Quantum Cascade Laser Theory
Rate Equations

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1.0 Introduction

Once all of the scattering rates are known, we apply the rate equations to determine the level populations. To use the rate equations, we assume that the system is in a state of equilibrium. This means that the total rate at which electrons transition into a given level equals the total rate at which electrons transition out. The total rate is the the transition rate of one electron times the number of electrons in the initial state. The rate equations therefore form a series of coupled equations. In this code, the photon populations are solved self-consistently with the electron populations. There is a photon population associated with each possible transition, and a rate equation for each photon population. In order to attain completeness and accuracy, all possible electron and photon populations in the three period structure are included in the rate equations.

2.0 Definitions and Notation

There are N quantum states in the three repetitions of the QCL core period, spanning from $i = 0$ to $i = N\text{-}1$. The code finds the electron population n_i of each level as well as the photon population m_{ij} of each possible transition. At this point in the calculations, the code has already found all transition rates W_{ij} from level i to level j: photon scattering, electron-electron scattering, and phonon scattering. Also known is the total electron density n_{tot} which is the sum of all the level populations in one period and remains constant. The code has already found the waveguide loss α_w, the mirror loss α_m, the confinement factor Γ, and the photon cavity loss rate W_p^{ij} at many frequencies.

We cannot assume we know the current because that depends on the populations. We must account for electrons flowing into and out of one period of the QCL by assuming the structure is periodic and at equilibrium so that all the electrons flowing out of the period must flow back into the period. The middle of the three numerically calculated QCL periods is taken to be the most accurate and is the one used. This raises the dilemma of how to handle wavefunctions and transitions that span several periods.

The best way is to find the center of mass of each wavefunction and treat the wavefunction as located in the period containing its center of mass. For the purpose of enforcing periodicity, transitions are considered to happen between the center-of-mass points of each state. Based on the center-of-mass approach, this reduces the periodicity problem to four cases:

(1) A transition starting in the central period and ending in the central period. This can be handled in the usual way.
(2) A transition starting in the central period and ending in the outer periods and vice versa. This must be handled by matching up corresponding wavefunctions in different periods and tying them to the same population variable.
(3) A transition starting in one outer period and ending in the other outer period. These are two-period transitions and are again handled by matching up equivalent wavefunctions.
(4) A transition starting and ending in the same outer period. These are ignored as they are redundant to case (1)

3.0 Derivations

At equilibrium, the sum of all possible transition rates into the level and out of the level are equal. This is the same as setting their difference equal to zero. The sum is done over every type of transition (electron-electron, LO phonon, etc.) and over every possible combination of initial and final level in all three periods.

$$0=\sum_{\substack{j=0\\ j\neq i}}^{N-1} W_{ji} n_j - n_i \sum_{\substack{j=0\\ j\neq i}}^{N-1} W_{ij} + \sum_{\substack{j=0\\ j\neq i}}^{N-1} W_{ji}^{\mathrm{st,1mode}} n_j - n_i \sum_{\substack{j=0\\ j\neq i}}^{N-1} W_{ij}^{\mathrm{st,1mode}}$$

The first term in the equation above is the sum over all non-stimulated photon emission transitions coming into level *i*. The second term is the sum over all non-stimulated photon emission transitions leaving level *i*. The third term is all of the stimulated photon emission transitions coming into level *i.* The fourth term is all of the stimulated photon emission transitions leaving level *i.*

The stimulated absorption and emission rates are equal, $W_{ji}^{\mathrm{st,1mode}} = W_{ij}^{\mathrm{st,1mode}}$, leading to

$$0=\sum_{\substack{j=0\\ j\neq i}}^{N-1} W_{ji} n_j - n_i \sum_{\substack{j=0\\ j\neq i}}^{N-1} W_{ij} - \sum_{j=0}^{N-1} W_{ij}^{\mathrm{st,1mode}} \left(n_i - n_j\right)$$

The total stimulated emission rate is just the one-mode spontaneous rate times the total *number* of photons M_{ij} available to stimulate:

$$W_{ij}^{\mathrm{st,1mode}} = M_{ij} W_{ij}^{\mathrm{sp,1mode}}$$

There is a photon number M_{ij} corresponding to every possible transition and we must keep track of each one. Each photon population also has a rate equation to be solved. Because both the stimulated absorption rate and stimulated emission rate equal, they are both dependent on the one-mode spontaneous emission rate. The best way to handle this in the code is to make the one-mode spontaneous emission matrix symmetric so that $W_{ij} = W_{ji}$. Even though spontaneous emission cannot happen for transition up the energy scale, this is still valid because the one-mode spontaneous emission rates are only used to determine the stimulated rates, which can go up and down.

It is easiest to speak of everything in terms of densities and not numbers because then it becomes independent of the bounding box. We set the number of photons in a certain mode in the cavity *that are available to stimulate emission* equal to the one-mode photon population density m_{ij} times the volume V of the active region.

$$M_{ij} = m_{ij} V$$

Insert this into the rate equations:

$$0 = \sum_{\substack{j=0 \\ j \neq i}}^{N-1} W_{ji} n_j - n_i \sum_{\substack{j=0 \\ j \neq i}}^{N-1} W_{ij} - \sum_{j=0}^{N-1} m_{ij} V W_{ij}^{\text{sp,1mode}} \left(n_i - n_j \right)$$

This expression represents a set of N coupled equations. This can be solved numerically by using fixed point iteration. Solve for n_i in terms of n_j in order to establish iteration equations. We start with a well estimated set of populations and apply the iteration equation repeatedly, treating n_i as the next iterated value of the population densities and n_j as the current value.

$$n_i = \frac{\sum_{\substack{j=0 \\ j \neq i}}^{N-1} n_j \left[W_{ji} + m_{ij} V W_{ij}^{\text{sp,1mode}} \right]}{\sum_{\substack{j=0 \\ j \neq i}}^{N-1} \left[W_{ij} + m_{ij} V W_{ij}^{\text{sp,1mode}} \right]}$$

Repeat this equation iteratively, setting $n_j = n_i$ after each step, until the population densities converge to a steady value. After each iteration, the populations must be normalized so that their sum equals the total average electron density. Mathematically speaking, one of the rate equations is redundant and the populations are under-specified by the rate equations. Applying the normalization is required to find a unique solution. The coupled rate equations could also be solved using matrix inversion techniques. However, fixed-point iteration was found to be easier to implement, and not significantly slower or less accurate then matrix techniques.

Periodic boundary conditions, which take into account the total current entering and leaving a period, are implemented by treating each level of the three period numerical array of data as independent, solving the rate equations as if they are independent, and then at the end of each iteration, copying the population densities from the levels in the central period to the equivalent levels in the outer periods. The wavefunction matching information is required to do this.

Each photon population present also has a rate equation at equilibrium:

$$0 = V\,W_{ij}^{\mathrm{st,1mode}}\,n_i - V\,W_{ji}^{\mathrm{st,1mode}}\,n_j + V\,W_{ij}^{\mathrm{sp,1mode}}\,n_i - V_p\,m_{ij}\,W_{ij}^{p}$$

The first term in the above equation is the total number rate at which photons are added to the cavity in mode *ij* due to stimulated emission. The second term is the total number rate at which photons are removed to the cavity in mode *ij* due to stimulated absorption. The third term is the total number rate at which photons are added to the cavity in mode *ij* due to spontaneous emission. The fourth term is the number rate at which photons are removed due to the waveguide losses and mirror losses, where W_{ij}^{p} is the total photon cavity loss rate at the frequency corresponding to the *ij* transition.

The photon loss rate is a function of the waveguide loss, mirror loss and group velocity according to $W_{ij}^{p} = (\alpha_w + \alpha_m)v_g$. These values are precalculated in the waveguide code as a frequency-dependent look-up table. In these rate equation calculations, the frequency of the transition concerned is used to look up the photon cavity loss rate for that photon population. The electrons able to be stimulated are only in the active region, so that the active region volume V must be multiplied by the electron population densities to get the total number, whereas all photons can be lost - those in the active region and in the outer waveguide layers - so that the cavity volume V_p must be used to find the total number of photons lost.

Divide every term by V_p and recognize the known confinement factor $\Gamma = V / V_p$ to find:

$$0 = \Gamma\,W_{ij}^{\mathrm{st,1mode}}\,n_i - \Gamma\,W_{ji}^{\mathrm{st,1mode}}\,n_j + \Gamma\,W_{ij}^{\mathrm{sp,1mode}}\,n_i - m_{ij}\,W_{ij}^{p}$$

This equation exists for every possible pair of initial electron level *i* and final electron level *j*. The density of photons m_{ij} with a frequency and polarization corresponding to the *ij* transition is assumed to be in equilibrium.

A photon population corresponds to a pair of levels involved in the transition and includes both *i*-to-*j* and *j*-to-*i* transitions. In order to avoid redundant calculations, this equation is only implemented when the initial level is higher in energy than the final level. The opposite calculation (lower to higher) should not be done because it gives redundant information (because $m_{ij} = m_{ji}$) and requires a different equation. The code simply calculates only down transitions when finding the photon populations, then copies the populations to the up transition slots for use in future calculations. This amounts to finding the lower-half triangle of the photon matrix and then making the matrix symmetric.

Use again $W_{ij}^{\mathrm{st,1mode}} = m_{ij}\,V\,W_{ij}^{\mathrm{sp,1mode}}$ and $W_{ji}^{\mathrm{st,1mode}} = W_{ij}^{\mathrm{st,1mode}}$ where V is the *active region volume*.

$$0 = \Gamma\,m_{ij}\,V\,W_{ij}^{\mathrm{sp,1mode}}(n_i - n_j) + \Gamma\,W_{ij}^{\mathrm{sp,1mode}}\,n_i - m_{ij}\,W_{ij}^{p}$$

Solve for the photon populations:

$$m_{ij} = \frac{n_i}{W_{ij}^{p} / (\Gamma W_{ij}^{\mathrm{sp,1mode}}) - V(n_i - n_j)}$$

3.1 Forcing Convergence

The photon and electron population equations now form another layer of coupled equations. We can iterate back and forth between then until we reach a solution that converges. Simply applying the above equations does not lead to a converging solution as the parameter space shape is not conducive to convergence. The solution, however, can be forced to converge by taking the previous photon population values and moving them slowly towards the photon population calculated by the above equation, instead of setting them outright equal to the photon population calculated by the above equation. What happens in practice is that through the course of the numerical iterative process, the electron population inversion temporarily goes higher than it ever would in the real laser. If the equation above is applied blindly, the photon density will go negative for high population inversions and unphysical trends will result. In reality, the population inversion asymptotically approaches a “pinned” value. To handle this numerically, the above equation is applied and if the photon population goes negative, the previous photon population was too low, so it is increased in the next iteration. In real QCL's, the stimulated emission of photons depletes the upper level enough that it never goes passed the pinned value.

3.2 Initial Populations

In order to implement iteration equations we must have some initial values for the electron population densities and photon population densities. The closer that the initial values are to the final values, the more quickly the solutions will converge. For the initial electron densities, we set them all equal so that total electron density is evenly divided among the levels. For the photon populations, we can pick some arbitrary number that has the right order of magnitude as experimental values, such as 10^{18} photons/m^3.