_{i\to f}(\mathbf{q},\mathbf{k}_i,\mathbf{k}_f)=\frac{2\pi}{\hbar}\frac{e^2}{(m^*)^2}\frac{\hbar}{2\epsilon V q c/n}\delta(E_f(\boldsymbol{k}_f)-E_i(\mathbf{k}_i)\pm E_{\mathbf{q}})|M|^2$$

where the matrix element is $M=<f,\mathbf{k}_f,m_{\mathbf{q},\sigma}\left|\left[\sum_{\sigma=1}^{2}\left[a_{\mathbf{q},\sigma}\boldsymbol{\epsilon}_{\mathbf{q},\boldsymbol{\sigma}}e^{i\mathbf{q}\cdot\mathbf{r}}+a^{\dagger}_{\mathbf{q},\sigma}\boldsymbol{\epsilon}_{\mathbf{q},\boldsymbol{\sigma}}e^{-i\mathbf{q}\cdot\mathbf{r}}\right]\right]\cdot\mathbf{P}\right|i,\mathbf{k}_i,n_{\mathbf{q},\sigma}>$

Let us evaluate the matrix element M as much as we can before turning back to the full equation.

$$M=\sum_{\sigma=1}^{2}<f,\mathbf{k}_f,m_{\mathbf{q},\sigma}|a_{\mathbf{q},\sigma}\boldsymbol{\epsilon}_{\mathbf{q},\boldsymbol{\sigma}}e^{i\mathbf{q}\cdot\mathbf{r}}\cdot\mathbf{P}|i,\mathbf{k}_i,n_{\mathbf{q},\sigma}>+<f,\mathbf{k}_f,m_{\mathbf{q},\sigma}|a^{\dagger}_{\mathbf{q},\sigma}\boldsymbol{\epsilon}_{\mathbf{q},\boldsymbol{\sigma}}e^{-i\mathbf{q}\cdot\mathbf{r}}\cdot\mathbf{P}|i,\mathbf{k}_i,n_{\mathbf{q},\sigma}>$$

$$M=\sum_{\sigma=1}^{2}<f,\mathbf{k}_f|\boldsymbol{\epsilon}_{\mathbf{q},\boldsymbol{\sigma}}e^{i\mathbf{q}\cdot\mathbf{r}}\cdot\mathbf{P}|i,\mathbf{k}_i><m_{\mathbf{q},\sigma}|a_{\mathbf{q},\sigma}|n_{\mathbf{q},\sigma}>+<f,\mathbf{k}_f|\boldsymbol{\epsilon}_{\mathbf{q},\boldsymbol{\sigma}}e^{-i\mathbf{q}\cdot\mathbf{r}}\cdot\mathbf{P}|i,\mathbf{k}_i><m_{\mathbf{q},\sigma}|a^{\dagger}_{\mathbf{q},\sigma}|n_{\mathbf{q},\sigma}>$$

$$M=\sum_{\sigma=1}^{2}<f,\mathbf{k}_f|\boldsymbol{\epsilon}_{\mathbf{q},\boldsymbol{\sigma}}e^{i\mathbf{q}\cdot\mathbf{r}}\cdot\mathbf{P}|i,\mathbf{k}_i>\sqrt{n_{\mathbf{q},\sigma}}<m_{\mathbf{q},\sigma}|n_{\mathbf{q},\sigma}-1>+<f,\mathbf{k}_f|\boldsymbol{\epsilon}_{\mathbf{q},\boldsymbol{\sigma}}e^{-i\mathbf{q}\cdot\mathbf{r}}\cdot\mathbf{P}|i,\mathbf{k}_i>\sqrt{n_{\mathbf{q},\sigma}+1}<m_{\mathbf{q},\sigma}|n_{\mathbf{q},\sigma}+1>$$

Due to orthogonality, the initial and final photon states directly above must be equal. Out of all the possible initial and final state combinations, all are zero except for two cases where each term above is satisfied.

CASE 1: If $m_{\mathbf{q},\sigma}=n_{\mathbf{q},\sigma}+1$ (photon created, emitted from electron) then

$$M^{\text{ems}}=\sum_{\sigma=1}^{2}\sqrt{n_{\mathbf{q},\sigma}+1}<f,\mathbf{k}_f|\boldsymbol{\epsilon}_{\mathbf{q},\boldsymbol{\sigma}}e^{-i\mathbf{q}\cdot\mathbf{r}}\cdot\mathbf{P}|i,\mathbf{k}_i>$$

CASE 2: If $m_{\mathbf{q},\sigma}=n_{\mathbf{q},\sigma}-1$ (photon destroyed, absorbed by electron) then

$$M^{\text{abs}}=\sum_{\sigma=1}^{2}\sqrt{n_{\mathbf{q},\sigma}}<f,\mathbf{k}_f|\boldsymbol{\epsilon}_{\mathbf{q},\boldsymbol{\sigma}}e^{i\mathbf{q}\cdot\mathbf{r}}\cdot\mathbf{P}|i,\mathbf{k}_i>$$

Combining the two cases:

$$M^{\text{ems,abs}}=\sum_{\sigma=1}^{2}\sqrt{n_{\mathbf{q},\sigma}+1/2\pm1/2}<f,\mathbf{k}_f|\boldsymbol{\epsilon}_{\mathbf{q},\boldsymbol{\sigma}}e^{\mp i\mathbf{q}\cdot\mathbf{r}}\cdot\mathbf{P}|i,\mathbf{k}_i>$$

Since we are dealing with Terahertz radiation and nanometer scales, the dipole approximation is valid (the exponent equals one):

$$M^{\text{ems,abs}}=\sum_{\sigma=1}^{2}\sqrt{n_{\mathbf{q},\sigma}+1/2\pm1/2}<f,\mathbf{k}_f|\boldsymbol{\epsilon}_{\mathbf{q},\boldsymbol{\sigma}}\cdot\mathbf{P}|i,\mathbf{k}_i>$$

$$M^{\text{ems,abs}}=\sum_{\sigma=1}^{2}\sqrt{n_{\mathbf{q},\sigma}+1/2\pm1/2}\left[<f,\mathbf{k}_f|\epsilon_{\sigma,x}P_x|i,\mathbf{k}_i>+<f,\mathbf{k}_f|\epsilon_{\sigma,y}P_y|i,\mathbf{k}_i>+<f,\mathbf{k}_f|\epsilon_{\sigma,z}P_z|i,\mathbf{k}_i>\right]$$

$$M^{\text{ems,abs}}=\sum_{\sigma=1}^{2}\sqrt{n_{\mathbf{q},\sigma}+1/2\pm1/2}\left[\epsilon_{\sigma,x}<f(z)|i(z)><\mathbf{k}_f|P_x|\mathbf{k}_i>+\epsilon_{\sigma,y}<f(z)|i(z)><\mathbf{k}_f|P_y|\mathbf{k}_i>+\epsilon_{\sigma,z}<\mathbf{k}_f(x,y)|\mathbf{k}_i(x,y)><f(z)|P_z|i(z)>\right]$$

Due to the orthogonality of the quantized states in the *z* dimension, several terms drop out, leaving:

$$M^{\text{ems, abs}} = \sum_{\sigma=1}^{2} \sqrt{n_{\mathbf{q},\sigma} + 1/2 \pm 1/2}\, \epsilon_{\sigma,z} < \mathbf{k}_f(x,y) | \mathbf{k}_i(x,y) > < f(z) | P_z | i(z) >$$

The first inner product is a statement of conservation of momentum. Because the photon carries away no momentum in the transverse directions, the initial electron's momentum must equal the final electron's momentum.

$$M^{\text{ems, abs}} = \sum_{\sigma=1}^{2} \sqrt{n_{\mathbf{q},\sigma} + 1/2 \pm 1/2}\, \epsilon_{\sigma,z} \delta_{\mathbf{k}_f,\mathbf{k}_i} < f(z) | P_z | i(z) >$$

We can use the commutation relation with the unperturbed Hamiltonian: $P_z = \frac{i m^*}{\hbar} [H_{0,} z]$

$$M^{\text{ems, abs}} = \sum_{\sigma=1}^{2} \sqrt{n_{\mathbf{q},\sigma} + 1/2 \pm 1/2}\, \epsilon_{\sigma,z} \delta_{\mathbf{k}_f,\mathbf{k}_i} \frac{i m^*}{\hbar} (E_f - E_i) < f(z) | z | i(z) >$$

We now substitute the matrix element *M* back into the original scattering rate equation:

$$W_{i\to f}^{\text{ems,abs}}(\mathbf{q}, \mathbf{k}_i, \mathbf{k}_f) = \frac{2\pi}{\hbar} \frac{e^2}{(m^*)^2} \frac{\hbar}{2\epsilon V q c/n} \delta(E_f(\boldsymbol{k}_f) - E_i(\mathbf{k}_i) \pm E_{\mathbf{q}}) \frac{(m^*)^2 (E_f - E_i)^2}{\hbar^2} | < f(z) | z | i(z) > |^2 \delta_{\mathbf{k}_f,\mathbf{k}_i} | \sum_{\sigma=1}^{2} \epsilon_{\sigma,z} \sqrt{n_{\mathbf{q},\sigma} + 1/2 \pm 1/2} |^2$$

Expand out the energies in the conservation-of-energy delta:

$$W_{i\to f}^{\text{ems,abs}}(\mathbf{q}, \mathbf{k}_i, \mathbf{k}_f) = \frac{2\pi}{\hbar} \frac{e^2}{(m^*)^2} \frac{\hbar}{2\epsilon V q c/n} \frac{(m^*)^2 (E_f - E_i)^2}{\hbar^2} | < f(z) | z | i(z) > |^2 | \sum_{\sigma=1}^{2} \epsilon_{\sigma,z} \sqrt{n_{\mathbf{q},\sigma} + 1/2 \pm 1/2} |^2$$
$$\times \delta\left(E_f + \frac{\hbar^2 k_f^2}{2m^*} - E_i - \frac{\hbar^2 k_i^2}{2m^*} \pm E_{\mathbf{q}}\right) \delta_{\mathbf{k}_f,\mathbf{k}_i}$$

With the initial and final electron momentum wavenumbers equal, the photon energy simplifies down to a difference of the subband minima:

$$W_{i\to f}^{\text{ems,abs}}(\mathbf{q}, \mathbf{k}_i, \mathbf{k}_f) = \frac{2\pi}{\hbar} \frac{e^2}{(m^*)^2} \frac{\hbar}{2\epsilon V q c/n} \frac{(m^*)^2 (E_f - E_i)^2}{\hbar^2} | < f(z) | z | i(z) > |^2 | \sum_{\sigma=1}^{2} \epsilon_{\sigma,z} \sqrt{n_{\mathbf{q},\sigma} + 1/2 \pm 1/2} |^2 \delta(E_f - E_i \pm E_{\mathbf{q}}) \delta_{\mathbf{k}_f,\mathbf{k}_i}$$

We sum over all possible final electron momenta. The Kronecker delta ensuring conservation of momentum dictates that only one term

remains:

$$W_{i\to f}^{\text{ems,abs}}(\mathbf{q})=\frac{2\pi}{\hbar}\frac{e^2}{(m^*)^2}\frac{\hbar}{2\epsilon V q c/n}\frac{(m^*)^2(E_f-E_i)^2}{\hbar^2}|<f(z)|z|i(z)>|^2\left|\sum_{\sigma=1}^{2}\epsilon_{\sigma,z}\sqrt{n_{\mathbf{q},\sigma}+1/2\pm 1/2}\right|^2\delta(E_f-E_i\pm E_{\mathbf{q}})$$

We define some parameters and simplify the constants to find:

$$\boxed{W_{i\to f}^{\text{ems,abs}}(\mathbf{q})=\frac{e^2 h\omega_{if}}{4m^*\sqrt{\epsilon_r}\epsilon_0 V q c}f_{i\to f}\left|\sum_{\sigma=1}^{2}\epsilon_{\sigma,z}\sqrt{n_{\mathbf{q},\sigma}+1/2\pm 1/2}\right|^2\delta(E_f-E_i\pm E_{\mathbf{q}})}$$

where the oscillator strength is: $f_{i\to f}=\frac{2m^*\omega_{if}}{\hbar}|<f(z)|z|i(z)>|^2$ and the resonant frequency is $\omega_{if}=\frac{E_i-E_f}{\hbar}$.

The oscillator strength is simplified to: $f_{i\to f}=\frac{2m^*\omega_{if}}{\hbar}\left|\int \psi_f^*(z)\,z\,\psi_i(z)\,dz\right|^2$

The integral is done numerically using the non-uniform-grid trapezoidal method.

3.0 Distinct Cases

There are many relevant cases that are handled differently for the different mode distributions, mechanisms, and assumptions:

1. Spontaneous Photon Emission into one mode
2. Stimulated Photon Emission/Absorption into one mode
3. Spontaneous Photon Emission into all modes
4. Stimulated Photon Emission/Absorption into a narrow mode distribution

We now handle one case at a time.

3.1 Spontaneous Photon Emission into one mode

$$W_{i\to f}^{\text{sp,1mode}}(\mathbf{q})=\frac{e^2 h\omega_{if}}{4m^*\sqrt{\epsilon_r}\epsilon_0 V q c}f_{i\to f}\left|\sum_{\sigma=1}^{2}\epsilon_{\sigma,z}\right|^2\delta(E_f-E_i\pm E_{\mathbf{q}})$$

All that contributes to the laser radiation out the front is one mode in one polarization. We set the sum over polarization unit vectors equal to one. This reduces the equation to:

$$W_{i\to f}^{\text{sp,1mode}}(q)=\frac{e^2 h\omega_{if}}{4m^*\sqrt{\epsilon_r}\epsilon_0 V q c} f_{i\to f}\,\delta(E_f-E_i+E_{\mathbf{q}})$$

Here V is the laser cavity volume. Note that the laser cavity volume is the active region volume over the confinement factor: $V=V_{active}/\Gamma$

Now integrate over all energies that may contribute to the mode:

$$W_{i\to f}^{\text{sp,1mode}}(q)=\frac{1}{2\pi/L}\int_0^\infty \frac{e^2 h\omega_{if}}{4m^*\sqrt{\epsilon_r}\epsilon_0 V q c} f_{i\to f}\,\delta(E_f-E_i+E_{\mathbf{q}})dq$$

$$\boxed{W_{i\to f}^{\text{sp,1mode}}(q)=\frac{e^2 L}{4m^*\sqrt{\epsilon_r}\epsilon_0 V c} f_{i\to f}}$$

This expression is not used directly in the code because spontaneous emission into one mode is negligible.

3.2 Stimulated Photon Emission/Absorption into one mode

Emission and absorption are handled with the same equation as they are so similar. The general equation states:

$$W_{i\to f}^{\text{stim,1mode}}(\mathbf{q})=\frac{e^2 h\omega_{if}}{4m^*\sqrt{\epsilon_r}\epsilon_0 V q c} f_{i\to f}\left|\sum_{\sigma=1}^{2}\epsilon_{\sigma,z}\sqrt{n_{\mathbf{q},\sigma}+1/2\pm1/2}\right|^2\delta(E_f-E_i\pm E_{\mathbf{q}})$$

We drop the halves because those represent spontaneous emission, and drop the sum over polarizations because we are only interested in one mode:

$$W_{i\to f}^{\text{stim,1mode}}(\mathbf{q})=\frac{e^2 h\omega_{if}}{4m^*\sqrt{\epsilon_r}\epsilon_0 V q c} f_{i\to f} n_{\mathbf{q},\sigma}\,\delta(E_f-E_i\pm E_{\mathbf{q}})$$

To avoid confusion with the photon density used elsewhere, let us relabel the *number* of photons $n_{\mathbf{q},\sigma}$ in this mode σ and in the frequency corresponding to wave vector $\mathbf{q}$ as M_{if} so that it is more clear that it is the total number and that it has a frequency corresponding to the i to f transition.

$$W_{i\to f}^{\text{stim,1mode}}(\mathbf{q}) = \frac{e^2 h \omega_{if}}{4 m^* \sqrt{\epsilon_r}\epsilon_0 V q c} f_{i\to f}\delta(E_f - E_i \pm E_{\mathbf{q}}) M_{if}$$

Now integrate over all energies that may contribute to the mode:

$$W_{i\to f}^{\text{stim,1mode}}(q) = \frac{e^2 L}{4 m^* \sqrt{\epsilon_r}\epsilon_0 V c} f_{i\to f} M_{if}$$

Comparing this expression to the spontaneous one-mode rate shows that they are identical apart from the number of photons in this mode:

$$\boxed{W_{i\to f}^{\text{st,1mode}} = M_{if} W_{i\to f}^{\text{sp,1mode}}}$$

This expression is generally applicable and very useful. It means that we can calculate the spontaneous rate once per main code loop iteration, and then find the stimulated rate by calculating the photon population using the rate equations. This expression is not currently used by the code because emission into a narrow range of modes (Case 4) matches experiment better than emission into one mode.

3.3 Spontaneous Photon Emission into all modes

$$W_{i\to f}^{\text{sp}}(\mathbf{q}) = \frac{e^2 h \omega_{if}}{4 m^* \sqrt{\epsilon_r}\epsilon_0 V q c} f_{i\to f} \left|\sum_{\sigma=1}^{2} \epsilon_{\sigma,z}\right|^2 \delta(E_f - E_i + E_{\mathbf{q}})$$

Sum over all modes in the cavity (assuming an effectively infinite cavity in all three dimensions)

$$W_{i\to f}^{\text{sp}} = \frac{1}{(2\pi/L)^3}\int d\,\mathbf{q}\, W_{i\to f}^{\text{sp}}(\mathbf{q})$$

$$W_{i\to f}^{\text{sp}} = \frac{1}{(2\pi/L)^3}\int d\,q\, q^2 \int d\,\theta \sin\theta \int d\,\phi\, W_{i\to f}^{\text{sp}}(\mathbf{q})$$

$$W_{i\to f}^{\text{sp}} = \frac{1}{(2\pi/L)^3}\int d\,q\, q^2 \int d\,\theta \sin\theta \int d\,\phi \frac{e^2 h \omega_{if}}{4 m^* \sqrt{\epsilon_r}\epsilon_0 V q c} f_{i\to f} \left|\sum_{\sigma=1}^{2} \epsilon_{\sigma,z}\right|^2 \delta(E_f - E_i + E_{\mathbf{q}})$$

If we choose the axis such that $\boldsymbol{\varepsilon}_1$ lies in the plane defined by **k** and **q**, then $\varepsilon_{2,z} = 0$ and $\varepsilon_{1,z} = \sin\theta$

$$W_{i\to f}^{\text{sp}} = \frac{1}{(2\pi/L)^3}\int dq\, q^2 \int d\theta \sin\theta \int d\phi \frac{e^2 h \omega_{if}}{4 m^* \sqrt{\epsilon_r}\epsilon_0 V q c} f_{i\to f} \sin^2\theta\, \delta(E_f - E_i + E_{\mathbf{q}})$$

$$W_{i\to f}^{\text{sp}} = \frac{1}{(2\pi/L)^3}\frac{e^2 h \omega_{if}}{4 m^* \sqrt{\epsilon_r}\epsilon_0 V c} f_{i\to f} \int dq\, q \int d\theta \sin^3\theta \int d\phi\, \delta(E_f - E_i + \hbar c q/n)$$

$$W_{i\to f}^{\text{sp}} = \frac{1}{(2\pi/L)^3}\frac{e^2 h \omega_{if} n}{4 m^* \sqrt{\epsilon_r}\epsilon_0 V c^2 \hbar} f_{i\to f} \omega_0 n/c \left(\frac{4}{3}\right)(2\pi)$$

$$\boxed{W_{i\to f}^{\text{sp}} = \frac{e^2 n \omega_{if}^2}{6\pi m^* \epsilon_0 c^3} f_{i\to f}}$$

This expression is used in the rate equations simply as another scattering mechanism that effects electron populations. The radiation due to spontaneous emission into all modes does not contribute to the laser radiation. Note that for typical QCL's, the spontaneous photon emission rate into all modes is so small compared to other scattering mechanisms that it is essentially negligible. However, this calculation is still included in the code because it is so easy to implement, runs quickly and establishes a more complete code.

3.4 Stimulated Photon Emission/Absorption into a narrow mode distribution at one polarization

We start with the one-mode expression before integrating over all energies:

$$W_{i\to f}^{\text{st}}(q) = \frac{e^2 h \omega_{if}}{4 m^* \sqrt{\epsilon_r}\epsilon_0 V q c} f_{i\to f} M_{if}\, \delta(E_f - E_i \pm E_{\mathbf{q}})$$

$$W_{i\to f}^{\text{st}}(q) = \frac{e^2 h \omega_{if}}{4 m^* \sqrt{\epsilon_r}\epsilon_0 V q c} f_{i\to f} M_{if} \frac{1}{h}\delta\left(\frac{(E_f - E_i)}{h} \pm \nu\right)$$

To mimic reality where the energy levels have finite widths due to their finite lifetimes, the Dirac delta is replaced with a normalized lineshape function in the form of a Lorentzian:

$$W_{i\to f}^{\text{st,band}}(q) = \frac{e^2 \omega_{if}}{4 m^* \sqrt{\epsilon_r}\epsilon_0 V q c} f_{i\to f} M_{if}\, \gamma_{if}(\nu) \quad \text{where} \quad \gamma_{if}(\nu) = \frac{\Delta\nu_{if}/2\pi}{(\nu - \nu_{if})^2 + (\Delta\nu_{if}/2)^2} \quad , \quad \nu_{if} = \frac{\omega_{if}}{2\pi} = \frac{E_i - E_f}{h}$$

and the full-width half maximum linewidth of the transition is:

$$\Delta\nu_{if}=\frac{1}{\pi}\left(\frac{1}{2\tau_i}+\frac{1}{2\tau_f}+\frac{1}{T_2^*}\right)$$

The parameters τ_i and τ_f are the initial and final state total lifetimes and T_2* is the pure dephasing time.

$$W_{i\to f}^{\text{st,band}}(\nu)=\frac{e^2\nu_{if}}{4m^*\epsilon V\nu}f_{i\to f}M_{if}\gamma_{if}(\nu)$$

We need to use the stimulated emission rate in the rate equations in order to determine the photon populations. The rate equations require a single number for the transition rate, but the expression above is an entire function. We solve this by taking the scattering rate at the peak frequency.

Set $\nu=\nu_{if}$:

$$\boxed{W_{i\to f}^{\text{st,band}}=M_{if}\frac{e^2}{2\pi m^*\epsilon V\Delta\nu_{if}}f_{i\to f}}$$ where $$\boxed{f_{i\to f}=\frac{2m^*\omega_{if}}{\hbar}\left|\int\psi_f^*(z)\,z\,\psi_i(z)\,dz\right|^2}$$ and $$\boxed{\Delta\nu_{if}=\frac{1}{\pi}\left(\frac{1}{2\tau_i}+\frac{1}{2\tau_f}+\frac{1}{T_2^*}\right)}$$

In the code, this expression is calculated without the photon number factor, and then the photon number is found using the rate equations. Note that there is great uncertainty in the literature as to what the pure dephasing time T_2* should be. The value used and published for mid-infrared QCL's was found to give poor results for Terahertz QCL's. The value of T_2* = 15 picoseconds was found to give the best code predictions for terahertz QCL's when compared to experiment and is the value currently used by the code.

The integral in the oscillator strength is done numerically using the non-uniform-grid trapezoidal method. The integral cannot be done over infinity, but is instead done over the three periods of the QCL core structure used in this code. Note that the location points *z* and the wavefunctions are defined on a non-uniform grid in order to preserve material layer widths exactly. Using a non-uniform grid means that traditional numerical integration methods such as Simpson's rule and the Boole rule cannot be used.