Quantum Cascade Laser Theory
Poisson Equation

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1.0 Introduction

The potential profile that determines the wavefunction in a QCL according to the one-dimensional one-electron Schrödinger equation includes the built-in potential. Physically, layers that are doped in a QCL readily see their electrons ionized into the conduction band and then spread out through the QCL. The electrons that spread out and the positive ions they left behind in the doped layers constitute the space charge ρ that creates the built-in potential. In order to avoid the intractable problem of a many-body Schrödinger equation involving billions upon billions of electrons, we calculate the built-in voltage Φ classically using the Poisson equation.

The charges are uniform in the *x* and *y* dimensions, so the built-in potential is independent of these dimensions. In the *z* dimension, the sequence of quantum wells in a QCL traps the electrons into quantum states with differing transition rates, so that the overall charge density becomes non-uniform and gives rise to the built-in potential. We therefore only need to use the one-dimensional Poisson equation.

2.0 Derivation

Gauss's Law in differential form states that a space charge density ρ gives rise to a diverging electric **D** field:

$$\nabla \cdot \mathbf{D} = \rho$$

We assume linear dielectric materials throughout the QCL so that $\mathbf{D} = \epsilon \mathbf{E}$ in terms of the electrical permittivity. We must be careful to remember that the material changes across the QCL in the *z* direction, and therefore the permittivity changes. The *z*-dependent permittivity cannot be take out of the divergence operator because it contains a derivative with respect to *z*.

$$\nabla \cdot (\epsilon \mathbf{E}) = \rho$$

Define the scalar potential Φ according to $\mathbf{E} = -\nabla \Phi$ and apply the fact that it only depends on *z* in order to derive the Poisson equation in one-dimension:

$$\boxed{-\frac{d}{dz}\left(\epsilon(z)\frac{d\,\Phi(z)}{dz}\right)=\rho(z)}$$

This is the final equation to be solved. The space charge profile ρ is typically complicated so that this equation can only be solved numerically.

3.0 Numerical Method

We choose to use the fourth-order Runge-Kutta (RK4) numerical method to solve the Poisson equation. This method requires that we transform one second-order differential equation into two coupled first-order differential equations. We define:

$$\frac{d\,\Phi(z)}{dz}=\frac{1}{\epsilon(z)}\Phi_2(z)$$

$$\frac{d\,\Phi_2(z)}{dz}=-\rho(z)$$

In order to apply the RK4 method in a straightforward manner and hide the details of this particular problem until the end, we define the functions f and g according to:

$$\frac{d\,\Phi(z)}{dz}=f(z,\Phi_2(z)) \quad \text{where} \quad f(z,\Phi_2(z))=\frac{1}{\epsilon(z)}\Phi_2(z)$$

$$\frac{d\,\Phi_2(z)}{dz}=g(z,\Phi(z)) \quad \text{where} \quad g(z,\Phi(z))=-\rho(z)$$

The RK4 method expands the differentials into finite differences, and approximates the right-hand sides by weighted averages at neighboring points:

$$\frac{\Phi(z_{n+1})-\Phi(z_n)}{z_{n+1}-z_n}=f_{ave}(z,\Phi_2(z)) \quad \text{where} \quad f_{ave}(z,\Phi_2(z))=\frac{1}{6}(f_1+2f_2+2f_3+f_4)$$

$$\frac{\Phi_2(z_{n+1})-\Phi_2(z_n)}{z_{n+1}-z_n}=g_{ave}(z,\Phi(z)) \quad \text{where} \quad g_{ave}(z,\Phi_2(z))=\frac{1}{6}(g_1+2g_2+2g_3+g_4)$$

We cannot replace the location differences (z_{n+1}-z_n) with a constant step size h because the grid points are not equally spaced. We have chosen to not equally space the grid points in order to accurately preserve the layer widths. A grid point is set at each layer boundary, and then equally spaced within layers.

We can now solve the differential equations for the potentials at the z_{n+1} locations in order to form iteration equations:

$$\boxed{\Phi(z_{n+1}) = \Phi(z_n) + (z_{n+1} - z_n) f_{ave}(z, \Phi_2(z))}$$

$$\boxed{\Phi_2(z_{n+1}) = \Phi_2(z_n) + (z_{n+1} - z_n) g_{ave}(z, \Phi(z))}$$

These iteration equations allow us to start with some known initial conditions $\Phi(z_0)$ and $\Phi_2(z_0)$ and calculate directly the rest of the functions, step by step. The RK4 method defines the points to be averaged according to:

$$f_1 = f(z_n, \Phi_2(z_n)) \quad \text{and} \quad g_1 = g(z_n, \Phi(z_n))$$

$$f_2 = f\left(\frac{1}{2}(z_{n+1} + z_n), \Phi_2(z_n) + \frac{1}{2}(z_{n+1} - z_n) g_1\right) \quad \text{and} \quad g_2 = g\left(\frac{1}{2}(z_{n+1} + z_n), \Phi(z_n) + \frac{1}{2}(z_{n+1} - z_n) f_1\right)$$

$$f_3 = f\left(\frac{1}{2}(z_{n+1} + z_n), \Phi_2(z_n) + \frac{1}{2}(z_{n+1} - z_n) g_2\right) \quad \text{and} \quad g_3 = g\left(\frac{1}{2}(z_{n+1} + z_n), \Phi(z_n) + \frac{1}{2}(z_{n+1} - z_n) f_2\right)$$

$$f_4 = f(z_{n+1}, \Phi_2(z_n) + (z_{n+1} - z_n) g_3) \quad \text{and} \quad g_4 = g(z_{n+1}, \Phi(z_n) + (z_{n+1} - z_n) f_3)$$

We substitute into these definitions the explicit forms for f and g to find:

$$f_1 = \frac{1}{\epsilon(z_n)} \Phi_2(z_n) \quad \text{and} \quad g_1 = -\rho(z_n)$$

$$f_2 = \frac{1}{\epsilon\left(\frac{1}{2}(z_{n+1} + z_n)\right)} \left[\Phi_2(z_n) + \frac{1}{2}(z_{n+1} - z_n) g_1\right] \quad \text{and} \quad g_2 = -\rho\left(\frac{1}{2}(z_{n+1} + z_n)\right)$$

$$f_3 = \frac{1}{\epsilon(\frac{1}{2}(z_{n+1}+z_n))}[\Phi_2(z_n)+\frac{1}{2}(z_{n+1}-z_n)g_2] \quad \text{and} \quad g_3 = -\rho(\frac{1}{2}(z_{n+1}+z_n))$$

$$f_4 = \frac{1}{\epsilon(z_{n+1})}[\Phi_2(z_n)+(z_{n+1}-z_n)g_3] \quad \text{and} \quad g_4 = -\rho(z_{n+1})$$

The charge density and permittivity are not known at the midpoints, but can be approximated as the average of the nearest points. Other parameters are also defined to speed up calculations.

$$h_n = z_{n+1}-z_n \quad , \quad \epsilon_{mid} = \frac{1}{2}(\epsilon(z_{n+1})+\epsilon(z_n)) \quad , \quad \rho_{mid} = \frac{1}{2}[\rho(z_{n+1})+\rho(z_n)]$$

$$f_1 = \frac{1}{\epsilon(z_n)}\Phi_2(z_n) \quad \text{and} \quad g_1 = -\rho(z_n)$$

$$f_2 = \frac{1}{\epsilon_{mid}}[\Phi_2(z_n)+\frac{h_n}{2}g_1] \quad \text{and} \quad g_2 = -\rho_{mid}$$

$$f_3 = \frac{1}{\epsilon_{mid}}[\Phi_2(z_n)+\frac{h_n}{2}g_2] \quad \text{and} \quad g_3 = -\rho_{mid}$$

$$f_4 = \frac{1}{\epsilon(z_{n+1})}[\Phi_2(z_n)+h_n g_3] \quad \text{and} \quad g_4 = -\rho(z_{n+1})$$

$$\Phi(z_{n+1}) = \Phi(z_n)+\frac{h_n}{6}(f_1+2f_2+2f_3+f_4)$$

$$\Phi_2(z_{n+1}) = \Phi_2(z_n)+\frac{h_n}{6}(g_1+2g_2+2g_3+g_4)$$

Because the Poisson equation is so simple, many of the parameters in the RK4 method end up redundant and the equations can be simplified down.

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: $h_n = z_{n+1} - z_n$

3. Calculate the midpoint values of the permittivity and charge: $\epsilon_{mid} = \frac{1}{2}(\epsilon(z_{n+1}) + \epsilon(z_n))$ and $\rho_{mid} = \frac{1}{2}[\rho(z_{n+1}) + \rho(z_n)]$

4. Calculate the potential values at the next point:

$$\Phi(z_{n+1}) = \Phi(z_n) + \frac{h_n}{6}[\Phi_2(z_n)(\frac{1}{\epsilon(z_n)} + \frac{4}{\epsilon_{mid}} + \frac{1}{\epsilon(z_{n+1})}) - h_n(\frac{\rho(z_n)}{\epsilon_{mid}} + \frac{\rho_{mid}}{\epsilon_{mid}} + \frac{\rho_{mid}}{\epsilon(z_{n+1})})]$$

$$\Phi_2(z_{n+1}) = \Phi_2(z_n) - \frac{h_n}{2}(\rho(z_n) + \rho(z_{n+1}))$$

4.1 Boundary Conditions

This method requires that we know the initial conditions $\Phi(z_0)$ and $\Phi_2(z_0)$, but we instead know the boundary conditions $\Phi(z_0) = 0$ and $\Phi(z_N) = \Delta V_{bias}$ where ΔV_{bias} is the external bias voltage applied across the grid of locations points (three periods in the current code). In order to get around this problem, we must use the shooting method. We guess some value for $\Phi_2(z_0)$, compute the entire function corresponding to this value using the methods above, then compute the error as the difference between the resulting boundary value and the desired boundary condition. The value of $\Phi_2(z_0)$ is then refined using a binary search method until the error is minimized.