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## Quantum Cascade Laser Theory Space Charge Density

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### 1.0 Introduction

The Poisson equation depends on the space charge present. The space charge, including ionized donor atoms in the valence band as well as electrons in the conduction band, gives rise to the built-in electrostatic potential described in the Poisson equation. The built-in potential is an effect which is additional to the conduction band-edge quantum-well profile created by stacking alternating layers of semiconductor material. The sum of both of these potentials is the potential that an electron experiences when it is spreading into a wavefunction via the Schrödinger equation. We must find the space charge density before we can solve the Poisson equation and the Schrödinger equation. But the space charge density ultimately depends on the Schrödinger equation because it dictates the wavefunctions' shapes, which for a large ensemble of electrons becomes the electron density. These equations must therefore be solved self-consistently; each equation is applied iteratively until the solution converges to the physical solution. But we must start with some initial guess for the space charge density before we can iterate to the correct solution. The best guess is to place the free electrons in the wells before the injection barrier.

Because the device material is uniform in the  $x$  and  $y$  dimensions, the space charge is also trivially uniform in these dimensions. The space charge density is therefore only dependent on the  $z$  dimension. The space charge density can be represented by the three-dimensional charge density  $\rho(z)$ , by the two-dimensional charge density  $\rho_{2D}(z)$ , or by the three- and two-dimensional number densities  $n(z)$  and  $n_{2D}(z)$ . It does not matter what form we use, and indeed it is often useful to use many of these forms at once, as long as we are aware of what we are doing. The Poisson equation depends on the three-dimensional charge density  $\rho(z)$ , so that is what we need to find in the end. The different forms are related in the following way:

$$\rho(z) = q n(z) \quad \text{and} \quad \rho_{2D}(z) = q n_{2D}(z) \quad \text{where } q \text{ is the charge on one charge carrier, } -e \text{ for electrons and } +e \text{ for ionized donor atoms,}$$

$$\rho_{2D}(z) = \rho(z)L \quad \text{and} \quad n_{2D}(z) = n(z)L \quad \text{where } L \text{ is the length of one period of the QCL core structure.}$$

### **1.1 Hole Densities**

We note that, by construction, QCL's are structures where the dynamics is completely concerned with electrons moving between states in the conduction band. In order to get a substantial number of electrons into the conduction band to sustain a current, some of the layers are doped with donor atoms. QCL's are rarely doped with acceptor atoms. As a result, the number of holes in the valence band is negligible and is assumed to make no contribution to space charge effects. While there may be some electrons in the conduction band because they left a

hole behind, the great majority of conduction electrons come from the donor atoms and leave behind fixed positively-charged donor ions. In the rare instances when holes are created in the valence band by regular thermal action, the abundance of excess electrons in the conduction band means that these holes are very quickly filled and destroyed. In the end, the dynamics of holes can be completely ignored in QCL's.

## **2.0 Total Space Charge Density**

The total charge density  $\rho(z)$ , as needed in the Poisson equation, is the sum of the positively charged ionized donor atoms  $\rho_{\text{donor}}(z)$ , and the negatively-charged electrons  $\rho_{\text{elec}}(z)$  that have left the donor atoms and been freed into the conduction band:

$$\rho(z) = \rho_{\text{donor}}(z) + \rho_{\text{elec}}(z)$$

$$\rho(z) = e n_{\text{donor}}(z) - e n_{\text{elec}}(z)$$

Only the semiconductor layers that are doped experience significant ionization levels. The doped atoms have an extra electron that is very loosely bound and very easily excited into the conduction band. An electron in the conduction band becomes delocalized and is pseudo-free within the effective-mass approximation because it is bound to the crystal as a whole rather than any local atom. The electron leaves behind a positively-charged atom that is fixed in the crystal lattice. The electron then becomes trapped in the wavefunction states of the quantum well structure, but moves from state to state when scattered. In this model, the donor density need only be found once at the beginning of the code because the donors are fixed, but the electron density must be self-consistently determined as part of the iterative process.

Note that the total charge in the QCL is zero because it is part of a grounded electric circuit. Integrating the charge density over the entire device must yield zero:

$$\int \rho(z) dz = 0$$

which leads to

$$\int n_{\text{elec}}(z) dz = \int n_{\text{donor}}(z) dz$$

Because the donor density is fixed and found at the beginning, this equation can be used repeatedly to normalize the electron density curve to its proper overall magnitude.

## **3.0 Space Charge Electron Density**

The space charge electron density is defined as the number of conduction electrons per unit volume at a point  $z$  in space. We assume all conduction electrons are trapped in the wavefunctions of the quantum well structure. We also assume that there are enough electrons in each wavefunction state (remembering the electrons have different wavevectors in the  $x$  and  $y$  dimensions, so that the Pauli exclusion principle is

not a problem), that the wave's probability density becomes the average charge density of that state. The electron space charge density is then just the sum over all wavefunctions:

$$n_{elec}(z) = \sum_i^{1 \text{ period}} n_{2D,elec}^i |\psi_i(z)|^2$$

Here,  $n_{2D,elec}^i$  is the overall electron number sheet density in the  $i^{\text{th}}$  quantum level and  $\psi_i$  is the wavefunction of that level. We must use the two-dimensional density because the wavefunction squared is the density in the third dimension. In practice, we find the charge density in the central period where the wavefunctions are the best and then copy this charge density profile to the outer periods to ensure periodicity. The electron densities in each level are referred to as populations and are found by solving the rate equations. The rate equations depend on the scattering rate calculations, which depend on the wavefunctions as well, so there are several iterative loops that must be carried out to ensure self-consistency.

### 3.1 Initial Space Charge Electron Density

The populations are found using the rate equations, but when the code begins, the rate equations have not been run yet. We must set some initial space charge density so that the code has somewhere to start before it converges to the true solution. In theory, the choice of initial electron density should be irrelevant to the final solution. In practice, using an initial electron density that is close to the final solution will dramatically reduce run-time and will lessen the effects of compounding numerical error. The model we use for the initial space charge electron density is one that assumes the electrons tend to bunch up behind the largest barrier, but extend backwards somewhat from this barrier because of thermal smearing. Our code therefore carries out the following algorithm:

- 1) Find the space charge donor density  $n_{donor}(z)$ .
- 2) Find the location of the thickest barrier in the QCL core structure.
- 3) Set up the initial space charge electron density profile as a decaying exponential curve  $n_{elec}(z) = f(z)$  with a peak at the barrier, extending uphill away from the barrier (in the opposite direction from the cascading electron motion).
- 4) Scale the electron density profile until the area under its curve matches the area under the donor density profile curve to ensure the overall total charge of the QCL is zero, according to  $\int n_{elec}(z) dz = \int n_{donor}(z) dz$ .
- 5) Find the total charge density as the sum of the donor and electron densities, according to  $\rho(z) = e n_{donor}(z) - e n_{elec}(z)$ .
- 6) Using this initial charge density, find the built-in potential using the Poisson equation, add the built-in potential to the conduction band-edge potential to get the total potential, insert this into Schrödinger's equations and find the wavefunctions.

7) Refine the initial charge density profile by using the wavefunctions multiplied by the exponential model,

$$n_{elec}(z) = f(z) \sum_i^{1 \text{ period}} |\psi_i(z)|^2, \text{ and again scale to proper magnitude.}$$

8) This refined initial charge density is then the starting point when we enter the main iterative loop of the code. From here on out, the populations are found using the rate equations and applied as described in Section 3.0.

### 3.2 Items of Caution Regarding Electron Densities

There are several opportunities for error when using electron densities because of the many ways this concept can be used and because of the three-period structure used for calculations in the code. There are two types of electron densities. There is the electron density of a single subband quantum state  $n_i$ . The electrons in this state spread out spatially through the quantum-well structure according to the wavefunction shapes found in Shroedinger's equation. These electron densities are referred to as “level populations” to avoid confusion. The level populations do not depend on the  $z$  dimension, but do depend on the level index. The level populations therefore represent the total number of electrons in level  $i$  divided by the volume occupied by the wavefunction. The characteristic length of a wavefunction is one period, so the length of one period, times the full width and depth of the device gives the volume used to define the density. The other type of electron density is the space charge electron density  $n(z)$ . This density measures the number of electrons in *all* quantum states, but only in a small volume  $Adz$  so that the density depends on spatial location, but not on level.

When approaching electron density definitions and programmatic implementations, error is best avoided by observing the following points:

- 1) An electron density is fundamentally the total number of electrons in a certain volume. We must define the volume carefully.
- 2) The characteristic length of a wavefunction is the length of one period of the core QCL structure. Electrons spread out in a quantum state can be considered to occupy the length of one period.
- 3) We must be careful to keep track of whether a certain variable represents the total number of electrons, the number density, the two-dimensional number density, or the charge density.

The total number of free electrons  $N_{tot}$  in the entire active region is the number of electrons in one period times the number of periods  $M$  in the whole QCL structure.

$$N_{tot} = M \sum_i^{1 \text{ period}} N_i$$

$$N_{tot} = M V_{1 \text{ period}} \sum_i^{1 \text{ period}} n_i$$

$$N_{tot} = V_{tot} \sum_i^{1 \text{ period}} n_i$$

Here,  $i$  iterates over all levels in one period,  $n_i$  is the three-dimensional density of electrons in level  $i$  as determined by the rate equations, and  $V_{tot}$  is the total volume of the active region.

The average density of electrons  $n_{tot}$  across the entire crystal is the total number of electrons divided by the volume of the active region  $V$ :

$$n_{tot} = \frac{N_{tot}}{V_{tot}}$$

$$n_{tot} = \sum_i^{1 \text{ period}} n_i$$

This is the total density across the whole crystal. Note that the sum is over only one period, not all periods. The total density can be thought of as the average of the space charge density.

Let us now approach it from the other type of electron density. Instead of summing over levels, we integrate over  $z$ :

$$N_{tot} = M \int_0^L n(z) A dz \quad \text{where } L \text{ is the length of one period.}$$

$$N_{tot} = M V_{1 \text{ period}} \frac{1}{L} \int_0^L n(z) dz$$

$$N_{tot} = V_{tot} \frac{1}{L} \int_0^L n(z) dz$$

$$n_{tot} = \frac{1}{L} \int_0^L n(z) dz$$

Set these two equal:

$$\sum_i^{1 \text{ period}} n_i = \frac{1}{L} \int_0^L n(z) dz$$

Consider the level population  $n_i$  to be the average space charge density in a single level. Because the wavefunction is properly normalized, the integral over the wavefunction squared is 1 so that we can expand according to:  $n_i = n_i \int_0^L |\psi(z)|^2 dz$

$$\sum_i^{1 \text{ period}} n_i \int_0^L |\psi(z)|^2 dz = \frac{1}{L} \int_0^L n(z) dz$$

We now set the integrands equal. We cannot do this on purely mathematical grounds. However, physically, we know that the probability density for a large number of electrons becomes the electron density, making this step valid.

$$n(z) = L \sum_i^{1 \text{ period}} n_i |\psi(z)|^2$$

$$n(z) = \sum_i^{1 \text{ period}} n_{i,2D} |\psi(z)|^2$$

We have therefore re-derived the main equation. This is the equation we use in the code's main iteration loop to take the level populations, as found from the rate equations, and turn them into the space charge density needed by the Poisson equation.

In order to start the rate equations, we must have some initial set of level populations. We assume the total number of electrons are initially evenly divided amongst all levels in one period.

$$n_{tot} = \sum_i^{1 \text{ period}} n_i$$

$$n_{tot} = M_{1 \text{ period}} n_i^{\text{initial}}$$

$$n_i^{\text{initial}} = \frac{n_{\text{tot}}}{M_{\text{1 period}}}$$

$$n_i^{\text{initial}} = \frac{1}{M_{\text{1 period}}} \frac{1}{L} \int_0^L n(z) dz$$

$$n_i^{\text{initial}} = \frac{1}{M_{\text{1 period}}} \frac{1}{L} \int_0^L n_{\text{donor}}(z) dz$$

In the process of iterating the rate equations, the populations become unnormalized and do not add up to the total electron density. We must force them to be normalized.

Consider the normalized populations to be equal to some overall normalization constant  $S$  times the unnormalized populations:

$$n_i = S n_i^{\text{unnorm}}$$

Plug this in the usual sum

$$n_{\text{tot}} = \sum_i^{\text{1 period}} S n_i^{\text{unnorm}}$$

Solve for  $S$

$$S = \frac{n_{\text{tot}}}{\sum_i^{\text{1 period}} n_i^{\text{unnorm}}}$$

Plug back in to see how the normalization is applied:

$$n_i = \left[ \frac{n_{\text{tot}}}{\sum_i^{\text{1 period}} n_i^{\text{unnorm}}} \right] n_i^{\text{unnorm}}$$

#### **4.0 Space Charge Ion Density**

The positive ions left behind when the electron leaves a donor atom for the conduction band are fixed in space and do not move. As a result, we only need to calculate the ionized donor space charge density  $\rho_{\text{donor}}(z)$  once at the beginning of the code and then store it for future use. We assume that the material layers are thick enough that they essentially act as infinite bulk pieces of material when it comes to donor ionization. We therefore calculate the  $z$ -dependent donor density by simply going through one  $z$  grid point at a time in the code's data structure, looking up the material and doping at that grid point as specified by the user, and calculating the ionization using a bulk model.

The ionization process actually involves a complex interaction of holes being created and destroyed, and donors being ionized and de-ionized according to the lattice temperature. We must therefore first find the bulk density of states and bulk Fermi energy level in order to determine the equilibrium point. All of the following derivations assume we are dealing with an infinite bulk uniform material, so there is no concept of subband levels or QCL periods. In the end, the bulk model ionization is applied point by point to the QCL structure.

Define the Fermi energy level  $E_F$  as bulk-material (non-junctioned) Fermi levels which include doping effects.

Using the free-electron/quasi-particle model for three-dimensional bulk material, the density of allowed states in  $k$ -space is given by:

$$g(\mathbf{k}) = 2 \left( \frac{2\pi}{L} \right)^{-3} = 2 \frac{V}{(2\pi)^3}$$

The number of states with wave number less than  $k$ , using the quasi-free particle relation  $k = \sqrt{2m^*E/\hbar^2}$  is the density times the volume in  $k$ -space.:

$$N(k) = V_k g(\mathbf{k})$$

$$N(k) = \left( \frac{4}{3} \pi k^3 \right) \left( 2 \frac{V}{(2\pi)^3} \right)$$

$$N(E) = \left( \frac{2m^*E}{\hbar^2} \right)^{3/2} \left( \frac{V}{3\pi^2} \right)$$

The density of states as a function of energy is the derivative of the number of states with respect to energy:

$$g(E) = \frac{dN(E)}{dE} = \left( \frac{2m^*}{\hbar^2} \right)^{3/2} \sqrt{E} \left( \frac{V}{2\pi^2} \right)$$



When applying this to the negatively-charged electrons in the conduction band the energy is defined as  $E \rightarrow E - E_c(z)$ , whereas for positively-charged holes in the valence band the energy becomes  $E \rightarrow E_v(z) - E$ :

$$g_n(E) = \left( \frac{2m_n^*}{\hbar^2} \right)^{3/2} \sqrt{E - E_c} \left( \frac{V}{2\pi^2} \right)$$

$$g_p(E) = \left( \frac{2m_p^*}{\hbar^2} \right)^{3/2} \sqrt{E_v - E} \left( \frac{V}{2\pi^2} \right)$$

The density of conduction-band states occupied by electrons using Fermi-Dirac statistics becomes the expression:

$$g_{n,occ}(E) = g_n(E) f_D(E) \quad \text{where} \quad f_D(E) = \frac{1}{1 + e^{(E - E_F)/k_B T}}$$

$$g_{n,occ}(E) = \left( \frac{2m_n^*}{\hbar^2} \right)^{3/2} \left( \frac{V}{2\pi^2} \right) \sqrt{E - E_c} \frac{1}{1 + e^{(E - E_F)/k_B T}}$$

The density of valence-band states occupied by holes using Fermi-Dirac statistics becomes the expression:

$$g_{p,occ}(E) = g_p(E) (1 - f_D(E))$$

$$g_{p,occ}(E) = \left( \frac{2m_p^*}{\hbar^2} \right)^{3/2} \left( \frac{V}{2\pi^2} \right) \sqrt{E_v - E} \frac{1}{1 + e^{(E_F - E)/k_B T}}$$

Using the approximation  $\frac{1}{1 + e^{(E - E_F)/k_B T}} \approx e^{(E_F - E)/k_B T}$ , we can now calculate the electron number density in the conduction band:

$$n = \frac{N}{V}$$

$$n = \frac{1}{V} \int_{E_c}^{\infty} g_{n,occ}(E) dE$$

$$n = \frac{1}{V} \int_{E_c}^{\infty} \left( \frac{2m_n^*}{\hbar^2} \right)^{3/2} \left( \frac{V}{2\pi^2} \right) \sqrt{E - E_c} \frac{1}{1 + e^{(E - E_F)/k_B T}} dE$$

$$n = \left( \frac{2m_n^*}{\hbar^2} \right)^{3/2} \left( \frac{1}{2\pi^2} \right) \int_{E_c}^{\infty} \sqrt{E - E_c} e^{(E_F - E)/k_B T} dE$$

$$n = \left( \frac{2m_n^*}{\hbar^2} \right)^{3/2} \left( \frac{1}{2\pi^2} \right) e^{(E_F - E_c)/k_B T} (k_B T)^{3/2} \int_0^{\infty} \sqrt{x} e^{-x} dx$$

$$n = 2 \left( \frac{m_n^*(z) k_B T}{2\pi \hbar^2} \right)^{3/2} e^{(E_F - E_c)/k_B T}$$

Using the same approximation again, the density of holes in the valence band can now be calculated:

$$p = \frac{P}{V}$$

$$p = \frac{1}{V} \int_{-\infty}^{E_v} g_{p, occ}(E) dE$$

$$p = \frac{1}{V} \int_{-\infty}^{E_v} \left( \frac{2m_p^*}{\hbar^2} \right)^{3/2} \left( \frac{V}{2\pi^2} \right) \sqrt{E_v - E} \frac{1}{1 + e^{(E_F - E)/k_B T}} dE$$

$$p = \left( \frac{2m_p^*}{\hbar^2} \right)^{3/2} \left( \frac{1}{2\pi^2} \right) \int_{-\infty}^{E_v} \sqrt{E_v - E} e^{(E - E_F)/k_B T} dE$$

$$p = \left( \frac{2m_p^* k_B T}{\hbar^2} \right)^{3/2} \left( \frac{1}{2\pi^2} \right) e^{(E_v - E_F)/k_B T} \int_0^{\infty} \sqrt{x} e^{-x} dx$$

$$p = 2 \left( \frac{m_p^* k_B T}{2 \pi \hbar^2} \right)^{3/2} e^{(E_v - E_{F0})/k_B T}$$

The density of positive donor ions at the donor level  $E_D$ , using the same approximation, is now found:

$$N_D^+ = N_D (1 - f_D(E_D))$$

$$N_D^+ = \frac{N_D}{1 + g_D e^{(E_{F0} - E_D)/k_B T}}$$

$$N_D^+ = N_D(z) (1 - g_D e^{(E_{F0} - E_D)/k_B T})$$

Using the charge neutrality of the crystal, we can solve for the Fermi energy:

$$n = p + N_D^+$$

$$2 \left( \frac{m_n^* k_B T}{2 \pi \hbar^2} \right)^{3/2} e^{(E_F - E_c)/k_B T} = 2 \left( \frac{m_p^* k_B T}{2 \pi \hbar^2} \right)^{3/2} e^{(E_v - E_F)/k_B T} + N_D(z) (1 - g_D e^{(E_F - E_D)/k_B T})$$

$$e^{2E_F/k_B T} \left[ (m_n^*)^{3/2} e^{-E_c/k_B T} + \frac{1}{2} \left( \frac{2 \pi \hbar^2}{k_B T} \right)^{3/2} N_D g_D e^{-E_D/k_B T} \right] - e^{E_F/k_B T} \frac{1}{2} \left( \frac{2 \pi \hbar^2}{k_B T} \right)^{3/2} N_D - (m_p^*)^{3/2} e^{E_v/k_B T} = 0$$

This equation has the form:

$$A x^2 + B x + C = 0$$

$$\text{where } x = e^{E_F/k_B T}, \quad A = \left[ (m_n^*)^{3/2} e^{-E_c/k_B T} + \frac{1}{2} \left( \frac{2 \pi \hbar^2}{k_B T} \right)^{3/2} N_D g_D e^{-E_D/k_B T} \right], \quad B = -\frac{1}{2} \left( \frac{2 \pi \hbar^2}{k_B T} \right)^{3/2} N_D, \quad \text{and} \quad C = -(m_p^*)^{3/2} e^{E_v/k_B T}$$

Applying the quadratic equation, we arrive at the final solution:

$$E_F = k_B T \ln \left[ \frac{G + \sqrt{G^2 + 4 \left[ (m_n^*)^{3/2} e^{-E_c/k_B T} + G g_D e^{-E_D/k_B T} \right] (m_p^*)^{3/2} e^{E_v/k_B T}}}{2 \left[ (m_n^*)^{3/2} e^{-E_c/k_B T} + G g_D e^{-E_D/k_B T} \right]} \right] \quad \text{where} \quad G = \frac{1}{2} \left( \frac{2\pi\hbar^2}{k_B T} \right)^{3/2} N_D$$

Because this is the bulk model, the conduction band edge energy  $E_c$  is just the valence band energy plus the temperature-dependent band gap, as calculated early in the code, and does not include the bias potential or the built-in potential. The donor doping density at each grid point  $N_D$  as well as the lattice temperature  $T$  is provided directly by the user as a design parameter at runtime. The electron effective mass  $m_n^*$ , the hole effective mass  $m_p^*$ , the donor valence band edge  $E_D$ , and the donor valley degeneracy  $g_D$  are all material parameters that can be found in the literature. Because the material and doping varies from layer to layer in the QCL core structure, all of these parameters will vary from grid point to grid point. At each  $z$  grid point, the material and doping must be received from the user, and then all these material-dependent parameters must be loaded from a material parameters file. The Fermi energy is therefore calculated at each grid point.

Once these Fermi levels are known, the ionized donor space charge density is calculated at each grid point:

$$\rho_{\text{donor}}(z) = \frac{e N_D}{1 + g_D e^{(E_F - E_D)/k_B T}}$$