1.0 Introduction

In order to strictly ensure periodic boundary conditions and periodic wavefunctions, but still model three full periods of the core structure, the wavefunctions in the central period are copied to the outer periods and replace the original wavefunctions there. Even though the wavefunctions typically extend across multiple periods, they can be determined to reside mostly in one period, and are assigned to that period by calculating the location of the center of mass of the wavefunction. All wavefunctions with a center of mass lying outside the central period are discarded, and then all remaining wavefunctions are copied and shifted left one period, and copied again and shifted right one period. The wavefunctions are shifted in space by the length of one period and shifted in energy by the potential energy drop across one period due to the bias.

Note that when some wavefunctions are copied to the outer periods, part of the waves' profile extends into regions not modeled by the three-period grid of location points and therefore must be discarded. The natural result is that such wavefunctions are no longer accurately normalized and are also unable to give accurate form factors. Such edge effects are inevitable but have minimal overall effect. These edge effects are minimized by always keeping only calculations performed in the central period and copying them to the outer periods for every type of calculations. One may wonder why the outer periods are used at all if their calculations are always thrown away. The answer is that if the outer periods were not used at all, the edge effects would be present in the central period. Using outer periods keeps the edge effects away from the central period where the meaningful calculations are performed. Additionally, wavefunctions that reside in the central period still extend into the outer periods.

2.0 Calculating Center of Masses

A given wavefunction $\psi_i(z)$ corresponding to the ith energy level has some spatial extent. If instead of treating its square as the quantum extent of one electron, we treat it as the population density of a large ensemble of electrons, then it becomes the spatially varying electron density of that level. Because the electrons all have the same mass (neglecting the fact that the effective mass varies from material layer to layer), the center of mass of the ith state is:

$$z_{i,cm} = \frac{\int |\psi_i(z)|^2 z \, dz}{\int |\psi_i(z)|^2 \, dz}$$

The wavefunctions are properly normalized as soon as they are found, so that the integral in the denominator is equal to one:

$$z_{i,cm} = \int |\psi_i(z)|^2 z \, dz$$

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 cannot be used.

Every time new wavefunctions are found using the Schrödinger equation, the code immediately calculates the center of mass of each wavefunction, assigns it to one of the three periods based on this center of mass, copies the central wavefunctions to the outer periods, and provides this information for use by later calculations.

3.0 Match up Levels
After copying wavefunctions to the outer periods, all periods have been forced to be numerically equivalent. Every wavefunction in an outer period matches exactly with one in the central period. This information can be used later on to optimize the rate equations as well as the scattering rate calculations. For this reason, all wavefunctions in the three periods are indexed in order of energy, the lowest energy being state zero. A list of equivalent wavefunctions according to index number is kept for later use. In this sense, the wavefunctions are automatically matched because we have forced them to be matched.