Quantum Cascade Laser Theory
Electron-Electron Scattering

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1.0 Introduction

We will first derive scattering without screening, then add in screening afterward in a separate document. The eigenstate of an electron in the unperturbed Hamiltonian of a QCL (neglecting the Bloch envelope function) can be projected into coordinate space:

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

where the L_x and L_y are the lengths of the crystal in the dimension perpendicular to the growth dimension z and are needed to normalize the effectively free-electron components of the wave function. The bound-state z-component wave functions Ψ_n are found by numerically solving the one-dimensional Schrödinger equation and the Poisson equation and is understood to be already normalized.

In the most general form, electron-electron scattering in a QCL involves the interaction of an electron in an initial quantum state level i in the z dimension and wavevector $\mathbf{k}_i$ in the x and y dimensions with an electron in level j with wavevector $\mathbf{k}_j$ so that they end up respectively in levels f and g and with wavevectors $\mathbf{k}_f$ and $\mathbf{k}_g$. In the x and y dimensions, the electron is considered pseudo-free within the effective mass approximation for bulk semiconductor materials. In these dimensions, the material is considered to be a bulk volume of the well material.

2.0 Variable Definitions

It is worthwhile to anticipate some of the features that will result in the formal derivation and make some variable definitions in advance. This will simplify the notation and help avoid error. We will also derive some useful relations between these variables. This will streamline the mathematics later on as well as bring the notation in line early on with the literature.

We start with four independent two-dimensional wavevectors, $\mathbf{k}_i$, $\mathbf{k}_j$, $\mathbf{k}_f$ and $\mathbf{k}_g$. Because the electrons are pseudo-free in the x-y plane, which is the same plane in which all these wave vectors lie, the law of conservation of momentum holds and removes both components of $\mathbf{k}_g$ as independent variables. In addition, the law of conservation of energy applies to the whole three-dimensional interaction and removes k_f as an independent variable. The remaining components, $k_i, \theta_{k_i}, k_j, \theta_{k_j}$, and θ_{k_f} are independent and any intermediate variables should be functions of these in the end.

Define $\mathbf{q}=\mathbf{k}_i-\mathbf{k}_f$ which leads to $q=\sqrt{k_i^2+k_f^2-2k_ik_f\cos(\theta_{k_i}-\theta_{k_f})}$. The variable **q** is the transition wave vector.

Define $k_u^2=k_ik_j\cos(\theta_{k_i}-\theta_{k_j})$ (Note k_u^2 can be negative and therefore k_u is complex valued.) The variable k_u^2 is the dot product of $\mathbf{k}_i$ and $\mathbf{k}_j$.

Define $g_0^2=\frac{4m^*}{\hbar^2}[E_i(0)+E_j(0)-E_f(0)-E_g(0)]$ (Note that g_0^2 can be negative.). The variable g_0 is the transition energy wavenumber.

Define $k_s=k_i\cos(\theta_{k_i}-\theta_{k_f})+k_j\cos(\theta_{k_j}-\theta_{k_f})$. The variable k_s is the sum of the initial wave vectors dotted by the unit vector $\mathbf{k}_f$.

Define $\mathbf{g}=\mathbf{k}_j-\mathbf{k}_i$ which can also be written in terms of magnitude and phase. This **g**, also labeled $\mathbf{k}_{ij}$, is the initial relative wavevector:

$$g=\sqrt{k_j^2+k_i^2-2k_u^2} \quad \text{and} \quad \tan\theta_g=\frac{k_j\sin\theta_{k_j}-k_i\sin\theta_{k_i}}{k_j\cos\theta_{k_j}-k_i\cos\theta_{k_i}}$$

Define $\mathbf{g}'=\mathbf{k}_g-\mathbf{k}_f$ which can also be written in terms of magnitude and phase. This **g′**, also labeled $\mathbf{k}_{fg}$, is the final relative wavevector:

$$g'=\sqrt{k_g^2+k_f^2-2k_gk_f\cos(\theta_{k_g}-\theta_{k_f})} \quad \text{and} \quad \tan\theta_{g'}=\frac{k_g\sin\theta_{k_g}-k_f\sin\theta_{k_f}}{k_g\cos\theta_{k_g}-k_f\cos\theta_{k_f}}$$

Define $\theta=\theta_g-\theta_{g'}$. The variable θ defined here is the relative angle. It is an alternate representations of θ_{k_f} and is related to it.

These definitions lead to the useful energy difference relation $g^2-g'^2=k_i^2+k_j^2-k_f^2-k_g^2-2k_u^2+2k_fk_g\cos(\theta_{k_f}-\theta_{k_g})$

2.1 Variable Definitions with Conservation of Momentum Applied

We now apply conservation of momentum $\mathbf{k}_i+\mathbf{k}_j=\mathbf{k}_f+\mathbf{k}_g$ and use it to simplify the variables defined above. It leads to:

$$k_g=\sqrt{k_i^2+k_j^2+k_f^2+2k_u^2-2k_fk_s} \quad , \quad \tan\theta_{k_g}=\frac{k_i\sin\theta_{k_i}+k_j\sin\theta_{k_j}-k_f\sin\theta_{k_f}}{k_i\cos\theta_{k_i}+k_j\cos\theta_{k_j}-k_f\cos\theta_{k_f}} \quad ,$$

$$\mathbf{q}=\frac{\mathbf{g}'-\mathbf{g}}{2} \quad , \quad q=\frac{1}{2}\sqrt{g'^2+g^2-2gg'\cos\theta} \quad ,$$

$\mathbf{g}' = \mathbf{k}_i + \mathbf{k}_j - 2\mathbf{k}_f$ with components $g' = \sqrt{k_i^2 + k_j^2 + 4k_f^2 + 2k_u^2 - 4k_f k_s}$, and $\tan\theta_{g'} = \frac{k_i \sin\theta_{k_i} + k_j \sin\theta_{k_j} - 2k_f \sin\theta_{k_f}}{k_i \cos\theta_{k_i} + k_j \cos\theta_{k_j} - 2k_f \cos\theta_{k_f}}$

as well as simplifying the useful energy difference relation to:

$$g^2 - g'^2 = -4k_f^2 - 4k_u^2 + 4k_f k_s$$

2.2 Variable Definitions with Conservation of Energy Applied

We now apply conservation of energy, $E_i + E_j = E_f + E_g$, and use it to further simplify the above defined variables. We must first expand the energy into *x*, *y*, and *z* components,

$$E_i(0) + \frac{\hbar^2 k_i^2}{2m^*} + E_j(0) + \frac{\hbar^2 k_j^2}{2m^*} = E_f(0) + \frac{\hbar^2 k_f^2}{2m^*} + E_g(0) + \frac{\hbar^2 k_g^2}{2m^*} \quad .$$

Using our definitions, this reduces to:

$$\frac{1}{2}g_0^2 + k_i^2 + k_j^2 = k_f^2 + k_g^2$$

Remove the dependence on k_g using the conservation of momentum relations found in Section 2.1 to obtain:

$$g_0^2 - 4k_f^2 - 4k_u^2 + 4k_f k_s = 0 \quad \textit{Simplified Conservation of Energy Equation}$$

There are two ways to solve this equation. We can solve for k_f directly or we can solve for g' which depends on k_f. Let us do it both ways and implement both ways computationally as a check that no errors have been made.

Solving the simplified conservation of energy equation for k_f reveals:

$$\boxed{k_f = \frac{1}{2}k_s \pm \frac{1}{2}\sqrt{k_s^2 + g_0^2 - 4k_u^2}}$$

Note that there are two possible solutions in this equation and sometimes both are valid, so we must calculate each possibility and in the end sum them together.

Alternatively, we can solve the simplified conservation of energy equation for g'. We do this by first transforming all variables into g and g'. This transformation is easy because we note the last three terms in the simplified conservation of energy equation equals ($g^2 - g'^2$) according to the useful energy difference relation. The simplified conservation-of-energy equation therefore reduces down to the intuitive statement that the transition energy equals the energy difference:

$$g_0^2 + g^2 - g'^2 = 0$$

Solving for g' leads to

$$\boxed{g' = \sqrt{g_0^2 + g^2}}$$

2.3 Variable Definitions within an Angular Integral Using the Two Approaches

Later on we will discover that we want to integrate a function of these variables over an angular integral. We can integrate over θ for the g' approach, or over θ_{k_f} for the k_f approach, and the two should be equivalent. We will do both to check for errors. How do these two equivalent integrals relate to each other? Using the definitions above, the variables θ and θ_{k_f} of the two approaches are found to relate to each other according to:

$$\tan(\theta) = \frac{-2k_i k_j \sin(\theta_{k_i} - \theta_{k_j}) + 2k_i k_f \sin(\theta_{k_i} - \theta_{k_f}) - 2k_j k_f \sin(\theta_{k_j} - \theta_{k_f})}{k_j^2 - k_i^2 + 2k_f k_s - 4k_f k_j \cos(\theta_{k_j} - \theta_{k_f})}$$

To set up an integral we need to know the incremental amounts $d\theta$ and $d\,\theta_{k_f}$. We hold everything constant in the above equation and vary incrementally only θ and θ_f. This is done mathematically by differentiating both sides, being careful to realize that several variables are implicit functions of θ_{k_f} and must be differentiated properly using the chain rule. We differentiate these intermediate variables first:

$$d\,k_s = k_i \sin(\theta_{k_i} - \theta_{k_f})\, d\,\theta_{k_f} + k_j \sin(\theta_{k_j} - \theta_{k_f})\, d\,\theta_{k_f} \quad , \quad d\,k_u = 0 \quad , \quad d\,g_0 = 0 \quad \text{, and therefore} \quad d\,k_f = \frac{1}{2} d\,k_s \left[1 + \frac{k_s}{2k_f - k_s}\right]$$

Differentiating the large equation above and using the pieces directly above, we finally find:

$$d\,\theta = \sum_{k_f} \frac{2k_f}{|k_s - 2k_f|} d\,\theta_{k_f}$$

We therefore find that the integrals of the two approaches are related according to

$$\boxed{\int U(\theta)d\theta=\sum_{k_f}\int U\left(\theta_{k_f}\right)\frac{2k_f}{\left|k_s-2k_f\right|}d\theta_{k_f}}$$

2.4 Final Form for the Variable Definitions using the g' Approach

The final form for an angular integral of any function of these wave-vectors using the **g'** approach is therefore

$$\int U(\theta,q,k_f,k_g)d\theta$$

where

$$k_f=\sqrt{k_i^2+k_j^2-k_g^2+\frac{1}{2}g_0^2}$$

$$k_g=\sqrt{q^2+k_u^2+\sqrt{1+\left(g_0/g\right)^2}\left[(k_j^2-k_u^2)\cos\theta-k_ik_j\sin(\theta_{k_i}-\theta_{k_j})\sin\theta\right]}$$

$$q=\frac{1}{2}\sqrt{g_0^2+2g^2-2g\sqrt{g_0^2+g^2}\cos\theta}$$

$$g^2=k_j^2+k_i^2-2k_u^2$$

$$k_u^2=k_ik_j\cos(\theta_{k_i}-\theta_{k_j})$$

$$g_0^2=\frac{4m^*}{\hbar^2}[E_i(0)+E_j(0)-E_f(0)-E_g(0)]$$

If $g = 0$ or $g_0^2 + g^2 \leq 0$, then the set of initial parameters does not obey the conservation laws and cannot happen physically. Such cases must be explicitly tested for and thrown out because they do not contribute to the integral. Note that computationally, between 10-1000 integration points must be used to get results accurate to 3 to 5 significant figures. Also remember that g_0^2 and k_u^2 often become negative and are still physically valid when they do. Therefore, the value of g_0 and k_u should never be found computationally and then squared as this can lead to errors.

2.5 Final Form for the Variable Definitions using the $\mathbf{k}_f$ Approach

The final form for an angular integral of any function of these wave-vectors using the $\mathbf{k}_f$ approach is:

$$\sum_{k_f} \int U(\theta_{k_f}, q, k_f, k_g) \frac{2k_f}{|k_s - 2k_f|} d\theta_{k_f}$$

where

$$q = \sqrt{k_i^2 + k_f^2 - 2k_f k_i \cos(\theta_{k_i} - \theta_{k_f})}$$

$$k_g = \sqrt{k_i^2 + k_j^2 + k_f^2 - 2k_f k_s + 2k_u^2}$$

$$k_f = \frac{1}{2} k_s \pm \frac{1}{2} \sqrt{k_s^2 + g_0^2 - 4k_u^2}$$

$$k_s = k_i \cos(\theta_{k_i} - \theta_{k_f}) + k_j \cos(\theta_{k_j} - \theta_{k_f})$$

$$k_u^2 = k_i k_j \cos(\theta_{k_i} - \theta_{k_j})$$

$$g_0^2 = \frac{4m^*}{\hbar^2} [E_i(0) + E_j(0) - E_f(0) - E_g(0)]$$

If ($k_i^2 + k_j^2 - 2k_u^2 + g_0^2 \leq 0$) or ($k_i^2 + k_j^2 - 2k_u^2 = 0$) or ($k_s^2 + g_0^2 - 4k_u^2 \leq 0$) or $k_f \leq 0$ then the set of initial parameters does not obey the conservation laws and cannot happen physically. Such cases must be explicitly tested for and thrown out because they do not contribute to the integral. Note that computationally, 100-10000 integration points must be used to get results accurate to 3 to 5 significant figures. Also note that g_0^2 and k_u^2 often become negative and are still physically valid when they do. Therefore, the value of g_0 and k_u should never be found computationally and then squared as this can lead to errors.

The final forms of the two approaches have been numerically tested and found to be equivalent. They produce the same numerical values for the integral when enough integration points are included.

3.0 Formal Derivation of the Scattering Rate for one $\mathbf{k}_i$

Let us now start from the beginning and pursue the derivation more formally. The conservation laws will appear automatically and will be applied as they appear. All of the variable definitions and relations found in the previous section will be used directly here without much need of further comment.

Within the approximation of first-order perturbation theory, the electron-electron scattering rate can be found using Fermi's Golden Rule:

$$W_{i,j\to f,g}(\mathbf{k}_i,\mathbf{k}_j,\mathbf{k}_f,\mathbf{k}_g)=\frac{2\pi}{\hbar}|M|^2\delta\left(E_f(\mathbf{k}_f)+E_g(\mathbf{k}_g)-E_i(\mathbf{k}_i)-E_j(\mathbf{k}_j)\right)$$

where the matrix element is $M=<f,\mathbf{k}_f,g,\mathbf{k}_g|H'|i,\mathbf{k}_i,j,\mathbf{k}_j>$.

The perturbed Hamiltonian is just Coulomb's Law, $H'=\frac{e^2}{4\pi\epsilon|\mathbf{r}_i-\mathbf{r}_j|}$,

where the position variables become operators. Here we are using SI units, which therefore lead to the appearance of 4π in the denominator. For now, the permittivity ϵ is the unscreened permittivity for a bulk volume of material consisting of the well material, but will become the screened version later on.

3.1 Project the Operators and Wavevectors into Coordinate Space

Expanding out the Hamiltonian explicitly in Cartesian coordinate operators, the matrix element becomes

$$M=\frac{e^2}{4\pi\epsilon}<f,\mathbf{k}_f,g,\mathbf{k}_g|\frac{1}{\sqrt{(x_i-x_j)^2+(y_i-y_j)^2+(z_i-z_j)^2}}|i,\mathbf{k}_i,j,\mathbf{k}_j>$$

Project the wave-vectors into coordinate space using the identities:

$$I=\int_0^{L_x}dx|x><x|,\quad I=\int_0^{L_y}dy|y><y|\ \text{etc.}$$

$$M=\frac{e^2}{4\pi\epsilon}<f,\mathbf{k}_f,g,\mathbf{k}_g|\left[\int_0^{L_x}dx|x><x|\right]\left[\int_0^{L_y}dy|y><y|\right]\left[\int_0^{L_z}dz|z><z|\right]\left[\int_0^{L_x}dx'|x'><x'|\right]\left[\int_0^{L_y}dy'|y'><y'|\right]\left[\int_0^{L_z}dz'|z'><z'|\right]\times$$
$$\frac{1}{\sqrt{(x_i-x_j)^2+(y_i-y_j)^2+(z_i-z_j)^2}}\times$$
$$\left[\int_0^{L_x}dx"|x"><x"|\right]\left[\int_0^{L_y}dy"|y"><y"|\right]\left[\int_0^{L_z}dz"|z"><z"|\right]\left[\int_0^{L_x}dx'''|x'''><x'''|\right]\left[\int_0^{L_y}dy'''|y'''><y'''|\right]\left[\int_0^{L_z}dz'''|z'''><z'''|\right]|i,\mathbf{k}_i,j,\mathbf{k}_j>$$

Collect all the integration symbols:

$$M=\frac{e^2}{4\pi\epsilon}\int_0^{L_x}dx\int_0^{L_x}dx'\int_0^{L_y}dy\int_0^{L_y}dy'\int_0^{L_z}dz\int_0^{L_z}dz'\int_0^{L_x}dx"\int_0^{L_x}dx'''\int_0^{L_y}dy"\int_0^{L_y}dy'''\int_0^{L_z}dz"\int_0^{L_z}dz'''<f,\mathbf{k}_f,g,\mathbf{k}_g|x>|y>|z>|x'>|y'>|z'>\times$$
$$<x|<y|<z|<x'|<y'|<z'|\frac{1}{\sqrt{(x_i-x_j)^2+(y_i-y_j)^2+(z_i-z_j)^2}}|x">|y">|z">|x'''>|y'''>|z'''>\times$$
$$<x"|<y"|<z"|<x'''|<y'''|<z'''|i,\mathbf{k}_i,j,\mathbf{k}_j>$$

The position operators, when operating on position eigenvectors, become position eigenvalues. Thus, for instance, the operator x_i becomes the eigenvalue x'' and the ket vector can be moved passed the scalar $x"$. For example, $<x|x_i|x">=<x|x">x"$.

$$M=\frac{e^2}{4\pi\epsilon}\int_0^{L_x}dx\int_0^{L_x}dx'\int_0^{L_y}dy\int_0^{L_y}dy'\int_0^{L_z}dz\int_0^{L_z}dz'\int_0^{L_x}dx"\int_0^{L_x}dx'''\int_0^{L_y}dy"\int_0^{L_y}dy'''\int_0^{L_z}dz"\int_0^{L_z}dz'''<f,\mathbf{k}_f,g,\mathbf{k}_g|x>|y>|z>|x'>|y'>|z'>\times$$
$$<x|x"><y|y"><z|z"><x'|x'''><y'|y'''><z'|z'''>\frac{1}{\sqrt{(x"-x''')^2+(y"-y''')^2+(z"-z''')^2}}<x"|<y"|<z"|<x'''|<y'''|<z'''|i,\mathbf{k}_i,j,\mathbf{k}_j>$$

The inner product of position eigenvectors is a Dirac delta:

$$M=\frac{e^2}{4\pi\epsilon}\int_0^{L_x}dx\int_0^{L_x}dx'\int_0^{L_y}dy\int_0^{L_y}dy'\int_0^{L_z}dz\int_0^{L_z}dz'\int_0^{L_x}dx''\int_0^{L_x}dx'''\int_0^{L_y}dy''\int_0^{L_y}dy'''\int_0^{L_z}dz''\int_0^{L_z}dz'''<f,\mathbf{k}_f,g,\mathbf{k}_g|x>|y>|z>|x'>|y'>|z'>\times$$
$$\delta(x-x'')\delta(y-y'')\delta(z-z'')\delta(x'-x''')\delta(y'-y''')\delta(z'-z''')\frac{1}{\sqrt{(x''-x''')^2+(y''-y''')^2+(z''-z''')^2}}\times$$
$$<x''|<y''|<z''|<x'''|<y'''|<z'''|i,\mathbf{k}_i,j,\mathbf{k}_j>$$

The Dirac deltas are evaluated in their integrals:

$$M=\frac{e^2}{4\pi\epsilon}\int_0^{L_x}dx\int_0^{L_x}dx'\int_0^{L_y}dy\int_0^{L_y}dy'\int_0^{L_z}dz\int_0^{L_z}dz'<f,\mathbf{k}_f,g,\mathbf{k}_g|x>|y>|z>|x'>|y'>|z'>\frac{1}{\sqrt{(x-x')^2+(y-y')^2+(z-z')^2}}\times$$
$$<x|<y|<z|<x'|<y'|<z'|i,\mathbf{k}_i,j,\mathbf{k}_j>$$

The state wave-functions are expanded into components and matched up with the proper inner products:

$$M=\frac{e^2}{4\pi\epsilon}\int_0^{L_x}dx\int_0^{L_x}dx'\int_0^{L_y}dy\int_0^{L_y}dy'\int_0^{L_z}dz\int_0^{L_z}dz'<f|z><k_{f,x}|x><k_{f,y}|y><g|z'><k_{g,x}|x'><k_{g,y}|y'>\frac{1}{\sqrt{(x-x')^2+(y-y')^2+(z-z')^2}}\times$$
$$<z|i><x|k_{i,x}><y|k_{i,y}><z'|j><x'|k_{j,x}><y'|k_{j,y}>$$

Now use the fact that $<z|i>=\psi_i(z)$, etc. , which are the wavefunctions found using Schrödinger's equations, and $<x|k_{i,x}>=\frac{1}{\sqrt{L_x}}e^{ik_x x}$, etc.

$$M=\frac{e^2}{4\pi\epsilon}\int_0^{L_x}dx\int_0^{L_x}dx'\int_0^{L_y}dy\int_0^{L_y}dy'\int_0^{L_z}dz\int_0^{L_z}dz'\psi_f^*(z)\frac{1}{\sqrt{L_x}}e^{-ik_{f,x}x}\frac{1}{\sqrt{L_y}}e^{-ik_{f,y}y}\psi_g^*(z')\frac{1}{\sqrt{L_x}}e^{-ik_{g,x}x'}\frac{1}{\sqrt{L_y}}e^{-ik_{g,y}y'}\frac{1}{\sqrt{(x-x')^2+(y-y')^2+(z-z')^2}}\times$$
$$\psi_i(z)\frac{1}{\sqrt{L_x}}e^{ik_{i,x}x}\frac{1}{\sqrt{L_y}}e^{ik_{i,y}y}\psi_j(z')\frac{1}{\sqrt{L_x}}e^{ik_{j,x}x'}\frac{1}{\sqrt{L_y}}e^{ik_{j,y}y'}$$

Collect terms:

$$M=\frac{1}{(L_x L_y)^2}\frac{e^2}{4\pi\epsilon}\int_0^{L_x}dx\int_0^{L_x}dx'\int_0^{L_y}dy\int_0^{L_y}dy'\int_0^{L_z}dz\int_0^{L_z}dz'\frac{1}{\sqrt{(x-x')^2+(y-y')^2+(z-z')^2}}\times$$
$$\psi_f^*(z)\psi_g^*(z')\psi_i(z)\psi_j(z')e^{i(k_{i,x}-k_{f,x})x}e^{i(k_{i,y}-k_{f,y})y}e^{i(k_{j,x}-k_{g,x})x'}e^{i(k_{j,y}-k_{g,y})y'}$$

3.2 Perform the First Integration After Rearranging

Move terms out of the integrals and rearrange:

$$M=\frac{1}{(L_x L_y)^2}\frac{e^2}{4\pi\epsilon}\int_0^{L_z}dz\int_0^{L_z}dz'\psi_f^*(z)\psi_g^*(z')\psi_i(z)\psi_j(z')\int_0^{L_x}dx'e^{i(k_{j,x}-k_{g,x})x'}\int_0^{L_y}dy'e^{i(k_{j,y}-k_{g,y})y'}\times$$
$$\int_0^{L_x}dx\,e^{i(k_{i,x}-k_{f,x})x}\int_0^{L_y}dy\,e^{i(k_{i,y}-k_{f,y})y}\frac{1}{\sqrt{(x-x')^2+(y-y')^2+(z-z')^2}}$$

Make a change of integration variables: $x\to x+x'$, $y\to y+y'$

$$M=\frac{1}{(L_x L_y)^2}\frac{e^2}{4\pi\epsilon}\int_0^{L_z}dz\int_0^{L_z}dz'\psi_f^*(z)\psi_g^*(z')\psi_i(z)\psi_j(z')\int_0^{L_x}dx'e^{i(k_{j,x}-k_{g,x})x'}\int_0^{L_y}dy'e^{i(k_{j,y}-k_{g,y})y'}\times$$
$$\int_{-x'}^{L_x-x'}dx\,e^{i(k_{i,x}-k_{f,x})(x+x')}\int_{-y'}^{L_y-y'}dy\,e^{i(k_{i,y}-k_{f,y})(y+y')}\frac{1}{\sqrt{(x)^2+(y)^2+(z-z')^2}}$$

Expand out the exponentials and move a part out of the integrals, and define I_1 for ease of notation:

$$M = \frac{1}{(L_x L_y)^2} \frac{e^2}{4\pi\epsilon} \int_0^{L_z} dz \int_0^{L_z} dz' \psi_f^*(z) \psi_g^*(z') \psi_i(z) \psi_j(z') \int_0^{L_x} dx' e^{i(k_{i,x} - k_{f,x} + k_{j,x} - k_{g,x})x'} \int_0^{L_y} dy' e^{i(k_{i,y} - k_{f,y} + k_{j,y} - k_{g,y})y'} I_1$$

$$\text{where} \quad I_1 = \int_{-x'}^{L_x - x'} dx \int_{-y'}^{L_y - y'} dy \frac{e^{i[(k_{i,x} - k_{f,x})x + (k_{i,y} - k_{f,y})y]}}{\sqrt{(x)^2 + (y)^2 + (z - z')^2}}$$

Let us now evaluate the integral I_1 before we move on. Express I_1 in polar coordinates and it can be solved analytically if one approximates that the area approaches infinity. Put the wavevector difference on the x-axis.

$$I_1 = \int_0^{\infty} dr\, r \frac{1}{\sqrt{r^2 + (z - z')^2}} \int_0^{2\pi} d\theta\, e^{iqr\cos\theta} \quad \text{where} \quad q = |\mathbf{k}_i - \mathbf{k}_f|$$

Expand the complex exponential and use the symmetry of the function to reduce to one integral:

$$I_1 = \int_0^{\infty} dr\, r \frac{1}{\sqrt{r^2 + (z - z')^2}} \left[2 \int_0^{\pi} d\theta \cos(q r \cos\theta) \right]$$

The factor in square brackets is related to the integral definition of the Bessel Function J_0:

$$I_1 = \int_0^{\infty} dr\, r \frac{1}{\sqrt{r^2 + (z - z')^2}} 2\pi J_0(qr)$$

Making a change of variables, let $u = qr$. Then also $r = u/q$ and $dr = du/q$:

$$I_1 = \frac{2\pi}{q} \int_0^{\infty} du \frac{u J_0(u)}{\sqrt{u^2 + (q|z - z'|)^2}}$$

This integral can be solved analytically and yields:

$$I_1 = \frac{2\pi}{q} e^{-q|z-z'|}$$

Substitute this integral's value back into the matrix element equation:

$$M = \frac{1}{(L_x L_y)^2} \frac{e^2}{4\pi\epsilon} \int_0^{L_z} dz \int_0^{L_z} dz' \psi_f^*(z) \psi_g^*(z') \psi_i(z) \psi_j(z') \int_0^{L_x} dx' e^{i(k_{i,x} - k_{f,x} + k_{j,x} - k_{g,x})x'} \int_0^{L_y} dy' e^{i(k_{i,y} - k_{f,y} + k_{j,y} - k_{g,y})y'} \frac{2\pi}{q} e^{-q|z-z'|}$$

$$M = \frac{1}{(L_x L_y)^2} \frac{e^2}{4\pi\epsilon} \frac{2\pi}{q} \int_0^{L_x} dx' e^{i(k_{i,x} - k_{f,x} + k_{j,x} - k_{g,x})x'} \int_0^{L_y} dy' e^{i(k_{i,y} - k_{f,y} + k_{j,y} - k_{g,y})y'} \int_0^{L_z} dz \int_0^{L_z} dz' \psi_f^*(z) \psi_g^*(z') \psi_i(z) \psi_j(z') e^{-q|z-z'|}$$

3.3 Identify the Form Factor and Conservation of Momentum

We note that the two-dimensional integral at the end depends only on q. Furthermore, having previously determined the wavefunctions, we can compute this part directly as a function of q without any further simplification. In fact, to speed up processing, we can pre-calculate this factor for a large set of typical q values, and then simply look up the factor's value for a certain q as we need it. Let us call this factor the overlap form factor $A(q)$ because it tells us that the more the wavefunctions overlap, the faster the transition rate.

$$A(q) = \int_0^{L_z} dz \int_0^{L_z} dz' \psi_f^*(z) \psi_g^*(z') \psi_i(z) \psi_j(z') e^{-|z-z'|q}$$

The matrix element now becomes:

$$M = \frac{1}{(L_x L_y)^2} \frac{e^2}{4\pi\epsilon} \frac{2\pi}{q} A(q) \int_0^{L_x} dx' e^{i(k_{i,x} - k_{f,x} + k_{j,x} - k_{g,x})x'} \int_0^{L_y} dy' e^{i(k_{i,y} - k_{f,y} + k_{j,y} - k_{g,y})y'}$$

Substitute into the full rate equation:

$$W_{i,j \to f,g}(\mathbf{k}_i, \mathbf{k}_j, \mathbf{k}_f, \mathbf{k}_g) = \frac{2\pi}{\hbar} |M|^2 \delta(E_f(\mathbf{k}_f) + E_g(\mathbf{k}_g) - E_i(\mathbf{k}_i) - E_j(\mathbf{k}_j))$$

$$W_{i,j\to f,g}(\mathbf{k}_i,\mathbf{k}_j,\mathbf{k}_f,\mathbf{k}_g)=\frac{1}{(L_xL_y)^4}\frac{e^4}{(4\pi\epsilon)^2}\frac{(2\pi)^2}{q^2}\frac{2\pi}{\hbar}\delta(E_f(\mathbf{k}_f)+E_g(\mathbf{k}_g)-E_i(\mathbf{k}_i)-E_j(\mathbf{k}_j))|A(q)|^2\times$$
$$\left|\int_0^{L_x}dx'e^{i(k_{i,x}-k_{f,x}+k_{j,x}-k_{g,x})x'}\right|^2\left|\int_0^{L_y}dy'e^{i(k_{i,y}-k_{f,y}+k_{j,y}-k_{g,y})y'}\right|^2$$

If the lengths approach infinity, then $\left|\int_0^{L_x}dx'e^{i(k_{i,x}-k_{f,x}+k_{j,x}-k_{g,x})x'}\right|^2=L_x2\pi\delta(k_{i,x}-k_{f,x}+k_{j,x}-k_{g,x})$, etc., leading to:

$$W_{i,j\to f,g}(\mathbf{k}_i,\mathbf{k}_j,\mathbf{k}_f,\mathbf{k}_g)=\frac{1}{(L_xL_y)^4}\frac{e^4}{(4\pi\epsilon)^2}\frac{(2\pi)^2}{q^2}\frac{2\pi}{\hbar}\delta(E_f(\mathbf{k}_f)+E_g(\mathbf{k}_g)-E_i(\mathbf{k}_i)-E_j(\mathbf{k}_j))|A(q)|^2L_xL_y(2\pi)^2\delta(\mathbf{k}_i-\mathbf{k}_f+\mathbf{k}_j-\mathbf{k}_g)$$

$$W_{i,j\to f,g}(\mathbf{k}_i,\mathbf{k}_j,\mathbf{k}_f,\mathbf{k}_g)=\frac{1}{(L_xL_y)^3}\frac{e^4}{(4\pi\epsilon)^2}\frac{(2\pi)^4}{q^2}\frac{2\pi}{\hbar}|A(q)|^2\delta(E_f(\mathbf{k}_f)+E_g(\mathbf{k}_g)-E_i(\mathbf{k}_i)-E_j(\mathbf{k}_j))\delta(\mathbf{k}_i-\mathbf{k}_f+\mathbf{k}_j-\mathbf{k}_g)$$

The Dirac deltas ensure conservation of energy and momentum. For them to be applied, we must integrate.

3.4 Add up All Possible Transitions by Integrating over all Possible States, Apply Conservation of Momentum

We care not just about one possible event, but all possible events that can happen to one electron state, so we sum over all possible interactions weighted by the carrier distributions to account for states occupied and state blocking. We have to be careful here. To get the total number of states in some interval $d\mathbf{k} = dk_x\,dk_y$, we multiply the probability of a state being occupied by the density of states. The density of states here is the two-dimensional density of states for an infinite rectangular crystal, which is $2L_x\,L_y/(2\pi)^2$. The two is there in front because of the two possible spin states of an electron at each level, thus doubling the number of possible states in the interval. However, because of exchange effects, we consider here only scattering of electrons with anti-parallel spins and must drop the two.

$$W_{i,j\to f,g}(\mathbf{k}_i)=\int\frac{L_xL_y}{(2\pi)^2}d\mathbf{k}_j\int\frac{L_xL_y}{(2\pi)^2}d\mathbf{k}_f\int\frac{L_xL_y}{(2\pi)^2}d\mathbf{k}_gW_{i,j\to f,g}(\mathbf{k}_i,\mathbf{k}_j,\mathbf{k}_f,\mathbf{k}_g)f_j(\mathbf{k}_j)(1-f_g(\mathbf{k}_g))(1-f_f(\mathbf{k}_f))$$

$$W_{i,j\to f,g}(\mathbf{k}_i)=\frac{(L_xL_y)^3}{(2\pi)^6}\int d\mathbf{k}_j\int d\mathbf{k}_f\int d\mathbf{k}_gW_{i,j\to f,g}(\mathbf{k}_i,\mathbf{k}_j,\mathbf{k}_f,\mathbf{k}_g)f_j(\mathbf{k}_j)(1-f_g(\mathbf{k}_g))(1-f_f(\mathbf{k}_f))$$

The Fermi distributions depend on the corresponding electron temperatures. Ideally, each subband distribution is different and therefore has

its own individual electron temperature to describe the distribution. The corresponding individual electron temperature is the one to be used in calculating the Fermi distributions. Note that currently the code sets the electron temperatures equal to the lattice temperature, but that in the future, the code will derive the individual temperatures using energy balance equations.

Substitute in:

$$W_{i,j\to f,g}(\mathbf{k}_i)=\frac{(L_xL_y)^3}{(2\pi)^6}\int d\,\mathbf{k}_j\int d\,\mathbf{k}_f\int d\,\mathbf{k}_g\,\frac{1}{(L_xL_y)^3}\frac{e^4}{(4\pi\epsilon)^2}\frac{(2\pi)^4}{q^2}\frac{2\pi}{\hbar}|A(q)|^2\delta(E_f(\mathbf{k}_f)+E_g(\mathbf{k}_g)-E_i(\mathbf{k}_i)-E_j(\mathbf{k}_j))\times$$
$$\delta(\mathbf{k}_i-\mathbf{k}_f+\mathbf{k}_j-\mathbf{k}_g)\,f_j(\mathbf{k}_j)(1-f_g(\mathbf{k}_g))(1-f_f(\mathbf{k}_f))$$

Simplify the constants:

$$W_{i,j\to f,g}(\mathbf{k}_i)=\frac{1}{(2\pi)^2}\frac{e^4}{(4\pi\epsilon)^2}\frac{2\pi}{\hbar}\int d\,\mathbf{k}_j\int d\,\mathbf{k}_f\int d\,\mathbf{k}_g\,\frac{1}{q^2}|A(q)|^2\delta(E_f(\mathbf{k}_f)+E_g(\mathbf{k}_g)-E_i(\mathbf{k}_i)-E_j(\mathbf{k}_j))\times$$
$$\delta(\mathbf{k}_i-\mathbf{k}_f+\mathbf{k}_j-\mathbf{k}_g)\,f_j(\mathbf{k}_j)(1-f_g(\mathbf{k}_g))(1-f_f(\mathbf{k}_f))$$

The conservation-of-momentum Dirac delta removes the integral over $\mathbf{k}_g$ and fixes both components of $\mathbf{k}_g$ to values dictated by the conservation of momentum. The details were handled in Sec. 2. The scattering rate now becomes:

$$W_{i,j\to f,g}(\mathbf{k}_i)=\frac{1}{(2\pi)^2}\frac{e^4}{(4\pi\epsilon)^2}\frac{2\pi}{\hbar}\int d\,\mathbf{k}_j\int d\,\mathbf{k}_f\frac{1}{q^2}|A(q)|^2\delta(E_f(\mathbf{k}_f)+E_g(\mathbf{k}_g)-E_i(\mathbf{k}_i)-E_j(\mathbf{k}_j))\,f_j(\mathbf{k}_j)(1-f_g(\mathbf{k}_g))(1-f_f(\mathbf{k}_f))$$

In order to use the conservation-of-energy Dirac delta, we must transform its argument into the dimensionality of a wavevector. We move the proper constants out of the Dirac delta using $\delta(ax)=\delta(x)/|a|$. Let us expand the energies and simplify at the same time.

$$W_{i,j\to f,g}(\mathbf{k}_i)=\frac{1}{(2\pi)^2}\frac{2m^*e^4}{(4\pi\epsilon)^2}\frac{2\pi}{\hbar^3}\int d\,\mathbf{k}_j\int d\,\mathbf{k}_f\frac{1}{q^2}|A(q)|^2\delta(\frac{1}{2}g_0^2+k_i^2+k_j^2-k_f^2-k_g^2)f_j(\mathbf{k}_j)(1-f_g(\mathbf{k}_g))(1-f_f(\mathbf{k}_f))$$

This is the point where we can now follow two different approaches, we can apply the integral over k_f directly and the Dirac delta gives us an equation which we can solve for k_f. Or we can transform the integral over k_f into one using relative wavevectors and solve for g'. We will use both approaches and implement both approaches computationally in order to check for errors.

3.5 Apply Conservation of Energy Using the Approach that Solves for k_f

First we use the approach that solves for k_f. Expand the integral into polar coordinates:

$$W_{i,j\to f,g}(\mathbf{k}_i)=\frac{1}{(2\pi)^2}\frac{2m^*e^4}{(4\pi\epsilon)^2}\frac{2\pi}{\hbar^3}\int d\,\mathbf{k}_j\int d\,\theta_{k_f}\int d\,k_f k_f\frac{1}{q^2}|A(q)|^2\,\delta\left(\frac{1}{2}g_0^2+k_i^2+k_j^2-k_f^2-k_g^2\right)f_j(\mathbf{k}_j)(1-f_g(\mathbf{k}_g))(1-f_f(\mathbf{k}_f))$$

We wish to use the identity $\delta(w(k_f))=\sum_i\frac{\delta(k_f-k_f^i)}{|w'(k_f^i)|}$ where k_f^i are the roots of $w(k_f)$

In this case, the argument of the Dirac delta becomes, after substituting in the value of k_g: $w(k_f)=\frac{1}{2}g_0^2-2k_f^2-2k_u^2+2k_fk_s$

The derivative of this is: $w'(k_f)=-4k_f+2k_s$

The roots k_f^i of $w(k_f)$ are: $k_f^{1,2}=\frac{1}{2}k_s\pm\frac{1}{2}\sqrt{k_s^2+g_0^2-4k_u^2}$

The absolute value of the derivative evaluated at the roots are found to be $|w'(k_f^{1,2})|=2\sqrt{k_s^2+g_0^2-4k_u^2}$

We now have all the pieces so that the Dirac delta identity for this case becomes:

$$\delta(g(k_f))=\frac{\delta\left(k_f-\left(\frac{1}{2}k_s+\frac{1}{2}\sqrt{k_s^2+g_0^2-4k_u^2}\right)\right)+\delta\left(k_f-\left(\frac{1}{2}k_s-\frac{1}{2}\sqrt{k_s^2+g_0^2-4k_u^2}\right)\right)}{2\sqrt{k_s^2+g_0^2-4k_u^2}}$$

Substitute back in and use the Dirac deltas to eliminate the integral:

$$W_{i,j\to f,g}(\mathbf{k}_i)=\frac{1}{(2\pi)^2}\frac{m^*e^4}{(4\pi\epsilon)^2}\frac{2\pi}{\hbar^3}\sum_{k_f}\int d\,\mathbf{k}_j\int d\,\theta_{k_f}\frac{k_f}{|k_s-2k_f|}\frac{1}{q^2}|A(q)|^2 f_j(\mathbf{k}_j)(1-f_g(\mathbf{k}_g))(1-f_f(\mathbf{k}_f))\quad\text{where}\quad k_f=\frac{k_s\pm\sqrt{k_s^2+g_0^2-4k_u^2}}{2}$$

Here the summation symbol is used to sum over the two roots of the delta function (the two possible final wave vectors k_f) with the understanding that each is sometimes not physical and must be thrown out.

The final form of the scattering rate for a given $\mathbf{k}_i$ using the $\mathbf{k}_f$ approach is:

$$\boxed{W_{i,j\to f,g}(\mathbf{k}_i)=\frac{1}{(2\pi)^2}\frac{m^* e^4}{(4\pi\epsilon)^2}\frac{2\pi}{\hbar^3}\sum_{k_f}\int d\,\mathbf{k}_j\int d\,\theta_{k_f}\frac{k_f}{|k_s-2k_f|}\frac{1}{q^2}|A(q)|^2 f_j(k_j)(1-f_g(k_g))(1-f_f(k_f))}$$ where

$$A(q)=\int_0^{L_z} dz\int_0^{L_z} dz'\,\psi_f^*(z)\psi_g^*(z')\psi_i(z)\psi_j(z')e^{-|z-z'|q}$$
$$q=\sqrt{k_i^2+k_f^2-2k_f k_i\cos(\theta_{k_i}-\theta_{k_f})}$$
$$k_g=\sqrt{k_i^2+k_j^2+k_f^2-2k_f k_s+2k_u^2}$$
$$k_f=\frac{1}{2}k_s\pm\frac{1}{2}\sqrt{k_s^2+g_0^2-4k_u^2}$$
$$k_s=k_i\cos(\theta_{k_i}-\theta_{k_f})+k_j\cos(\theta_{k_j}-\theta_{k_f})$$
$$k_u^2=k_i k_j\cos(\theta_{k_i}-\theta_{k_j})$$
$$g_0^2=\frac{4m^*}{\hbar^2}[E_i(0)+E_j(0)-E_f(0)-E_g(0)]$$

All of the limitations apply as discussed in Sec. 2.

3.6 Apply Conservation of Energy Using the Approach that Solves for g'

$$W_{i,j\to f,g}(\mathbf{k}_i)=\frac{1}{(2\pi)^2}\frac{2m^* e^4}{(4\pi\epsilon)^2}\frac{2\pi}{\hbar^3}\int d\,\mathbf{k}_j\int d\,\mathbf{k}_f\frac{1}{q^2}|A(q)|^2\delta(\frac{1}{2}g_0^2+k_i^2+k_j^2-k_f^2-k_g^2)f_j(\mathbf{k}_j)(1-f_g(\mathbf{k}_g))(1-f_f(\mathbf{k}_f))$$

Switch the variables inside the Dirac delta to the g and g' notation.

$$W_{i,j\to f,g}(\mathbf{k}_i)=\frac{1}{(2\pi)^2}\frac{4m^* e^4}{(4\pi\epsilon)^2}\frac{2\pi}{\hbar^3}\int d\,\mathbf{k}_j\int d\,\mathbf{k}_f\frac{1}{q^2}|A(q)|^2\delta(g_0^2+g^2-g'^2)f_j(\mathbf{k}_j)(1-f_g(\mathbf{k}_g))(1-f_f(\mathbf{k}_f))$$

Using this notation, $d\,\mathbf{k}_f=d\,k_{fx}d\,k_{fy}$

Using $\mathbf{k}_f = \frac{\mathbf{k}_i + \mathbf{k}_j - \mathbf{g}'}{2}$, this becomes:

$$d\,\mathbf{k}_f = \frac{1}{4} d(k_{ix} + k_{jx} - g_x') d(k_{iy} + k_{jy} - g_y')$$

Within the integration, $\mathbf{k}_i$ and $\mathbf{k}_j$ are independent constants, so their derivative is zero.

$$d\,\mathbf{k}_f = \frac{1}{4} d(g_x') d(g_y')$$

$$d\,\mathbf{k}_f = \frac{1}{4} d\,\mathbf{g}'$$

Making this transformation we get:

$$W_{i,j\to f,g}(\mathbf{k}_i) = \frac{1}{(2\pi)^2} \frac{m^* e^4}{(4\pi\epsilon)^2} \frac{2\pi}{\hbar^3} \int d\,\mathbf{k}_j \int d\,\theta_{g'} \int d\,g' \frac{1}{q^2} |A(q)|^2 g' \delta(g'^2 - (g_0^2 + g^2)) f_j(\mathbf{k}_j)(1 - f_g(\mathbf{k}_g))(1 - f_f(\mathbf{k}_f))$$

Apply the conservation of energy delta and use the rule $x\,\delta(x^2 - a^2) = \frac{x}{2|a|}(\delta(x+a) + \delta(x-a))$

The first possibility is non-physical and is dropped. Once the Dirac delta is applied, it leads to $x = a$, so that the ratio in front goes away:

$$x\,\delta(x^2 - a^2) = \frac{1}{2}\delta(x - a)$$

Applying this and simplifying finally leads to:

$$W_{i,j\to f,g}(\mathbf{k}_i) = \frac{1}{(2\pi)^2} \frac{m^* e^4}{(4\pi\epsilon)^2} \frac{2\pi}{\hbar^3} \frac{1}{2} \int d\,\mathbf{k}_j \int d\,\theta_{g'} \frac{1}{q^2} |A(q)|^2 f_j(\mathbf{k}_j)(1 - f_g(\mathbf{k}_g))(1 - f_f(\mathbf{k}_f)) \quad \text{where} \quad g' = \sqrt{g_0^2 + g^2}$$

Make the transformation $\theta = \theta_g - \theta_{g'}$, $d\,\theta = -d\,\theta_{g'}$ (the negative sign goes away when we flip the limits on the integral).

The final form of the scattering rate for a given $\mathbf{k}_i$ using the $\mathbf{g}'$ approach is:

$$\boxed{W_{i,j\to f,g}(\mathbf{k}_i)=\frac{1}{(2\pi)^2}\frac{m^* e^4}{(4\pi\epsilon)^2}\frac{2\pi}{\hbar^3}\frac{1}{2}\int d\,\mathbf{k}_j\int d\,\theta\frac{1}{q^2}|A(q)|^2 f_j(k_j)(1-f_g(k_g))(1-f_f(k_f))}$$ where

$$A(q)=\int_0^{L_z} dz\int_0^{L_z} dz'\,\psi_f^*(z)\psi_g^*(z')\psi_i(z)\psi_j(z')e^{-|z-z'|q}$$

$$k_f=\sqrt{k_i^2+k_j^2-k_g^2+\frac{1}{2}g_0^2}$$

$$k_g=\sqrt{q^2+k_u^2+\sqrt{1+\left(g_0/g\right)^2}\left[(k_j^2-k_u^2)\cos\theta-k_i k_j\sin(\theta_{k_i}-\theta_{k_j})\sin\theta\right]}$$

$$q=\frac{1}{2}\sqrt{g_0^2+2g^2-2g\sqrt{g_0^2+g^2}\cos\theta}$$

$$g^2=k_j^2+k_i^2-2k_u^2$$

$$k_u^2=k_i k_j\cos(\theta_{k_i}-\theta_{k_i})$$

$$g_0^2=\frac{4m^*}{\hbar^2}[E_i(0)+E_j(0)-E_f(0)-E_g(0)]$$

All of the limitations apply as discussed in Sec. 2.

3.7 Check that the Two Approaches Yield Solutions that Match.
Apply the transformation:

$$\int U(\theta)d\,\theta=\sum_{k_f}\int U\left(\theta_{k_f}\right)\frac{2k_f}{|k_s-2k_f|}d\,\theta_{k_f}$$

to the solution found using the **g'** approach:

$$W_{i,j\to f,g}(\mathbf{k}_i)=\frac{1}{(2\pi)^2}\frac{m^* e^4}{(4\pi\epsilon)^2}\frac{2\pi}{\hbar^3}\frac{1}{2}\int d\,\mathbf{k}_j\int d\,\theta\frac{1}{q^2}|A(q)|^2 f_j(k_j)(1-f_g(k_g))(1-f_f(k_f))$$

so that it becomes

$$W_{i,j\to f,g}(\mathbf{k}_i)=\frac{1}{(2\pi)^2}\frac{m^* e^4}{(4\pi\epsilon)^2}\frac{2\pi}{\hbar^3}\int d\,\mathbf{k}_j\int d\,\theta_{k_f}\frac{k_f}{|k_s-2k_f|}\frac{1}{q^2}|A(q)|^2 f_j(k_j)(1-f_g(k_g))(1-f_f(k_f))$$

This matches exactly the solution found using the $\mathbf{k}_f$ approach and the two expressions are therefore equivalent.

4.0 Scattering Rate Averaged Over $\mathbf{k}_i$

We don't know the actual wavevector $\mathbf{k}_i$ of the specific electron of interest, so we must average over a typical distribution of $\mathbf{k}_i$ to get an average scattering rate. This is done by summing up all the scattering rates for all the different states and dividing by the number of states. As before, the density of occupied states in an interval $d\mathbf{k}_i$ is the density of states at this value times the probability of occupation, which is the Fermi function.

$$W_{i,j\to f,g}=\frac{\int\frac{L_x L_y}{(2\pi)^2}d\,\mathbf{k}_i W_{i,j\to f,g}(\mathbf{k}_i)f_i(\mathbf{k}_i)}{\int\frac{L_x L_y}{(2\pi)^2}d\,\mathbf{k}_i f_i(\mathbf{k}_i)}$$

The constants cancel out top and bottom. Expand the integral into polar coordinates:

$$W_{i,j\to f,g}=\frac{\int dk_i\int k_i d\,\theta_{k_i}W_{i,j\to f,g}(\mathbf{k}_i)f_i(\mathbf{k}_i)}{\int dk_i\int k_i d\,\theta_{k_i}f_i(\mathbf{k}_i)}$$

The Fermi function in the denominator does not depend on angles, so the angular integral in the denominator just evaluates to 2π.

$$W_{i,j\to f,g}=\frac{\int dk_i\int k_i d\,\theta_{k_i}W_{i,j\to f,g}(\mathbf{k}_i)f_i(\mathbf{k}_i)}{2\pi\int dk_i k_i f_i(\mathbf{k}_i)}$$

Plug in the scattering rate for the two different approaches and get the final averaged forms:

$$W_{i,j\to f,g}=\frac{1}{2\pi\int dk_i k_i f_i(k_i)}\frac{1}{(2\pi)^2}\frac{m^* e^4}{(4\pi\epsilon)^2}\frac{2\pi}{\hbar^3}\frac{1}{2}\int dk_i\int d\,\theta_{k_i}\int d\,k_j\int d\,\theta_{k_j}\int d\,\theta\frac{k_i k_j}{q^2}|A(q)|^2 f_j(k_j)(1-f_g(k_g))(1-f_f(k_f))f_i(k_i)$$

Note that we can make a transformation $\theta_{k_i}-\theta_{k_j}=\theta_{ij}$ that leaves the entire integrand independent of θ_{k_i} so that the integral over θ_{k_i} evaluates to 2π. This is equivalent to aligning the *x* axis on θ_{k_i} so that it always equals zero.

$$W_{i,j\to f,g}=\frac{1}{\int dk_i k_i f_i(k_i)}\frac{1}{(2\pi)^2}\frac{m^* e^4}{(4\pi\epsilon)^2}\frac{2\pi}{\hbar^3}\frac{1}{2}\int d k_i\int d k_j\int d\theta_{ij}\int d\theta\frac{k_i k_j}{q^2}|A(q)|^2 f_j(k_j)(1-f_g(k_g))(1-f_f(k_f))f_i(k_i)$$

$$A(q)=\int_0^{L_z} dz\int_0^{L_z} dz'\,\psi_f^*(z)\psi_g^*(z')\psi_i(z)\psi_j(z')e^{-|z-z'|q}$$

$$k_f=\sqrt{k_i^2+k_j^2-k_g^2+\frac{1}{2}g_0^2}$$

$$k_g=\sqrt{q^2+k_u^2+\sqrt{1+\left(g_0/g\right)^2}[(k_j^2-k_u^2)\cos\theta-k_i k_j\sin\theta_{ij}\sin\theta]}$$

$$q=\frac{1}{2}\sqrt{g_0^2+2g^2-2g\sqrt{g_0^2+g^2}\cos\theta}$$

$$g^2=k_j^2+k_i^2-2k_u^2$$

$$k_u^2=k_i k_j\cos\theta_{ij}$$

$$g_0^2=\frac{4m^*}{\hbar^2}[E_i(0)+E_j(0)-E_f(0)-E_g(0)]$$

Alternatively,

$$W_{i,j\to f,g}=\frac{1}{\int dk_i k_i f_i(k_i)}\frac{1}{(2\pi)^2}\frac{m^* e^4}{(4\pi\epsilon)^2}\frac{2\pi}{\hbar^3}\sum_{k_f}\int d k_i\int d k_j\int d\theta_{ij}\int d\theta_{k_f}\frac{k_i k_j k_f}{|k_s-2k_f|}\frac{1}{q^2}|A(q)|^2 f_j(k_j)(1-f_g(k_g))(1-f_f(k_f))f_i(k_i)$$

$$A(q)=\int_0^{L_z} dz\int_0^{L_z} dz'\,\psi_f^*(z)\psi_g^*(z')\psi_i(z)\psi_j(z')e^{-|z-z'|q}$$

$$q=\sqrt{k_i^2+k_f^2-2k_f k_i\cos\theta_{k_f}}$$

$$k_g=\sqrt{k_i^2+k_j^2+k_f^2-2k_f k_s+2k_u^2}$$

$$k_f=\frac{1}{2}k_s\pm\frac{1}{2}\sqrt{k_s^2+g_0^2-4k_u^2}$$

$$k_s=k_i\cos\theta_{k_f}+k_j\cos(\theta_{ij}+\theta_{k_f})$$

$$k_u^2 = k_i k_j \cos\theta_{ij}$$

$$g_0^2 = \frac{4m^*}{\hbar^2}[E_i(0) + E_j(0) - E_f(0) - E_g(0)]$$

5.0 Computational Implementation

The two approaches were found to give similar results with regards to numerical accuracy. We choose the relative wave-vector approach because it is simpler. It is the one implemented and is the only one considered in the rest of this documentation. Also, state-blocking was found to be negligible in terahertz QCL's. For this reason, the final states are assumed to be empty, $f_f = 0, f_g = 0$. Upon dropping state blocking, we find that nothing else depends on k_f or k_g. For this reason, we do not need to calculate them.

A. Calculate the form factor $A(q)$ look-up table for a large set of q points using the non-uniform trapezoidal method.

$$A(q)=\int_0^{L_z} dz \int_0^{L_z} dz' \, \psi_f^*(z)\psi_g^*(z')\psi_i(z)\psi_j(z')e^{-|z-z'|q}$$

B. Calculate the front constant:

$$C=\frac{1}{\int k_i f_i(k_i)dk_i}\frac{m^* e^4}{64\pi^3\epsilon^2\hbar^3}$$

C. Calculate the energy difference constant:

$$g_0^2=\frac{4m^*}{\hbar^2}[E_i(0)+E_j(0)-E_f(0)-E_g(0)]$$

D. Calculate the scattering rate by performing the integrals and calling a sub-routine to calculate the innermost integral. The integrals are calculated over a uniform grid of points. The user chooses between 10 to 1000 points per integral, depending on the accuracy desired. Experience has shown that using more than 50 integration points per integral has no discernible effect on the final results of the entire code. The wavenumber integrals are calculated from a lower limit of zero to an upper limit of k_{max}, where k_{max} corresponds to the height of the energy barriers. Any electrons with energies beyond the barrier height will not be contained in the quantum wells. The angular integrals are performed over the whole unit circle. Because the integrals are defined over uniform grids, we can use standard methods such Simpson's Rule or the Boole (Bode) rule.

$$W_{i,j\to f,g}=C\int d\,k_i k_i f_i(k_i)\int d\,k_j k_j f_j(k_j)\int d\,\theta_{ij}U(k_i,k_j,\theta_{ij})$$

E. Calculate the inner integral U by performing the following steps:

$k_u^2 = k_i k_j \cos\theta_{ij}$

$g^2 = k_j^2 + k_i^2 - 2k_u^2$ If $g = 0$ then $W = 0$ for this set of integration points

$q = \frac{1}{2}\sqrt{g_0^2 + 2g^2 - 2g\sqrt{g_0^2 + g^2}\cos\theta}$ If $g_0^2 + g^2 \leq 0$ then $W = 0$ for this set of integration points

$U(k_i, k_j, \theta_{ij}) = \int d\theta \left|\frac{A(q)}{q}\right|^2$

5.1 Additional Computational Optimizations

When including all antisymmetric transitions, calculating the form factor look-up tables can take a long time. For instance, a structure with 30 levels across the three periods will require $30^4 = 810{,}000$ look-up tables to cover all possible interactions of the states i, j to f, g. However, the number of calculations to perform can be reduced if we skip redundant calculations.

5.1.1 Skip Redundancies due to Multiple Periods

Because of the periodic nature of the QCL structure, transitions completely happening in the first period are identical to those happening solely in the second period. If we locate every wavefunction to either period 1, 2, or 3 based on its center of mass (period 3 being the lowest in energy), then we can skip all redundant calculations by applying the following rules. Later on, the whole data structure can be populated by copying the original data to its appropriate redundant locations. The notation used below is $ij \rightarrow fg$ so that for instance 11→23 means an electron in period 1 scatters with another electron in period 1 and they end up in periods 2 and 3 respectively.
Skip all of the following types of transitions:

1) If $i, j, f,$ and g are all not equal to 1 for a given transition, except for 22→22 transitions.

2) Skip all 11→11 transitions

3) Skip double period transitions, when $|i - f| = 2$ or $|j - g| = 2$. Technically, this is not a redundancy, but is instead an assumption that double period transitions are negligible.

These rules can be summarized with the following statement:

Skip when: {[($i \neq 1$) AND ($j \neq 1$) AND ($f \neq 1$) AND ($g \neq 1$)] AND [($i \neq 2$) OR ($j \neq 2$) OR ($f \neq 2$) OR ($g \neq 2$)]}
OR [($i = 1$) AND ($j = 1$) AND ($f = 1$) AND ($g = 1$)]
OR ($|i - f| = 2$) OR ($|j - g| = 2$)

5.1.2 Skip Redundancies due to the Symmetry of the Form Factor $A(q)$

Scrutiny of the form factor equation reproduced below reveals that there are several symmetries:

$$A(q) = \int_0^{L_z} dz \int_0^{L_z} dz' \psi_f^*(z) \psi_g^*(z') \psi_i(z) \psi_j(z') e^{-|z-z'|q}$$

$$A_{ijfg} = A_{fjig} = A_{igfj} = A_{jigf} = A_{jfgi} = A_{gijf} = A_{gfji} = A_{fgij}$$

The way to skip these redundancies computationally is through the following rules. These symbols represent level numbers as opposed to the period numbers in the previous section.

Skip when: ($j > g$) OR ($i > j$) OR ($i > f$) OR ($i > g$) OR (($i = j$) AND ($f > g$))

Note that these symmetries only apply to the form factor and not the entire e-e scattering rate.

5.1.3 Final Recipe for fully optimized implementation 4D electron-electron scattering calculations

A. Outside of the inner two loops, pre-calculate all form factors.

- Iterate through all possible 4D transition indices and create a one-dimensional job list that excludes all period redundancies and form factor redundancies according to Sections 5.1.1 and 5.1.2. Each job is a cluster containing $i, j, f, g, i_2, j_2, f_2, g_2, i_3, j_3, f_3, g_3, A(q)$ where $A(q)$ is a 15 element array of single float-type fractional numbers preset to 0, later to contain the form factor table for this transition. All other elements are 8-bit integers that are indices tracking the levels involved in the transition $ij \rightarrow fg$. The indices with subscripts 2 and 3 are the equivalent transitions in other periods which are redundant to this one. If there are no equivalent transitions, these indices are set to -1.

- Calculate the location of the equivalent redundant transitions in the other periods and store their indices in the job cluster.

- Split the job list into 8 sub-lists to be handed off to 8 identical loops in order to enable multi-processing.

- Loop through each job list directly, and calculate the form factor $A(q)$ of each transition job at the 15 points in q space that will constitute the look-up table and place the results in the job structure. Values of the form factors at other points will be found later using interpolation. The points range from 0 to q_{max}, where q_{max} is the wavenumber equivalent to the barrier height. Wavenumbers above this value represent electrons that escape the quantum well structure and do no contribute. The points are not spread out uniformly, but are rather spread out exponentially as the form factor curves have large wiggles for small q but are very smooth for large q. Instead of saving an array of the q values used for later use, the q_{max} is saved and the exponential function that produces the q values is saved as a subroutine and reapplied as needed.

- Directly after each table is calculated, within the loops, test to see if the maximum value of $A(q)$ is below some threshold. If so, set the entire array equal to -1, as a flag that this job should later be skipped.

- Recombine the jobs from the 8 different processor loops.

- After completely calculating the form factors for all jobs, iterate directly through the job list and if the job contains a symmetric transition such as 33 → 11, insert its form factor table into the 2D transition array at the appropriate place for later use by the phonon scattering algorithm.

B. Calculate Phonon Scattering Rates

- Iterate directly though the 2D transition array and calculate the phonon scattering rates using the form-factor table already loaded in this array.

- If $A(q) = -1$, skip this entire calculation and store the phonon rate for this calculation as zero.

- Expand the 15 point form factor table to 300 point by interpolation outside all loops.

- When an $A(q)$ is needed by the phonon calculations at a certain q, look-up the nearest value in the 300 point table.

C. Calculate electron-electron Scattering Rates

- Split the one-dimensional job list into 8 sub-lists and feed into 8 identical loops to enable multi-processing.

- Initialize a four-dimensional array of single-type fractional numbers to 0 as place holders for all e-e scattering rates and pass to all inner loops.

- Iterate directly through each one-dimensional job list of 4D e-e transitions.

- For each job, skip the entire calculation if $A(q) = -1$

- For each job, interpolate the form factor from the 15 non-uniform points to 300 uniform points, outside of all of the e-e loops.

- For each job, make a list of the 8 equivalent jobs according to Section 5.1.2. The reason for this is that the symmetries that exist in the form factor do not exist in the e-e scattering equation, so we must calculate all of them separately. Iterate through all 8 equivalent jobs using the same form factor, and calculate the unique e-e rate for each.

- Insert the resulting e-e rates into the initially blank 4D e-e rate matrix at the standard position, but also at the period-equivalent positions is they exist according to the indices pre-calculated in the job structure.

- Combine the 8 4D e-e matrices from the different multi-processor threads by adding them directly.

- Collapse the final 4D e-e matrix to a 2D matrix for use in the rate equations by summing over j and g. Be careful to double symmetric rates at they lead to two electrons transitioning, and skip rates where the electron count of interest does not change such as $ij \rightarrow ig$ and $ij \rightarrow ji$.

6.0 Comparison with Literature

In Goodnick's 1988 paper[1], there are many obvious errors in Equation 2.13. The term $|\mathbf{r}-\mathbf{r}'|$ in the denominator should be squared. The exponentials in the numerator should read $e^{-i(\mathbf{k}'\cdot\mathbf{r}+\mathbf{k}_0'\cdot\mathbf{r}')}e^{i(\mathbf{k}\cdot\mathbf{r}+\mathbf{k}_0\cdot\mathbf{r}')}$. This equation is also missing an A^{-4} out front.

Equation 2.17 of Goodnick's 1988 paper has errors in the constants out front. All of the constants before the summation symbol should read

$$\frac{m^* e^4}{\pi \kappa^2 \hbar^3}$$

In a similar way, the constants in the front of Eq. 2.19 should read:

$$\frac{m^* e^4}{4\pi \kappa^2 \hbar^3}$$

Goodnick's 1993 paper[2] also is missing the ¼ factor and all of their data is uniformly 4 times too large.

Goodnick himself published a later correction[3] in 1995 where he recognized the omission of the ¼ factor that appears when transforming to relative wave vectors. However, his published correction oddly does not mention any of the other various errors in his 1988 paper. The final equation in this correction paper is reassuringly finally correct down to the last constant.

In Smet's dissertation[4], which draws heavily from Goodnick's work, Eq. 3.31 is missing a factor A^{-2}.

Equation 3.32 of Smet's disseration is missing a factor q^{-1} which appears later in the derivation.

Equation 3.37 of Smet's dissertation is missing the same ¼ factor that Goodnick neglected in his earlier work.

William's disseration[5] draws from Smet's. Equation 2.50 of William's thesis is consequently missing a factor q^{-1} similar to Smet.

Callebaut's disseration[6] is refreshingly free of errors. Unfortunately, despite being a a fairly recent work, Callebaut's dissertation continues to omit the ¼ factor as can be seen in Eq. 2.47.

The first edition of Harrison's book[7], as well as the accompanying online data, is off by the common ¼ factor. However, the second edition of Harrison's book has this error corrected.

[1] Goodnick, S. M., Lugi, P., "Effect of electron-electron scattering on nonequilibrium transport in quantum well systems." Physical Review B 37:5 p. 2578 (1988).

[2] Physical Review B 48:8, p. 5708 (1993).

[3] Tomita, A., Shah, J., Cunningham, J. E., Goodnick, S. M., Lugni, P, Chuang, S. L., "Erratum: Femtosecond hole relaxation in n-type modulation-doped quantum wells." Physical Review B 52:7 p. 5445 (1995).

[4] Smet, J. H., "Intrawell and Interwell Intersubband Transitions in Single and Multiple Quantum Well Heterostructures." Ph.D. Dissertation, MIT (1995).

[5] Williams, B. S., "Terahertz Quantum Cascade Lasers," Ph.D. Dissertation, MIT, (2003).

[6] Callebaut, H., "Analysis of the Electron Transport Properties in Quantum Cascade Lasers," Ph.D. Disseration, MIT (2006).

[7] Harrison, P., "Quantum Wells, Wires and Dots," Wiley, (2000).