Quantum Cascade Laser Theory
Phonon Scattering

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1.0 Introduction

Only longitudinal optical (LO) phonon scattering is assumed to be significant in QCL's. The phonon spectrum available to a QCL electron for scattering is approximated to be the phonon spectrum of a bulk sample of the material used in the quantum wells. The assumption is also made that the bulk crystal is dispersionless such that every LO photon that can be created or destroyed in a transition is at the frequency $\omega_{\text{LO}}(\mathbf{q}) = \omega_{\text{LO}}(0)$ regardless of the wave vector **q.** This is equivalent to a constant phonon energy of $E_{\text{LO}} = \hbar\omega_{\text{LO}}$.

2.0 Derivation

Phonon scattering in a crystal is described by the Fröhlich interaction. By applying the Fröhlich Hamiltonian to Fermi's golden rule, we can calculate the phonon scattering rate. Inside a QCL, the electron is quantized in the z dimension, as it sits in a quantum well wavefunction state, and is pseudo-free in the x and y dimensions according to the effective mass model.

2.1 Hamiltonian

Fermi's Golden Rule can be written for the transition rate $W_{i\to f}$ from an initial quantized intersubband state i in the z dimension and initial free state with wave vector $\mathbf{k}_i$ in the x-y dimension and initial crystal phonon state $n_{i,\mathbf{q}}$ to a final intersubband state f in the z dimension and final free state with wave vector $\mathbf{k}_f$ in the x-y dimension and final crystal phonon state $n_{f,\mathbf{q}}$.

$$W_{i\to f}^{\text{ems,abs}}(\mathbf{k}_i,\mathbf{k}_f)=\frac{2\pi}{\hbar}|<f,\mathbf{k}_f,n_{f,\mathbf{q}}|H'|i,\mathbf{k}_i,n_{i,\mathbf{q}}>|^2\,\delta(E_f(\boldsymbol{k}_f)-E_i(\mathbf{k}_i)\pm E_{LO})$$

The delta factor is a statement of the conservation of energy. If a phonon is emitted, then $E_{before} = E_{after}$, and $E_i = E_f + E_{LO}$, and therefore $E_f - E_i + E_{LO} = 0$. If a phonon is absorbed, then $E_{before} = E_{after}$, and $E_i + E_{LO} = E_f$, and therefore $E_f - E_i - E_{LO} = 0$

The interaction Hamiltonian between an electron and a phonon is given by:

$$H'=\sum_{\mathbf{q}}[\alpha(\mathbf{q})(e^{i\,\mathbf{q}\cdot\mathbf{r}}b_{\mathbf{q}}+e^{-i\,\mathbf{q}\cdot\mathbf{r}}b_{\mathbf{q}}^{\dagger})]$$

where the interaction strength is given by the Fröhlich representation:

$$|\alpha(\mathbf{q})|^2 = \frac{E_{LO}}{2}\frac{e^2}{V q^2}\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_s}\right)$$

The interaction Hamiltonian is a sum of all the possible phonon wave vectors (modes) **q**. Although the modes are discreet, the crystal is large enough that the modes are assumed to be infinitesimally close and the sum is approximated by an integral:

$$H' = \sum_{q_x}\sum_{q_y}\sum_{q_z}[\alpha(q_x\hat{i}+q_y\hat{j}+q_z\hat{k})(e^{i(q_x x+q_y y+q_z z)} b_{(q_x\hat{i}+q_y\hat{j}+q_z\hat{k})} + e^{-i(q_x x+q_y y+q_z z)} b^\dagger_{(q_x\hat{i}+q_y\hat{j}+q_z\hat{k})})]$$

$$H' = \frac{L^3}{(2\pi)^3}\int d q_x \int d q_y \int d q_z [\alpha(q_x\hat{i}+q_y\hat{j}+q_z\hat{k})(e^{i(q_x x+q_y y+q_z z)} b_{(q_x\hat{i}+q_y\hat{j}+q_z\hat{k})} + e^{-i(q_x x+q_y y+q_z z)} b^\dagger_{(q_x\hat{i}+q_y\hat{j}+q_z\hat{k})})]$$

2.2 Phonon Creation and Destruction

Plug the Hamiltonian into Fermi's golden rule:

$$W^{\text{ems,abs}}_{i\to f}(\mathbf{k}_i,\mathbf{k}_f) = \frac{L^6}{(2\pi)^6}\frac{2\pi}{\hbar}\delta(E_f(\boldsymbol{k}_f) - E_i(\mathbf{k}_i) \pm E_{LO})$$
$$\times|<f,\mathbf{k}_f,n_{f,\mathbf{q}}|\int d q_x \int d q_y \int d q_z [\alpha(q_x\hat{i}+q_y\hat{j}+q_z\hat{k})(e^{i(q_x x+q_y y+q_z z)} b_{(q_x\hat{i}+q_y\hat{j}+q_z\hat{k})} + e^{-i(q_x x+q_y y+q_z z)} b^\dagger_{(q_x\hat{i}+q_y\hat{j}+q_z\hat{k})})]|i,\mathbf{k}_i,n_{i,\mathbf{q}}>|^2$$

Move the integrals outside of the bra and ket vectors:

$$W^{\text{ems,abs}}_{i\to f}(\mathbf{k}_i,\mathbf{k}_f) = \frac{L^6}{(2\pi)^6}\frac{2\pi}{\hbar}\delta(E_f(\boldsymbol{k}_f) - E_i(\mathbf{k}_i) \pm E_{LO})$$
$$\times|\int d q_x \int d q_y \int d q_z \alpha(q_x\hat{i}+q_y\hat{j}+q_z\hat{k}) <f,\mathbf{k}_f,n_{f,\mathbf{q}}|(e^{i(q_x x+q_y y+q_z z)} b_{(q_x\hat{i}+q_y\hat{j}+q_z\hat{k})} + e^{-i(q_x x+q_y y+q_z z)} b^\dagger_{(q_x\hat{i}+q_y\hat{j}+q_z\hat{k})})|i,\mathbf{k}_i,n_{i,\mathbf{q}}>|^2$$

Define the matrix element $M_{\mathbf{q}}$ in the standard way:

$$W^{\text{ems,abs}}_{i\to f}(\mathbf{k}_i,\mathbf{k}_f) = \frac{L^6}{(2\pi)^6}\frac{2\pi}{\hbar}|\int d q_x \int d q_y \int d q_z \alpha(q_x\hat{i}+q_y\hat{j}+q_z\hat{k}) M_{\mathbf{q}}|^2 \delta(E_f(\boldsymbol{k}_f) - E_i(\mathbf{k}_i) \pm E_{LO})$$

where $M_{\mathbf{q}} = <f,\mathbf{k}_f,n_{f,\mathbf{q}}|(e^{i(q_x x+q_y y+q_z z)} b_{(q_x\hat{i}+q_y\hat{j}+q_z\hat{k})} + e^{-i(q_x x+q_y y+q_z z)} b^\dagger_{(q_x\hat{i}+q_y\hat{j}+q_z\hat{k})})|i,\mathbf{k}_i,n_{i,\mathbf{q}}>$

Let us simplify as much as possible the matrix element $M_{\mathbf{q}}$ for phonon mode $\mathbf{q}$ separately. Distribute out the sum:

$$M_{\mathbf{q}} = < f, \mathbf{k}_f, n_{f,\mathbf{q}} | e^{i(q_x x + q_y y + q_z z)} b_{(q_x \hat{i} + q_y \hat{j} + q_z \hat{k})} | i, \mathbf{k}_i, n_{i,\mathbf{q}} > + < f, \mathbf{k}_f, n_{f,\mathbf{q}} | e^{-i(q_x x + q_y y + q_z z)} b^{\dagger}_{(q_x \hat{i} + q_y \hat{j} + q_z \hat{k})} | i, \mathbf{k}_i, n_{i,\mathbf{q}} >$$

Apply the phonon annihilation and creation operators:

$$M_{\mathbf{q}} = < f, \mathbf{k}_f, n_{f,\mathbf{q}} | e^{i(q_x x + q_y y + q_z z)} \sqrt{n_{i,\mathbf{q}}} | i, \mathbf{k}_i, n_{i,\mathbf{q}} - 1 > + < f, \mathbf{k}_f, n_{f,\mathbf{q}} | e^{-i(q_x x + q_y y + q_z z)} \sqrt{n_{i,\mathbf{q}} + 1} | i, \mathbf{k}_i, n_{i,\mathbf{q}} + 1 >$$

Due to orthogonality, the initial and final crystal states must be equal. Out of all the possible initial and final state combinations, all are zero except for two cases where each term above is satisfied.

CASE 1: If $n_{f,\mathbf{q}} = n_{i,\mathbf{q}} + 1$ (phonon created, emitted from electron)

$$M_{\mathbf{q}}^{\text{ems}} = < f, \mathbf{k}_f, n_{i,\mathbf{q}} + 1 | e^{-i(q_x x + q_y y + q_z z)} \sqrt{n_{i,\mathbf{q}} + 1} | i, \mathbf{k}_i, n_{i,\mathbf{q}} + 1 >$$

The before and after phonon states are orthonormal and collapse down to the number one.

$$M_{\mathbf{q}}^{\text{ems}} = \sqrt{n_{i,\mathbf{q}} + 1} < f, \mathbf{k}_f | e^{-i(q_x x + q_y y + q_z z)} | i, \mathbf{k}_i >$$

CASE 2: If $n_{f,\mathbf{q}} = n_{i,\mathbf{q}} - 1$ (phonon destroyed, absorbed by electron)

$$M_{\mathbf{q}}^{\text{abs}} = < f, \mathbf{k}_f, n_{i,\mathbf{q}} - 1 | e^{i(q_x x + q_y y + q_z z)} \sqrt{n_{i,\mathbf{q}}} | i, \mathbf{k}_i, n_{i,\mathbf{q}} - 1 >$$

The before and after phonon states are orthonormal and collapse down to the number one.

$$M_{\mathbf{q}}^{\text{abs}} = \sqrt{n_{i,\mathbf{q}}} < f, \mathbf{k}_f, | e^{i(q_x x + q_y y + q_z z)} | i, \mathbf{k}_i >$$

Combining the two cases into one statement, we have:

$$M_{\mathbf{q}}^{\text{ems,abs}} = \sqrt{n_{i,\mathbf{q}} + 1/2 \pm 1/2} < f, \mathbf{k}_f | e^{\mp i(q_x x + q_y y + q_z z)} | i, \mathbf{k}_i >$$

2.3 Electron Eigenstate Evaluation

With the phonon eigenstates evaluated, we now turn to evaluating the electron eigenstates. The electron that emits or absorbs a phonon is not itself created or destroyed. Rather, the electron transitions to a new quantum level $f(z)$ and new transverse wavevector $\mathbf{k}_f$. We expand out the state vectors into their independent dimensions:

$$M_{\mathbf{q}}^{\text{ems,abs}}=\sqrt{n_{i,\mathbf{q}}+1/2\pm 1/2}<f(z)|\times<\mathbf{k}_f(x,y)|e^{\mp i q_x x}e^{\mp i q_y y}e^{\mp i q_z z}|i(z)>\times|\mathbf{k}_i(x,y)>$$

Expand out the harmonic operator into its independent dimensions.

$$M_{\mathbf{q}}^{\text{ems,abs}}=\sqrt{n_{i,\mathbf{q}}+1/2\pm 1/2}<f(z)|e^{\mp i q_z z}|i(z)><k_{f,x}|e^{\mp i q_x x}|k_{i,x}><k_{f,y}|e^{\mp i q_y y}|k_{i,y}>$$

We now project the transverse operators and state vectors into coordinate space. We do this by inserting identities such as $\mathrm{I}=\left[\int dx|x><x|\right]$:

$$M_{\mathbf{q}}^{\text{ems,abs}}=\sqrt{n_{i,\mathbf{q}}+1/2\pm 1/2}<f(z)|e^{\mp i q_z z}|i(z)><k_{f,x}|\left[\int dx|x><x|\right]e^{\mp i q_x x}\left[\int dx'|x'><x'|\right]|k_{i,x}>$$
$$\times<k_{f,y}|\left[\int dy|y><y|\right]e^{\mp i q_y y}\left[\int dy'|y'><y'|\right]|k_{i,y}>$$

Move the coordinate vectors to where they can be applied:

$$M_{\mathbf{q}}^{\text{ems,abs}}=\sqrt{n_{i,\mathbf{q}}+1/2\pm 1/2}<f(z)|e^{\mp i q_z z}|i(z)>\int dx\int dx'<k_{f,x}|x><x|e^{\mp i q_x x}|x'><x'|k_{i,x}>$$
$$\times\int dy\int dy'<k_{f,y}|y><y|e^{\mp i q_y y}|y'><y'|k_{i,y}>$$

Write out the explicit forms for the transverse electron state vectors in coordinate space. The electron is free in the transverse directions, so that state function is just an exponential:

$$M_{\mathbf{q}}^{\text{ems,abs}}=\sqrt{n_{i,\mathbf{q}}+1/2\pm 1/2}<f(z)|e^{\mp i q_z z}|i(z)>\int dx\int dx'\frac{1}{\sqrt{L}}e^{-ik_{f,x}x}<x|e^{\mp i q_x x}|x'>\frac{1}{\sqrt{L}}e^{ik_{i,x}x'}$$
$$\times\int dy\int dy'\frac{1}{\sqrt{L}}e^{-ik_{f,y}y}<y|e^{\mp i q_y y}|y'>\frac{1}{\sqrt{L}}e^{ik_{i,y}y'}$$

Move all the constants out:

$$M_{\mathbf{q}}^{\text{ems,abs}}=\frac{1}{L^2}\sqrt{n_{i,\mathbf{q}}+1/2\pm 1/2}<f(z)|e^{\mp i q_z z}|i(z)>\int dx\int dx'e^{-ik_{f,x}x}<x|e^{\mp i q_x x}|x'>e^{ik_{i,x}x'}\int dy\int dy'e^{-ik_{f,y}y}<y|e^{\mp i q_y y}|y'>e^{ik_{i,y}y'}$$

Evaluate the harmonic operator's matrix elements:

$$M_{\mathbf{q}}^{\text{ems,abs}}=\frac{1}{L^2}\sqrt{n_{i,\mathbf{q}}+1/2\pm1/2}<f(z)|e^{\mp iq_z z}|i(z)>\int dx\int dx' e^{-ik_{f,x}x}e^{\mp iq_x x}\delta(x-x')e^{ik_{i,x}x'}\int dy\int dy' e^{-ik_{f,y}y}e^{\mp iq_y y}\delta(y-y')e^{ik_{i,y}y'}$$

Evaluate the Dirac deltas:

$$M_{\mathbf{q}}^{\text{ems,abs}}=\frac{1}{L^2}\sqrt{n_{i,\mathbf{q}}+1/2\pm1/2}<f(z)|e^{\mp iq_z z}|i(z)>\int dx\, e^{-ik_{f,x}x}e^{\mp iq_x x}e^{ik_{i,x}x}\int dy\, e^{-ik_{f,y}y}e^{\mp iq_y y}e^{ik_{i,y}y}$$

Consolidate the exponentials:

$$M_{\mathbf{q}}^{\text{ems,abs}}=\frac{1}{L^2}\sqrt{n_{i,\mathbf{q}}+1/2\pm1/2}<f(z)|e^{\mp iq_z z}|i(z)>\int dx\, e^{ix(-k_{f,x}\mp q_x+k_{i,x})}\int dy\, e^{iy(-k_{f,y}\mp q_y+k_{i,y})}$$

Recognize the integrals as Dirac deltas. These deltas enforce conservation of momentum:

$$M_{\mathbf{q}}^{\text{ems,abs}}=\frac{(2\pi)^2}{L^2}\sqrt{n_{i,\mathbf{q}}+1/2\pm1/2}<f(z)|e^{\mp iq_z z}|i(z)>\delta(k_{f,x}\pm q_x-k_{i,x})\,\delta(k_{f,y}\pm q_y-k_{i,y})$$

Put this matrix element back in the original scattering rate equation:

$$W_{i\to f}^{\text{ems,abs}}(\mathbf{k}_i,\mathbf{k}_f)=\frac{L^6}{(2\pi)^6}\frac{2\pi}{\hbar}\delta(E_f(\boldsymbol{k}_f)-E_i(\mathbf{k}_i)\pm E_{LO})$$
$$\times\left|\int dq_x\int dq_y\int dq_z\,\alpha(q_x\hat{i}+q_y\hat{j}+q_z\hat{k})\frac{(2\pi)^2}{L^2}\sqrt{n_{i,\mathbf{q}}+1/2\pm1/2}<f(z)|e^{\mp iq_z z}|i(z)>\delta(k_{f,x}\pm q_x-k_{i,x})\delta(k_{f,y}\pm q_y-k_{i,y})\right|^2$$

By replacing the **q**-momentum-specific occupation numbers with an average occupation number, it can be removed out of the integrals:

$$W_{i\to f}^{\text{ems,abs}}(\mathbf{k}_i,\mathbf{k}_f)=\frac{(2\pi)^4}{L^4}\frac{L^6}{(2\pi)^6}\frac{2\pi}{\hbar}(n_{\text{LO}}+1/2\pm1/2)\delta(E_f(\boldsymbol{k}_f)-E_i(\mathbf{k}_i)\pm E_{LO})$$
$$\times\left|\int dq_x\int dq_y\int dq_z\,\alpha(q_x\hat{i}+q_y\hat{j}+q_z\hat{k})<f(z)|e^{\mp iq_z z}|i(z)>\delta(k_{f,x}\pm q_x-k_{i,x})\delta(k_{f,y}\pm q_y-k_{i,y})\right|^2$$

2.4 Evaluation of the Conservation-of-Momentum Dirac Deltas

Upon applying the Dirac deltas we find that the transverse component of the interaction wavevector $\mathbf{q}_T$ is just the difference of the initial and final wavevectors. In subsequent derivations, we drop the subscript "T" and take the symbol **q** to represent the transverse interaction wavevector and not the full interaction wavevector.

$$W_{i\to f}^{\text{ems,abs}}(\mathbf{k}_i,\mathbf{k}_f)=\frac{(2\pi)^4}{L^4}\frac{L^6}{(2\pi)^6}\frac{2\pi}{\hbar}(n_{\text{LO}}+1/2\pm1/2)\delta(E_f(\boldsymbol{k}_f)-E_i(\mathbf{k}_i)\pm E_{LO})\left|\int d\,q_z\alpha(\mp\mathbf{q}+q_z\hat{k})<f(z)|e^{\mp iq_z z}|i(z)>\right|^2$$

where $\mathbf{q}=\mathbf{k_f}-\mathbf{k_i}$ so that $\boxed{q^2=k_i^2+k_f^2-2k_ik_f\cos(\theta)}$

Assume cross-terms in the square of the integral are zero due to the orthogonality of the different wave vector states:

$$W_{i\to f}^{\text{ems,abs}}(\mathbf{k}_i,\mathbf{k}_f)=\frac{(2\pi)^4}{L^4}\frac{L^6}{(2\pi)^6}\frac{2\pi}{\hbar}(n_{\text{LO}}+1/2\pm1/2)\delta(E_f(\boldsymbol{k}_f)-E_i(\mathbf{k}_i)\pm E_{LO})\int d\,q_z|\alpha(\mp\mathbf{q}+q_z\hat{k})|^2|<f(z)|e^{\mp iq_z z}|i(z)>|^2$$

Now substitute the explicit form of the interaction parameter:

$$W_{i\to f}^{\text{ems,abs}}(\mathbf{k}_i,\mathbf{k}_f)=\frac{2\pi}{L}\frac{(2\pi)^4}{L^4}\frac{L^6}{(2\pi)^6}\frac{2\pi}{\hbar}(n_{\text{LO}}+1/2\pm1/2)\delta(E_f(\boldsymbol{k}_f)-E_i(\mathbf{k}_i)\pm E_{LO})\int d\,q_z\frac{E_{LO}}{2}\frac{e^2}{V(q^2+q_z^2)}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_s}\right)|<f(z)|e^{\mp iq_z z}|i(z)>|^2$$

Move all the constants out:

$$W_{i\to f}^{\text{ems,abs}}(\mathbf{k}_i,\mathbf{k}_f)=\frac{2\pi}{L}\frac{(2\pi)^4}{L^4}\frac{L^6}{(2\pi)^6}\frac{2\pi}{\hbar}\frac{e^2}{V}(n_{\text{LO}}+1/2\pm1/2)\frac{E_{LO}}{2}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_s}\right)\delta(E_f(\boldsymbol{k}_f)-E_i(\mathbf{k}_i)\pm E_{LO})\int d\,q_z\frac{1}{(q^2+q_z^2)}|<f(z)|e^{\mp iq_z z}|i(z)>|^2$$

2.5 Sum over all Final Subband States

The transition rate to a specific quantum state *f* in the *z* dimension but any final state in the *x-y* dimensions is the integral over all possible final states in the *x-y* dimension.

$$W_{i\to f}^{\text{ems,abs}}(\mathbf{k}_i)=\frac{1}{(2\pi/L)^2}\int W_{i\to f}^{\text{ems,abs}}(\mathbf{k}_i,\mathbf{k}_f)\,d\,\mathbf{k}_f$$

Apply this sum explicitly:

$$W_{i\to f}^{\text{ems,abs}}(\mathbf{k}_i)=\frac{1}{(2\pi/L)^2}\frac{2\pi}{L}\frac{(2\pi)^4}{L^4}\frac{L^6}{(2\pi)^6}\frac{2\pi}{\hbar}\frac{e^2}{V}(n_{\text{LO}}+1/2\pm1/2)\frac{E_{LO}}{2}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_s}\right)$$
$$\times\int d\,\mathbf{k}_f\,\delta(E_f(\boldsymbol{k}_f)-E_i(\mathbf{k}_i)\pm E_{LO})\int d\,q_z\frac{1}{(q^2+q_z^2)}|<f(z)|e^{\mp i q_z z}|i(z)>|^2$$

Expand the two-dimensional final wavevector integral into polar coordinates:

$$W_{i\to f}^{\text{ems,abs}}(\mathbf{k}_i)=\frac{1}{(2\pi/L)^2}\frac{2\pi}{L}\frac{(2\pi)^4}{L^4}\frac{L^6}{(2\pi)^6}\frac{2\pi}{\hbar}\frac{e^2}{V}(n_{\text{LO}}+1/2\pm1/2)\frac{E_{LO}}{2}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_s}\right)$$
$$\times\int_0^{2\pi}d\,\theta\int_0^{\infty}d\,k_f\,k_f\,\delta(E_f(0)+\frac{\hbar^2k_f^2}{2m^*}-E_i(0)-\frac{\hbar^2k_i^2}{2m^*}\pm E_{LO})\int d\,q_z\frac{1}{(q^2+q_z^2)}|<f(z)|e^{\mp i q_z z}|i(z)>|^2$$

Rearrange integrals:

$$W_{i\to f}^{\text{ems,abs}}(\mathbf{k}_i)=\frac{1}{(2\pi/L)^2}\frac{2\pi}{L}\frac{(2\pi)^4}{L^4}\frac{L^6}{(2\pi)^6}\frac{2\pi}{\hbar}\frac{e^2}{V}(n_{\text{LO}}+1/2\pm1/2)\frac{E_{LO}}{2}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_s}\right)\int_0^{2\pi}d\,\theta\int d\,q_z|<f(z)|e^{\mp i q_z z}|i(z)>|^2\,I_k(\theta,q_z)$$

where $I_k(\theta,q_z)=\int_0^{\infty}d\,k_f\,k_f\,\delta(E_f(0)+\frac{\hbar^2k_f^2}{2m^*}-E_i(0)-\frac{\hbar^2k_i^2}{2m^*}\pm E_{LO})\frac{1}{(q^2+q_z^2)}$

2.6 Evaluation of the Conservation-of-Energy Dirac Delta

We evaluate the conservation-of-energy integral separately:

$$I_k(\theta,q_z)=\int_0^{\infty}d\,k_f\,k_f\,\delta(E_f(0)+\frac{\hbar^2k_f^2}{2m^*}-E_i(0)-\frac{\hbar^2k_i^2}{2m^*}\pm E_{LO})\frac{1}{(q^2+q_z^2)}$$

$$I_k(\theta,q_z)=\int_0^{\infty}d\,k_f\frac{k_f}{(q^2+q_z^2)}\delta(\left(E_f(0)-E_i(0)\pm E_{LO}-\frac{\hbar^2k_i^2}{2m^*}\right)+\left(\frac{\hbar^2}{2m^*}\right)k_f^2)$$

Consider the identity: $\int d k_f F(k_f)\delta(A+B k_f^2)=\frac{1}{2|B|\sqrt{\frac{-A}{B}}}\left[F(\sqrt{\frac{-A}{B}})+F(-\sqrt{\frac{-A}{B}})\right]$

The interaction is only over positive wavenumbers, so the second term is never integrated over. This makes sense because the negative momentum possibility for this particular energy was already accounted for in the theta integral. We have:

$$\int_0^\infty d k_f F(k_f)\delta(A+B k_f^2)=\frac{1}{2|B|\sqrt{\frac{-A}{B}}}\left[F(\sqrt{\frac{-A}{B}})\right]$$

Now apply this identity to find:

$$I_k(\theta,q_z)=\frac{1}{2\left(\frac{\hbar^2}{2m^*}\right)k_f}\left[\frac{k_f}{(q^2+q_z^2)}\right] \quad \text{where} \quad \boxed{k_f^2=k_i^2+\frac{2m^*}{\hbar^2}\left(E_i(0)-E_f(0)\mp E_{LO}\right)}$$

Simplify the constants:

$$I_k(\theta,q_z)=\frac{1}{2}\left(\frac{2m^*}{\hbar^2}\right)\left[\frac{1}{q^2+q_z^2}\right]$$

Plug this integral's value back into the scattering rate equation:

$$W_{i\to f}^{\text{ems,abs}}(\mathbf{k}_i)=\frac{1}{(2\pi/L)^2}\frac{2\pi}{L}\frac{(2\pi)^4}{L^4}\frac{L^6}{(2\pi)^6}\frac{2\pi}{\hbar}\frac{e^2}{V}(n_{\text{LO}}+1/2\pm1/2)\frac{E_{LO}}{2}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_s}\right)\int_0^{2\pi}d\theta\int d q_z|<f(z)|e^{\mp i q_z z}|i(z)>|^2\frac{1}{2}\left(\frac{2m^*}{\hbar^2}\right)\left[\frac{1}{q^2+q_z^2}\right]$$

Now separate out the integral over q_z for further evaluation:

$$W_{i\to f}^{\text{ems,abs}}(\mathbf{k}_i)=\frac{1}{2}\left(\frac{2m^*}{\hbar^2}\right)\frac{1}{(2\pi/L)^2}\frac{2\pi}{L}\frac{(2\pi)^4}{L^4}\frac{L^6}{(2\pi)^6}\frac{2\pi}{\hbar}\frac{e^2}{V}(n_{\text{LO}}+1/2\pm1/2)\frac{E_{LO}}{2}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_s}\right)\int_0^{2\pi}d\theta\, I_{q_z}(\theta)$$

where $I_{q_z}(\theta)=\int d\,q_z |<f(z)|\,e^{\mp i q_z z}|i(z)>|^2 \left[\frac{1}{q^2+q_z^2}\right]$

2.7 Evaluation of the z-Dimension State Vectors
We now solve this inner integral. This involves expanding the square of the matrix element into the element times its conjugate, as well as projecting the state vectors and operator into coordinate space:

$$I_{q_z}(\theta)=\int d\,q_z <i(z)|e^{\pm i q_z z}|\,f(z)><f(z')|e^{\mp i q_z z'}|i(z')>\left[\frac{1}{q^2+q_z^2}\right]$$

To project the operators and state vectors into coordinate space, we use identities such as $\mathrm{I}=\left[\int d\,z|z><z|\right]$:

$$I_{q_z}(\theta)=\int d\,q_z <i(z)|\left[\int d\,z|z><z|\right]e^{\pm i q_z z}\left[\int d\,z''|z''><z''|\right]|\,f(z)><f(z')|\left[\int d\,z'|z'><z'|\right]e^{\mp i q_z z'}\left[\int d\,z'''|z'''><z'''|\right]|i(z')>$$
$$\times\left[\frac{1}{q^2+q_z^2}\right]$$

Collect out to the front all of the integral symbols:

$$I_{q_z}(\theta)=\int d\,q_z \int d\,z \int d\,z'' \int d\,z' \int d\,z''' <i(z)|z><z|e^{\pm i q_z z}|z''><z''|\,f(z)><f(z')|z'><z'|e^{\mp i q_z z'}|z'''><z'''|i(z')>$$
$$\times\left[\frac{1}{q^2+q_z^2}\right]$$

Recognize the *z*-dimension electron state vectors projected into coordinate space as just the wavefunctions already found using Schrödinger's equation:

$$I_{q_z}(\theta)=\int d\,q_z \int d\,z \int d\,z'' \int d\,z' \int d\,z''' \psi_i(z)\psi_f(z'')\psi_f(z')\psi_i(z''')<z|e^{\pm i q_z z}|z''><z'|e^{\mp i q_z z'}|z'''>\left[\frac{1}{q^2+q_z^2}\right]$$

Evaluate the exponential operators:

$$I_{q_z}(\theta)=\int d q_z \int d z \int d z'' \int d z' \int d z''' \psi_i(z)\psi_f(z'')\psi_f(z')\psi_i(z''') e^{\pm i q_z z}\delta(z-z'') e^{\mp i q_z z'}\delta(z'-z''')\left[\frac{1}{q^2+q_z^2}\right]$$

Apply the Dirac deltas:

$$I_{q_z}(\theta)=\int d q_z \int d z \int d z' \psi_i(z)\psi_f(z)\psi_f(z')\psi_i(z') e^{\pm i q_z (z-z')}\left[\frac{1}{q^2+q_z^2}\right]$$

Move in the integral over q_z

$$I_{q_z}(\theta)=\int d z \int d z' \psi_i(z)\psi_f(z)\psi_f(z')\psi_i(z')\int d q_z e^{\pm i q_z (z-z')}\left[\frac{1}{q^2+q_z^2}\right]$$

Isolate the integral over q_z for evaluation:

$$I_{q_z}(\theta)=\int d z \int d z' \psi_i(z)\psi_f(z)\psi_f(z')\psi_i(z') I_2(\theta) \quad \text{where} \quad I_2(\theta)=\int d q_z e^{\pm i q_z (z-z')}\left[\frac{1}{q^2+q_z^2}\right]$$

2.8 Evaluation of the q_z Integral

The q_z integral spans all possible phonon states, limited by the crystal lattice parameter a:

$$I_2(\theta)=\int_{-2\pi/a}^{2\pi/a} d q_z e^{\pm i q_z (z-z')}\left[\frac{1}{q^2+q_z^2}\right]$$

Expand out the exponential using Euler's formula:

$$I_2(\theta)=\int_{-2\pi/a}^{2\pi/a} d q_z \frac{\cos(q_z(z-z'))}{q^2+q_z^2} \pm i \int_{-2\pi/a}^{2\pi/a} d q_z \frac{\sin(q_z(z-z'))}{q^2+q_z^2}$$

The last integral is over an odd function and thus evaluates to zero, leaving:

$$I_2(\theta)=\int_{-2\pi/a}^{2\pi/a} d\,q_z \frac{\cos(q_z(z-z'))}{q^2+q_z^2}$$

Looking up this integral in integral tables or using integration software reveals that the analytic solution involves the Cosine and Sine integrals:

$$I_2(\theta)=\frac{1}{2q} i\cosh(-q(z-z'))\left[Ci((-q_z-iq)(z-z'))-Ci((-q_z+iq)(z-z'))\right]_{-2\pi/a}^{2\pi/a}$$
$$-\frac{1}{2q}\sinh(-q(z-z'))\left[Si((-q_z-iq)(z-z'))+Si((-q_z+iq)(z-z'))\right]_{-2\pi/a}^{2\pi/a}$$

where $Ci(z)=-\int_z^{\infty}\cos(t)/t\,dt$ and $Si(z)=\int_0^z \sin(t)/t\,dt$

Expand out each term in brackets into real and imaginary parts, because we can make use of some identities:

$$I_2(\theta)=\frac{1}{2q} i\cosh(-q(z-z'))$$
$$\times\left[\Re[Ci((-q_z-iq)(z-z'))]+i\,\Im[Ci((-q_z-iq)(z-z'))]-\Re[Ci((-q_z+iq)(z-z'))]-i\,\Im[Ci((-q_z+iq)(z-z'))]\right]_{-2\pi/a}^{2\pi/a}+$$
$$-\frac{1}{2q}\sinh(-q(z-z'))$$
$$\times\left[\Re[Si((-q_z-iq)(z-z'))]+i\,\Im[Si((-q_z-iq)(z-z'))]+\Re[Si((-q_z+iq)(z-z'))]+i\,\Im[Si((-q_z+iq)(z-z'))]\right]_{-2\pi/a}^{2\pi/a}$$

Now use the identities: $\Re[Ci(x+iy)]=\Re[Ci(x-iy)]=\Re[Ci(-x+iy)]=\Re[Ci(-x-iy)]$ and $\Im[Ci(x+iy)]=-\Im[Ci(x-iy)]$

and $\Re[Si(x+iy)]=\Re[Si(x-iy)]=-\Re[Si(-x+iy)]=-\Re[Si(-x-iy)]$

and $\Im[Si(x+iy)]=\Im[Si(-x+iy)]=-\Im[Si(x-iy)]=-\Im[Si(-x-iy)]$

$$I_2(\theta)=\frac{1}{2q} i\cosh(-q(z-z'))\left[2i\,\Im[Ci((-q_z-iq)(z-z'))]\right]_{-2\pi/a}^{2\pi/a}$$
$$-\frac{1}{2A}\sinh(-q(z-z'))\left[2\,\Re[Si((-q_z-iq)(z-z'))]\right]_{-2\pi/a}^{2\pi/a}$$

Evaluate the limits:

$$I_2(\theta)=\frac{1}{2q}i\cosh(-q(z-z'))[2i\Im[Ci((-(2\pi/a)-iq)(z-z'))]-2i\Im[Ci((-(-2\pi/a)-iq)(z-z'))]]$$
$$-\frac{1}{2q}\sinh(-q(z-z'))[2\Re[Si((-(2\pi/a)-iq)(z-z'))]-2\Re[Si((-(-2\pi/a)-iq)(z-z'))]]$$

Let the lattice parameter *a* approach zero as it is very small compared to the QCL structure:

$$I_2(\theta)=\frac{1}{2q}i\cosh(-q(z-z'))[2i\Im[Ci((-\infty-iq)(z-z'))]-2i\Im[Ci((\infty-iq)(z-z'))]]$$
$$-\frac{1}{2q}\sinh(-q(z-z'))[2\Re[Si((-\infty-iq)(z-z'))]-2\Re[Si((\infty-iq)(z-z'))]]$$

We need to break this up into two cases:

If $(z-z')>0$ then we know the limits of the Cosine and Sine integrals at infinity, leading to:

$$I_2(\theta)=\frac{\pi}{q}[\cosh(-q(z-z'))+\sinh(-q(z-z'))]$$

$$I_2(\theta)=\frac{\pi}{q}e^{-q(z-z')}$$

If $(z-z')<0$ then

$$I_2(\theta)=\frac{\pi}{q}[\cosh(-q(z-z'))-\sinh(-q(z-z'))]$$

$$I_2(\theta)=\frac{\pi}{q}e^{q(z-z')}$$

Put the cases back together:

$$\boxed{I_2(\theta)=\frac{\pi}{q}e^{-q|z-z'|}}$$

Substituting the solution to this inner integral back into the outer integrals:

$$I_{q_z}(\theta)=\int dz\int dz'\psi_i(z)\psi_f(z)\psi_f(z')\psi_i(z')I_2(\theta)$$

$$I_{q_z}(\theta)=\int dz\int dz'\psi_i(z)\psi_f(z)\psi_f(z')\psi_i(z')\frac{\pi}{q}e^{-q|z-z'|}$$

2.9 Identifying the Form Factor

Finally, substituting the outer integrals back into the main scattering rate expression, we find:

$$W_{i\to f}^{\text{ems,abs}}(\mathbf{k}_i)=\frac{1}{2}\left(\frac{2m^*}{\hbar^2}\right)\frac{1}{(2\pi/L)^2}\frac{2\pi}{L}\frac{(2\pi)^4}{L^4}\frac{L^6}{(2\pi)^6}\frac{2\pi}{\hbar}\frac{e^2}{V}(n_{\text{LO}}+1/2\pm1/2)\frac{E_{LO}}{2}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_s}\right)\pi\int_0^{2\pi}d\theta\,\frac{1}{q}$$
$$\times\int dz\int dz'\psi_i(z)\psi_f(z)\psi_f(z')\psi_i(z')\,e^{-q|z-z'|}$$

We recognize the inner two integrals as the form factor: $A(q)=\int dz\int dz'\psi_i(z)\psi_f(z)\psi_f(z')\psi_i(z')e^{-q|z-z'|}$ so that

$$W_{i\to f}^{\text{ems,abs}}(\mathbf{k}_i)=\frac{1}{2}\left(\frac{2m^*}{\hbar^2}\right)\frac{1}{(2\pi/L)^2}\frac{2\pi}{L}\frac{(2\pi)^4}{L^4}\frac{L^6}{(2\pi)^6}\frac{2\pi}{\hbar}\frac{e^2}{V}(n_{\text{LO}}+1/2\pm1/2)\frac{E_{LO}}{2}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_s}\right)\pi\int_0^{2\pi}\frac{A(q)}{q}d\theta$$

The form factor $A(q)$ is the same one that appears in electron-electron scattering calculations. To avoid recalculating the same parameters, the form factors are calculated in advance, before the electron-electron scattering or phonon scattering calculations. The form factor depends only on the wavefunctions and the transverse interaction wavenumber q. We can significantly improve the code's runtime by precalculating the form factor outside of the other integrals to form a look-up table in q. When the phonon scattering integrals are calculated and specific form factor values are needed for certain q values, they are interpolated from the look-up table.

After simplifying the constants, our final expression is:

$$W_{i\to f}^{\text{ems,abs}}(\mathbf{k}_i)=\frac{m^*e^2E_{LO}}{8\pi\hbar^3}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_s}\right)(n_{\text{LO}}+1/2\pm1/2)\int_0^{2\pi}\frac{A(q)}{q}d\theta \quad\text{where}\quad A(q)=\int dz\int dz'\psi_i(z)\psi_f(z)\psi_f(z')\psi_i(z')e^{-q|z-z'|}\ ,$$

$$q^2 = k_i^2 + k_f^2 - 2 k_i k_f \cos(\theta) \quad , \quad k_f^2 = k_i^2 + \frac{2 m^*}{\hbar^2}\left(E_i(0) - E_f(0) \mp E_{LO}\right)$$

2.10 Average over All Initial Wavevectors

Now average over all initial wave vectors:

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

The constants cancel out

$$W_{i,j\to f,g} = \frac{\int dk_{i,x} \int dk_{i,y} W_{i,j\to f,g}(\mathbf{k}_i) f_i(\mathbf{k}_i)}{\int dk_{i,x} \int dk_{i,y} f_i(\mathbf{k}_i)}$$

Switch to polar coordinates:

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

All of the functions are independent of θ_{k_i}, so its integral is evaluated to 2π on the top and bottom and they cancel out

$$W_{i,j\to f,g} = \frac{\int dk_i k_i W_{i,j\to f,g}(k_i) f_i(k_i)}{\int dk_i k_i f_i(k_i)}$$

3.0 Final Expression

Apply the averaging to get the final expression:

$$W_{i,j\to f,g}^{\text{ems,abs}} = \frac{m^* e^2 E_{LO}}{8\pi\hbar^3}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_s}\right)(n_{\text{LO}}+1/2\pm 1/2)\frac{1}{\int dk_i k_i f_i(k_i)}\int dk_i k_i f_i(k_i)\int_0^{2\pi} d\theta \frac{A(q)}{q}$$

$$\text{where} \quad A(q)=\int dz \int dz' \psi_i(z)\psi_f(z)\psi_f(z')\psi_i(z')e^{-q|z-z'|} \quad , \quad q^2=k_i^2+k_f^2-2k_i k_f \cos(\theta) \quad , \quad k_f^2=k_i^2+\frac{2m^*}{\hbar^2}\left(E_i(0)-E_f(0)\mp E_{LO}\right)$$

The form factor integrands are defined over a non-uniform grid, so their integrals are done using the non-uniform trapezoidal method. The rest of the integrals are defined on a uniform grid, so they are calculated using Simpson's rule or the Bode (Boole) rule. The form factor integrals are performed over the full three periods of the QCL structure. The wavenumber integral runs from zero to the maximum wavenumber possible. The maximum wavenumber is the one corresponding to the well height in energy space, because wavenumbers greater than this are not confined in the quantum well structures and do not contribute to the process.

The LO phonon energy E_{LO} is taken to be a constant of the material. The phonon occupation number n_{LO} is taken to be its bulk material value, which is given by Bose-Einstein statistics to be:

$$n_{LO}=\frac{1}{e^{E_{LO}/kT}-1}$$