Quantum Cascade Laser Theory
Schrödinger Equation
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1.0 Introduction

Quantum cascade lasers (QCL's) are fabricated by stacking up alternating layers of semiconducting material with nanoscale thicknesses. This heterostructure of layers forms a series of conduction-band quantum wells in the z direction which trap the electrons into subband states. The eigenstate of an electron in the unperturbed Hamiltonian of a QCL is the product of the Bloch envelope function $B(x, y, z)$, the free electron wavefunction in the x and y direction, and the bound quantum-well eigenfunctions $\psi_n(z)$ in the z direction.

$$<\mathbf{r}|\psi> = <x|\psi_x><y|\psi_y><z|\psi_z> = B(x,y,z)\frac{1}{\sqrt{L_x}}e^{ik_x x}\frac{1}{\sqrt{L_y}}e^{ik_y y}\psi_n(z)$$

The Bloch function factor contains the effects on the electron state due to the non-uniform nature of the crystal potential on the atomic scale. We assume the semiconductor layer widths are large compared to the atoms, so we make the approximation that the Bloch function factor is negligible. Each electron is pseudo-free in the x and y dimensions because the material is uniform in those dimensions. Even though each electron is bound to the crystal in these dimensions, we can treat each as free if we use the effective mass of the electron. The bound-state z-component wave functions $\psi_n(z)$ are found by numerically solving the one-dimensional Schrödinger equation when the potential profile is known. As developed elsewhere, the potential profile is a combination of the conduction-band edge quantum well profile of the material layers, the bias voltage, and the built-in potential which accounts for the effects of space charge. The built-in potential is found by solving the Poisson equation.

2.0 Derivation

The one-dimensional time-independent Schrödinger equation for a single electron in the potential $V(z)$ is the Hamiltonian eigenvalue equation, where E is the total energy of the electron in the eigenstate:

$$H\psi = E\psi$$

The Hamiltonian operator H is just the total energy operator, so we can expand it into a sum of the kinetic energy operator T and the potential energy operator V,

$$(T+V)\psi = E\psi$$

$$T\psi = (E-V)\psi$$

Expand the kinetic energy T, being careful to preserve the operator nature of the expression and recognizing that the effective mass m^* is a function of position z because the material changes along this dimension:

$$\left(\frac{1}{2}m^*(z)\dot{Z}\dot{Z}\right)\psi(z) = (E-V(z))\psi(z)$$

Expand the velocity operators in terms of momentum operators, again being careful with the effective mass:

$$\left(\frac{1}{2}m^*(z)\left(\frac{1}{m^*(z)}P\right)\left(\frac{1}{m^*(z)}P\right)\right)\psi(z) = (E-V(z))\psi(z)$$

$$\left[\frac{1}{2}\left(-i\hbar\frac{d}{dz}\right)\left(\frac{1}{m^*(z)}\left(-i\hbar\frac{d}{dz}\right)\right)\right]\psi(z) = (E-V(z))\psi(z)$$

$$\boxed{\frac{d}{dz}\left[\frac{1}{m^*(z)}\frac{d\,\psi(z)}{dz}\right] = -\frac{2}{\hbar^2}(E-V(z))\psi(z)}$$

The is the fundamental physical equation to be solved. Note that if we make the approximation that the effective mass $m^*(z)$ is constant, this expression reduces down to the simple textbook form. However, we may not be justified in making such an approximation as the effective mass is clearly not constant. In addition, incorporating the z-dependent effective mass is trivial in its implementation.

3.0 Numerical Method
The potential $V(z)$ is too complicated to allow the Schrödinger equation to be solved analytically. We must turn to numerical methods and implement them computationally. We choose the fourth-order Runge-Kutta (RK4)numerical method.

We must first break the single second-order differential equation into two first-order differential equations before we can apply the RK4 method.

$$\frac{d\,\psi(z)}{dz} = m^*(z)\psi_2(z)$$

$$\frac{d\psi_2(z)}{dz} = -\frac{2}{\hbar^2}(E - V(z))\psi(z)$$

In order to apply the RK4 method in a straightforward manner, we define the right side of the equations as the function f and g.

$$\frac{d\psi(z)}{dz} = f(z, \psi_2(z)) \quad \text{where} \quad f(z, \psi_2(z)) = m*(z)\psi_2(z)$$

$$\frac{d\psi_2(z)}{dz} = g(z, \psi(z)) \quad \text{where} \quad g(z, \psi(z)) = -\frac{2}{\hbar^2}(E - V(z))\psi(z)$$

The RK4 method specifies that the derivatives are expanded into finite differences and the slopes that they equal are set to the weighted averages. At this point we have transferred the functions from the continuous dimension z to the discrete dimension z_n which is needed for numerical computation.

$$\frac{(\psi(z_{n+1}) - \psi(z_n))}{(z_{n+1} - z_n)} = f_{ave}(z, \psi_2(z)) \quad \text{where} \quad f_{ave} = \frac{1}{6}(f_1 + 2f_2 + 2f_3 + f_4)$$

$$\frac{(\psi_2(z_{n+1}) - \psi_2(z_n))}{(z_{n+1} - z_n)} = g_{ave}(z, \psi(z)) \quad \text{where} \quad g_{ave} = \frac{1}{6}(g_1 + 2g_2 + 2g_3 + g_4)$$

Note that for reasons of accuracy, we do not assume that the points z_n are evenly spaced, so that we are *not* assuming $z_n = nh$ where h is some constant step size. Although this assumption would simplify the equations considerably, the varying thickness of the semiconductor layers does not allow it. Instead, we have chosen to set points z_n at every boundary between semiconductor layers, and then disperse them evenly within the layers. The non-uniform grid of computational points z_n must therefore be set up in advance, but remains known and constant for the remainder of the calculations.

The finite difference expansions can be solved for the wavefunctions at the advanced points to yield iteration equations:

$$\boxed{\psi(z_{n+1}) = \psi(z_n) + (z_{n+1} - z_n)f_{ave}(z, \psi_2(z))}$$

$$\boxed{\psi_2(z_{n+1}) = \psi_2(z_n) + (z_{n+1} - z_n)g_{ave}(z, \psi(z))}$$

After calculating f_{ave} and g_{ave}, these equations can be used iteratively to calculate the entire wavefunctions if the initial values $\psi(z_0)$ and $\psi_2(z_0)$ are given.

The RK4 method defines the weighted average slopes to be:

$$f_{ave}=\frac{1}{6}(f_1+2f_2+2f_3+f_4) \quad \text{and} \quad g_{ave}=\frac{1}{6}(g_1+2g_2+2g_3+g_4)$$

where

$$f_1=f(z_n,\psi_2(z_n)) \quad \text{and} \quad g_1=g(z_n,\psi(z_n))$$

$$f_2=f(\frac{1}{2}(z_{n+1}+z_n),\psi_2(z_n)+\frac{1}{2}(z_{n+1}-z_n)g_1) \quad \text{and} \quad g_2=g(\frac{1}{2}(z_{n+1}+z_n),\psi(z_n)+\frac{1}{2}(z_{n+1}-z_n)f_1)$$

$$f_3=f(\frac{1}{2}(z_{n+1}+z_n),\psi_2(z_n)+\frac{1}{2}(z_{n+1}-z_n)g_2) \quad \text{and} \quad g_3=g(\frac{1}{2}(z_{n+1}+z_n),\psi(z_n)+\frac{1}{2}(z_{n+1}-z_n)f_2)$$

$$f_4=f(z_{n+1},\psi_2(z_n)+(z_{n+1}-z_n)g_3) \quad \text{and} \quad g_4=g(z_{n+1},\psi(z_n)+(z_{n+1}-z_n)f_3)$$

We apply these definitions to our problem by explicitly inserting the expressions for f and g and evaluating:

$$f_1=m*(z_n)\psi_2(z_n) \quad \text{and} \quad g_1=-\frac{2}{\hbar^2}(E-V(z_n))\psi(z_n)$$

$$f_2=m*(\frac{1}{2}(z_{n+1}+z_n))[\psi_2(z_n)+\frac{1}{2}(z_{n+1}-z_n)g_1] \quad \text{and} \quad g_2=-\frac{2}{\hbar^2}(E-V(\frac{1}{2}(z_{n+1}+z_n)))[\psi(z_n)+\frac{1}{2}(z_{n+1}-z_n)f_1]$$

$$f_3=m*(\frac{1}{2}(z_{n+1}+z_n))[\psi_2(z_n)+\frac{1}{2}(z_{n+1}-z_n)g_2] \quad \text{and} \quad g_3=-\frac{2}{\hbar^2}(E-V(\frac{1}{2}(z_{n+1}+z_n)))[\psi(z_n)+\frac{1}{2}(z_{n+1}-z_n)f_2]$$

$$f_4=m*(z_{n+1})[\psi_2(z_n)+(z_{n+1}-z_n)g_3] \quad \text{and} \quad g_4=-\frac{2}{\hbar^2}(E-V(z_{n+1}))[\psi(z_n)+(z_{n+1}-z_n)f_3]$$

We do not know the effective masses or the potential energies at the midpoints as required by these equations. We therefore approximate them as the average of the two nearest neighbors. After making this approximation, the final computational algorithm is obtained.

4.0 Final Numerical Algorithm

1. Starting at the point z_0, apply the following equations iteratively, one point at a time, until the entire function is known.

2. Calculate the current location's step size: $\boxed{h_n = z_{n+1} - z_n}$ as well as the constant $\boxed{a = -\dfrac{2}{\hbar^2}}$

3. Calculate the midpoint values of the potential and effective mass: $\boxed{V_{mid} = \dfrac{1}{2}(V(z_{n+1}) + V(z_n))}$, $\boxed{m*_{mid} = \dfrac{1}{2}(m*(z_{n+1}) + m*(z_n))}$

4. Calculate the RK4 slopes. Note that these must be done in this order as they are interdependent:

$\boxed{f_1 = m*(z_n)\psi_2(z_n)}$ and $\boxed{g_1 = a(E - V(z_n))\psi(z_n)}$

$\boxed{f_2 = m*_{mid}\left[\psi_2(z_n) + \dfrac{h_n}{2}g_1\right]}$ and $\boxed{g_2 = a(E - V_{mid})\left[\psi(z_n) + \dfrac{h_n}{2}f_1\right]}$

$\boxed{f_3 = m*_{mid}\left[\psi_2(z_n) + \dfrac{h_n}{2}g_2\right]}$ and $\boxed{g_3 = a(E - V_{mid})\left[\psi(z_n) + \dfrac{h_n}{2}f_2\right]}$

$\boxed{f_4 = m*(z_{n+1})\left[\psi_2(z_n) + h_n g_3\right]}$ and $\boxed{g_4 = a(E - V(z_{n+1}))\left[\psi(z_n) + h_n f_3\right]}$

5. Calculate the wavefunction values at the next point:

$\boxed{\psi(z_{n+1}) = \psi(z_n) + \dfrac{h_n}{6}(f_1 + 2f_2 + 2f_3 + f_4)}$

$\boxed{\psi_2(z_{n+1}) = \psi_2(z_n) + \dfrac{h_n}{6}(g_1 + 2g_2 + 2g_3 + g_4)}$

4.1 Boundary Conditions

This method requires the initial conditions $\psi(z_0)$ and $\psi_2(z_0)$ to be known. However, the boundary conditions that we have are $\psi(z_0) = 0$ and $\psi(z_{last}) = 0$. We are therefore using the boundary conditions $\psi(z_0) = 0$ and $\psi_2(z_0) = 1$, understanding that the entire wavefunction will be off by an overall scale factor. This scale factor error goes away however when we normalize the wavefunction at the end to ensure that there is 100% probability of finding the electron anywhere in its wavefunction. The actual boundary conditions that should be implemented are pseudo-periodic boundary conditions because a typical QCL has 100 repetitions of the same core period structure. However, periodic boundary conditions are difficult to implement directly without requiring substantial computational cost. Instead, we apply the Dirichlet boundary conditions, but solve for the wavefunctions across three periods of the QCL core structure. After finding all valid wavefunctions, we throw away all wavefunctions with a center of mass that lies in the outer periods, and copy all wavefunctions with a center of mass in the central period to the outer periods for future use. This process ensures periodic boundary conditions.
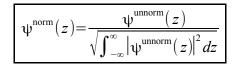
4.2 Eigenvalues

These equations depend on the energy E of the electron in its state, but E is not known beforehand. There are actually several possible solutions to a certain potential; the eigenstate wavefunctions ψ_n of the system; each with its own energy E_n. The correct eigenenergies E_n are the ones that yield valid bound wavefunctions; wavefunctions that do not blow up towards infinity outside the wells. Programatically, we must guess E_n, calculate the corresponding wavefunction using the algorithm listed above, then iteratively refine our guess for E_n by minimizing the error in the wavefunction. Because the wavefunction is supposed to match the boundary condition $\psi(z_{last}) = 0$, the actual amplitude squared at the bounadary $|\psi(z_{last})|^2$ can be taken as the error. By calculating a sweep of possible E_n values and their corresponding wavefunction errors, an error landscape can be generated. The correct energies are the minima in such an energy landscape. The minima are identified, and then refined using a binary search method.

4.3 Normalization

Electron wave functions should always be *normalized* before being used in any subsequent calculations. The wave functions should *not* be magnitude squared unless explicitly required, as the complex phase of the wavefunction is needed is some subsequent calculations. The squared wave functions constitute a probability *density*, thus the proper way to normalize each is by integrating:

Define $\psi^{norm}(z) = A\,\psi^{unnorm}(z)$ and apply the concept that the probability of being found anywhere is 1:

$$1 = \int_{-\infty}^{\infty} \left|\psi^{norm}(z)\right|^2 dz$$

$$1 = \int_{-\infty}^{\infty} A^2 \left|\psi^{unnorm}(z)\right|^2 dz$$

$$A = \frac{1}{\sqrt{\int_{-\infty}^{\infty} \left|\psi^{unnorm}(z)\right|^2 dz}}$$

$$\psi^{\text{norm}}(z) = \frac{\psi^{\text{unnorm}}(z)}{\sqrt{\int_{-\infty}^{\infty} \left| \psi^{\text{unnorm}}(z) \right|^2 dz}}$$

The integral 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 layers 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.