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Quantum Cascade Laser Theory Individual Fermi Levels

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1.0 Introduction

Every quantized level in a QCL has a different electron population and temperature. We assume that each subband thermalizes much quicker than electrons transition out of the subband, so that all subbands are always thermalized. This means that all the electrons in a subband are in a Fermi distribution, which depends on the subband's Fermi level (which depends on the populations) and electron temperature. The populations are determined by the rate equations. The temperatures will be determined in the future by the energy balance equations, but are currently set to the lattice temperature in the code. The individual Fermi levels are found from the populations and temperatures, and the Fermi levels are used in the scattering calculations. Because the rate equations depend on scattering calculations, all these properties are circularly dependent and must be found iteratively.

When dealing with individual levels, we can no longer safely make the approximation that the material acts as bulk. Instead we must assume we know the level populations and from there find the corresponding Fermi levels.

2.0 Derivation

Using the two-dimensional quasi-free electron model, the density of allowed states in k -space is:

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

The number of states with wave number less than k , using the quasi-free particle relation $k = \sqrt{2m^*(z)E/\hbar^2}$ is the area in k -space of the circle containing the points where the wave number is less than k :

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

$$N(k) = (\pi k^2) \left(2 \frac{A}{(2\pi)^2} \right)$$

$$N(E) = \frac{A \pi 4 m^* E}{(2\pi)^2 \hbar^2}$$

The density of states as a function of energy $g(E)$ is the change in the number of states with respect to energy:

$$g(E) = \frac{dN(E)}{dE} = \frac{A m^*}{\pi \hbar^2}$$

The density of subband states *occupied* by electrons $g_{n,occ}(E)$ is found by multiplying the density of states by a Fermi distribution:

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

$$g_{n,occ}(E) = \frac{A m^*}{\pi \hbar^2} \frac{1}{1 + e^{(E - E_{F,i})/k_B T}}$$

The spatial sheet density of electrons n^{2D} in the subband is defined as the total number of electrons N in the subband divided by the spatial area of interest A :

$$n^{2D} = \frac{N}{A}$$

The total number of electrons N in the subband is the integral over all occupied states:

$$n^{2D} = \frac{1}{A} \int_{E_i}^{\infty} g_{n,occ}(E) dE$$

$$n^{2D} = \frac{1}{A} \int_{E_i}^{\infty} \frac{A m^*}{\pi \hbar^2} \frac{1}{1 + e^{(E - E_{F,i})/k_B T}} dE$$

$$n^{2D} = \frac{m^*}{\pi \hbar^2} \int_{E_i}^{\infty} \frac{1}{1 + e^{(E - E_{F,i})/k_B T}} dE$$

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Substitute $u = (E - E_{F,i})/k_B T$, $du = dE/k_B T$

$$n^{2D} = \frac{m^* k_B T}{\pi \hbar^2} \int_{(E_i - E_{F,i})/k_B T}^{\infty} \frac{1}{1 + e^u} du$$

$$n^{2D} = \frac{m^* k_B T}{\pi \hbar^2} [u - \ln(1 + e^u)]_{(E_i - E_{F,i})/k_B T}^{\infty}$$

$$n^{2D} = \frac{m^*}{\pi \hbar^2} [E_{F,i} - E_i + k_B T \ln(1 + e^{((E_i - E_{F,i})/k_B T)})]$$

Now invert this to solve for the Fermi energy:

$$E_{F,i} = E_i + k_B T \ln[\exp(\pi \hbar^2 n^{2D} / k_B T m^*) - 1]$$

The sheet density is related to the regular density by $n^{2D} = L n$ where L is the length of one period of the QCL (which represents the average width of the wavefunctions). When the level's population and electron temperature T are known, this equation is applied directly to calculate the individual Fermi energy. Note that the subband energy minimum E_i and the Fermi energy $E_{F,i}$ are measured on the same absolute energy scale. For high temperatures and low populations, the Fermi level necessarily becomes smaller than the subband minimum. The code should be careful to never assume otherwise. These individual Fermi levels are then used in calculating scattering rates.

2.1 Initial populations

The first time the individual Fermi levels are calculated, the populations have not yet been determined. As an initial set of values from which the code can iteratively converge, we set all of the populations equal and normalize them so that the total of all the populations equals the overall crystal electron density. We are therefore assuming that the electrons are uniformly distributed across all of the states as an initial setting.