1.0 Introduction

We have derived the scattering of one electron with one other electron. While the problem really involves a multi-electron interaction, the multi-electron Hamiltonian is too complicated to be solved. Instead, we can take into account the effect of the multi-electron interaction in an approximate way. We assume that only one electron is close enough to the original electron to actually scatter off it in a fully quantum way, and thus the previous treatment still applies. We then assume all the other electrons are not negligible, but are far enough way that they behave semi-classically as a sea of electrons that exert a net influence. The other electrons tend to block and weaken the interaction between the two close electrons and therefore their effect is described as screening. Classically, this macroscopic screening effect in matter is handled by replacing the permittivity of free space with a permittivity value that is representative of the material. We have in effect already incorporated some level of screening in our treatment by using the material's permittivity. The problem is that that permittivity is for a bulk volume of material. In QCL's we have nano-scale layers of differing materials leading to quantum wells and quantized states for the electrons which do the screening. So, to incorporate a more exact form of screening, we should replace the bulk permittivity in the above equations with a new permittivity that depends on the quantized states. Because it depends on the quantized states, this new permittivity must appear within all of the integrals in the electron-electron scattering equation. Once we have found the screening constant, we simply divide it into the innermost integrand of the e-e scattering equation.

2.0 Two-dimensional Electron Gas Properties

Let us investigate a two-dimensional electron gas. Electrons in quantum wells, such as in a QCL, are trapped in the z dimension and pseudo-free in the x and y dimensions. They act as a two-dimensional gas of electrons.

The density of electron states for a two-dimensional gas, per unit area is:

$$g(k) = \frac{2 g_v}{(2\pi)^2}$$

where g_v is the valley degeneracy factor of the material ($g_v = 1$ for GaAs), and the factor two in the numerator accounts for both electron spin states.

We want a density of electron states in terms of energy and not wave number. By "density of electron states in terms of energy", we mean the total number of electron states in a unit swath of energy, so that:

$$g(E) = \frac{d N(E)}{d E}$$

The number of electron state at a given energy $N(E)$ is just the area in k-space A_k times the density of electron states $g(k)$:

$$g(E) = \frac{d}{d E}\left[A_k g(k) \right]$$

$$g(E) = \frac{d}{d E}\left[(\pi k^2)\left(\frac{2 g_v}{(2\pi)^2} \right) \right]$$

In order to do the derivative, we must switch k to E using the standard relation: $E = \hbar^2 k^2 / 2 m^*$

$$g(E) = \frac{d}{d E}\left[(\pi\, 2 m^* \frac{E}{\hbar^2})\left(\frac{2 g_v}{(2\pi)^2} \right) \right]$$

$$\boxed{g(E) = \frac{g_v m^*}{\pi \hbar^2}}$$ *electron states per unit energy per unit area in a two-dimensional electron gas*

This is a surprisingly simple result. We must remember that $g(E)$ drops to zero outside the subband (if $E < E_n$).

2.1 Fermi Energy of a Two-dimensional Electron Gas
The total 2D electron density in a subband at absolute zero temperature is just the total number of electron states from the zero energy of the subband to the Fermi energy:

$$N = \int_0^{E_F} g(E)\, d E$$

$$N = \frac{g_v m^*}{\pi \hbar^2} \int\limits_0^{E_F} dE$$

$$N = \frac{g_v m^*}{\pi \hbar^2} E_F \quad \text{where the Fermi energy is measured relative to the subband minimum.}$$

$$N = \frac{g_v}{\pi} \frac{k_F^2}{2}$$

Solve for the Fermi wavenumber

$$\boxed{k_F = \sqrt{\frac{2\pi N_i}{g_v}}}$$

Here k_F is the two-dimensional Fermi wavevector magnitude of the subband i relative to the subband minimum, defined at $T=0$. Also, N_i is the electron density of the subband i, and g_v is the degeneracy of the material where $g_v = 1$ for GaAs. This entire treatment has been two-dimensional, so it should be obvious that N_i is the two-dimensional electron density. This expression is only valid at zero temperature. We need the general expression which is valid at all temperatures.

The total 2D electron density in a subband at any temperature is:

$$N = \int\limits_0^\infty g(E) f(E) dE$$

$$N = \frac{g_v m^*}{\pi \hbar^2} \int\limits_0^\infty f(E) dE$$

$$N = \frac{g_v m^*}{\pi \hbar^2} \int\limits_0^\infty \frac{1}{1 + e^{(E - E_F)/k_B T}} dE$$

$$N = \frac{g_v m^*}{\pi \hbar^2} \left[E_F + k_B T \ln\left(1 + e^{-E_F/k_B T}\right) \right]$$

$$N = \frac{g_v m^*}{\pi \hbar^2} k_B T \ln\left(1 + e^{\frac{E_F}{k_B T}}\right)$$

Solve for the Fermi energy:

$$\boxed{E_F = k_B T \ln\left[\exp\left(\frac{\pi \hbar^2 N}{k_B T g_v m^*}\right) - 1\right]}$$

Now let's try to derive the general expression for the permittivity of a solid using a self-consistent field (SCF) approach, which has been shown to be equivalent to a random-phase approximation (RPA) approach.

3.0 General Screening Expression

By definition, the relative permittivity connects the polarization field **P** with the total electric field **E** inside a material:

$$\mathbf{P} = \epsilon_0 (\epsilon_r - 1) \mathbf{E}$$

We must remember that in the general realm of electrodynamics, causality means that induced polarization fields at different times and places all add together to a total field at a certain time and place. This means that the solution would be an integral over many time points. Instead let us transform to frequency space and work with just one wave number component **q** of the total solution. Let us show this explicitly:

$$\mathbf{P}(\mathbf{q}, t) = \epsilon_s (\epsilon_r(\omega, \mathbf{q}) - 1) \mathbf{E}(\mathbf{q}, t)$$

Here, ϵ_s is the static permittivity of the material and ϵ_r is a relative permittivity screening constant that represents how the total permittivity deviates from the static value. Solve for the screening constant:

$$\epsilon_r(\omega, \mathbf{q}) = 1 + \frac{\mathbf{P}(\mathbf{q}, t)}{\epsilon_s \mathbf{E}(\mathbf{q}, t)}$$

Express the electric field in terms of the negative gradient of some total potential V, Fourier transform, and plug in:

$$\mathbf{E}(\mathbf{x}, t) = -\nabla V(\mathbf{x}, t)$$

$$\mathbf{E}(\mathbf{q},t)=-i\,\mathbf{q}\,V(\mathbf{q},t)$$

$$\epsilon_r(\omega,\mathbf{q})=1-\frac{\mathbf{P}(\mathbf{q},t)}{\epsilon_s i\,\mathbf{q}\,V(\mathbf{q},t)}$$

The polarization field is created by the induced charge density ρ_{pol}. Let us Fourier transform this and plug it into the permittivity relation:

$$\nabla\cdot\mathbf{P}(\mathbf{x},t)=-\rho_{pol}(\mathbf{x},t)$$

$$i\,\mathbf{q}\cdot\mathbf{P}(\mathbf{q},t)=-\rho_{pol}(\mathbf{q},t)$$

$$\epsilon_r(\omega,\mathbf{q})=1-\frac{\mathbf{P}(\mathbf{q},t)}{\epsilon_s i\,\mathbf{q}\,V(\mathbf{q},t)}$$

$$\epsilon_r(\omega,\mathbf{q})=1+\frac{i\,\mathbf{q}\cdot\mathbf{P}(\mathbf{q},t)}{\epsilon_s q^2 V(\mathbf{q},t)}$$

$$\epsilon_r(\omega,\mathbf{q})=1-\frac{1}{\epsilon_s q^2}\frac{\rho_{pol}(\mathbf{q},t)}{V(\mathbf{q},t)}$$

The classical induced charge density is the sum over the different energy states of the quantum density matrix:

$$\rho_{pol}(\mathbf{q},t)=-\frac{e}{L^3}\sum_{\mathbf{k}}<\mathbf{k}|\rho_1|\mathbf{k}+\mathbf{q}>$$

$$\epsilon_r(\omega,\mathbf{q})=1+\frac{e}{\epsilon_s q^2 L^3}\sum_{\mathbf{k}}\frac{<\mathbf{k}|\rho_1|\mathbf{k}+\mathbf{q}>}{V(\mathbf{q},t)}$$

We want the ratio of the density matrix to the potential in terms of quantum statistical distributions. We turn to the Louisville equation and apply first-order perturbation theory to get it.

Just as the Schrödinger equation describes how a pure quantum state evolves in time, an analog can be derived from it that describes the time evolution of a mixed statistical ensemble of quantum states, known as the density matrix ρ. The analog equation is known as Von Neumann's (or Louisville's) equation:

$$i\hbar\frac{\partial\rho}{\partial t}=[H,\rho]$$

Apply first order perturbation theory. The interaction Hamiltonian H is a sum of the unperturbed Hamiltonian H_0 and the perturbation H_1:

$$H=H_0+H_1$$

Here the unperturbed state is that of the pseudo-free electron inside the solid (according to the effective mass approach):

$$H_0=\frac{P^2}{2m^*}\quad\text{and}\quad H_0|\mathbf{k}>=E_\mathbf{k}|\mathbf{k}>$$

The perturbing interaction is that of the total potential, so that $H_1 = eV$. The factor e is there because the perturbing Hamiltonian is the potential energy of the electron, and we have defined V as the scalar potential.

Similarly, the density matrix operator is expanded into a sum of unperturbed and perturbed contributions:

$$\rho=\rho_0+\rho_1$$

The unperturbed density matrix operator just gives the electron distribution in a solid in equilibrium, namely the Fermi distribution:

$$\rho_0|\mathbf{k}>=f(E_\mathbf{k})|\mathbf{k}>$$

Put these expansions in the Louisville equation:

$$i\hbar\frac{\partial\rho}{\partial t}=[H,\rho]$$

$$i\hbar\frac{\partial\rho}{\partial t}=H\rho-\rho H$$

$$i\hbar\frac{\partial(\rho_0+\rho_1)}{\partial t}=(H_0+H_1)(\rho_0+\rho_1)-(\rho_0+\rho_1)(H_0+H_1)$$

$$i\hbar\frac{\partial\rho_0}{\partial t}-(H_0\rho_0-\rho_0 H_0)+i\hbar\frac{\partial\rho_1}{\partial t}=H_0\rho_1+H_1\rho_0+H_1\rho_1-\rho_0 H_1-\rho_1 H_0-\rho_1 H_1$$

The first three terms on the left are the Louisville equation without any perturbation present and equates to zero. Also, because we are only using first order perturbation theory, all second order terms can be canceled, namely $H_1\rho_1$ and $\rho_1 H_1$

$$i\hbar\frac{\partial\rho_1}{\partial t}=H_0\rho_1+H_1\rho_0-\rho_0 H_1-\rho_1 H_0$$

Apply these operators between states **k** and **k + q**:

$$i\hbar\frac{\partial}{\partial t}<\mathbf{k}|\rho_1|\mathbf{k+q}>=<\mathbf{k}|H_0\rho_1|\mathbf{k+q}>+<\mathbf{k}|H_1\rho_0|\mathbf{k+q}>-<\mathbf{k}|\rho_0 H_1|\mathbf{k+q}>-<\mathbf{k}|\rho_1 H_0|\mathbf{k+q}>$$

Apply the operators as defined above:

$$i\hbar\frac{\partial}{\partial t}<\mathbf{k}|\rho_1|\mathbf{k+q}>=(E_{\mathbf{k}}-E_{\mathbf{k+q}})<\mathbf{k}|\rho_1|\mathbf{k+q}>+(f(E_{\mathbf{k+q}})-f(E_{\mathbf{k}}))e\,V(\mathbf{q},t)$$

Assume the matrix element varies harmonically in time with the fields and do the derivative, then solve for the ratio of matrix element to potential:

$$\frac{<\mathbf{k}|\rho_1|\mathbf{k+q}>}{V(\mathbf{q},t)}=e\frac{f(E_{\mathbf{k+q}})-f(E_{\mathbf{k}})}{E_{\mathbf{k+q}}-E_{\mathbf{k}}-\hbar\omega}$$

This is the ratio we were looking for, so let us plug it back into the permittivity equation:

$$\boxed{\epsilon_r(\omega,\mathbf{q})=1+\frac{e^2}{\epsilon_s q^2 L^3}\sum_{\mathbf{k}}\frac{f(E_{\mathbf{k+q}})-f(E_{\mathbf{k}})}{E_{\mathbf{k+q}}-E_{\mathbf{k}}-\hbar\omega}}$$ *General expression for the relative permittivity in terms of quantum distributions, in SI units*

For a two-dimensional system with a quantized third dimension, and in the static limit, this becomes:

$$\epsilon_r(\mathbf{q}) = 1 + \frac{e^2}{\epsilon_s q L^2} A_{ii \to ii}(q) \sum_{\mathbf{k}} \frac{f(E_{\mathbf{k+q}}) - f(E_{\mathbf{k}})}{E_{\mathbf{k+q}} - E_{\mathbf{k}}}$$

Define a polarizability such that:

$$\epsilon_r(q) = 1 + \frac{e^2}{2\epsilon_s q} \Pi_{ii}(q) A_{ii\,ii}(q) \quad \text{where} \quad \Pi_{ii}(Q) = \frac{2}{L^2} \sum_{\mathbf{k}} \frac{f(E_{\mathbf{k+q}}) - f(E_{\mathbf{k}})}{E_{\mathbf{k+q}} - E_{\mathbf{k}}}$$

In reality, an electron is screened by all the electrons in all subbands, not just its own. We therefore sum over subbands:

$$\epsilon_r(q) = 1 + \frac{e^2}{2\epsilon_s q} \sum_i \Pi_{ii}(q) A_{ii\,ii}(q) \quad \text{where} \quad \Pi_{ii}(Q) = \frac{2}{L^2} \sum_{\mathbf{k}} \frac{f(E_{\mathbf{k+q}}) - f(E_{\mathbf{k}})}{E_{\mathbf{k+q}} - E_{\mathbf{k}}}$$

4.0 Evaluation of the General Expression

Expand out the Fermi distributions and energies into their explicit forms:

$$\Pi_{ii}(q) = \frac{2}{L^2} \sum_{\mathbf{k}} \frac{\dfrac{1}{1+e^{(\frac{\hbar^2|\mathbf{k+q}|^2}{2m^*} - E_F)/k_B T}} - \dfrac{1}{1+e^{(\frac{\hbar^2 k^2}{2m^*} - E_F)/k_B T}}}{\dfrac{\hbar^2|\mathbf{k+q}|^2}{2m^*} - \dfrac{\hbar^2 k^2}{2m^*}}$$

Define the Fermi wave-vector $k_F = \sqrt{2m^* E_F}/\hbar$, being careful to remember that the Fermi energy can go negative relative to the subband minimum, and therefore the Fermi wave-vector can be imaginary. Assume that the crystal is large enough that the set of quantum states for the electron becomes a continuous band of states. The sum therefore becomes an integral:

$$\Pi_{ii}(q) = \frac{4m^*}{\hbar^2(2\pi)^2} \int d\mathbf{k} \left(\frac{1}{q^2 + 2\mathbf{k}\cdot\mathbf{q}} \right) \left[\frac{1}{1+e^{(k^2+q^2+2\mathbf{k}\cdot\mathbf{q}-k_F^2)\hbar^2/2m^* k_B T}} - \frac{1}{1+e^{(k^2-k_F^2)\hbar^2/2m^* k_B T}} \right]$$

$$\Pi_{ii}(q) = \frac{4m^*}{\hbar^2(2\pi)^2} \int_0^\infty dk \int_0^{2\pi} k\, d\theta \left(\frac{1}{q^2 + 2kq\cos(\theta)} \right) \left[\frac{1}{1+e^{(k^2+q^2+2kq\cos\theta-k_F^2)\hbar^2/2m^* k_B T}} - \frac{1}{1+e^{(k^2-k_F^2)\hbar^2/2m^* k_B T}} \right]$$

4.1 Polarizability at Zero Temperature

For the special case of zero temperature, $T=0$, this reduces to:

$$\Pi_{ii}(q,k_f,T=0)=\frac{4m^*}{\hbar^2(2\pi)^2}\int_0^\infty dk\int_0^{2\pi}k\,d\theta\left(\frac{1}{q^2+2kq\cos(\theta)}\right)\left[\theta(k_F^2-k^2-q^2-2kq\cos\theta)-\theta(k_F^2-k^2)\right]$$

$$\Pi_{ii}(q,k_f,T=0)=\frac{4m^*}{\hbar^2(2\pi)^2}\left[\int_0^{2\pi}k\,d\theta\int_0^\infty dk\left(\frac{1}{q^2+2kq\cos(\theta)}\right)\theta(k_F^2-k^2-q^2-2kq\cos\theta)+\pi\left[\sqrt{(1/2)^2-(k_F/q)^2}-1/2\right]\right]$$

$$\boxed{\Pi_{ii}(q,k_f,T=0)=\frac{m^*}{\hbar^2\pi}\left[1-\theta(q-2k_F)\sqrt{1-(2k_F/q)^2}\right]}$$

4.2 Polarizability at Any Temperature

To solve for any temperature, we want to express the Fermi functions differently.
Start with the definition of the hyperbolic tangent:

$$\tanh x=\frac{e^x-e^{-x}}{e^x+e^{-x}}$$

Solve partially for the exponential to find:

$$\frac{1}{1+e^x}=\frac{1}{2}\left(1-\tanh\left(\frac{x}{2}\right)\right)$$

Looking up in an integral table, we find that the the hyperbolic tangent is the solution to the integral:

$$\left[\tanh x'\right]_a^b=\int_a^b\frac{dx'}{\cosh^2 x'}$$

Take the upper limit to be infinity and the lower limit as x.

$$\left[\tanh x'\right]_x^\infty = \int_x^\infty \frac{d\,x'}{\cosh^2 x'}$$

$$1 - \tanh x = \int_x^\infty \frac{d\,x'}{\cosh^2 x'}$$

so that

$$\frac{1}{1+e^x} = \frac{1}{2} \int_{x/2}^\infty \frac{d\,x'}{\cosh^2 x'}$$

We can make the integral span all positive numbers if we force the lower contribution to be zero using the Heaviside step function:

$\theta(x) = 1$ if $x > 0$, $\theta(x) = 0$ if $x < 0$, so that

$$\frac{1}{1+e^x} = \frac{1}{2} \int_0^\infty \frac{\theta(x'-x/2)d\,x'}{\cosh^2 x'}$$

Substitute $x = \dfrac{E_k - E_F}{k_B T}$

$$\frac{1}{1+e^{\frac{E_k-E_F}{k_B T}}} = \frac{1}{2} \int_0^\infty \frac{\theta\left(x' - \dfrac{E_k - E_F}{2k_B T}\right)d\,x'}{\cosh^2 x'}$$

Substitute $\quad x' = \dfrac{E - E_F}{2\,k_B T} \quad$ and $\quad d\,x' = \dfrac{d\,E}{2\,k_B T}$

$$\frac{1}{1+e^{\frac{E_k-E_F}{k_BT}}}=\frac{1}{2}\int_0^\infty \frac{\theta\left(\frac{E-E_F}{2k_BT}-\frac{E_k-E_F}{2k_BT}\right)\frac{dE}{2k_BT}}{\cosh^2\left(\frac{E-E_F}{2k_BT}\right)}$$

$$\boxed{\frac{1}{1+e^{\frac{E_k-E_F}{k_BT}}}=\int_0^\infty \frac{\theta\left(E-E_k\right)dE}{4k_BT\cosh^2\left(\frac{E-E_F}{2k_BT}\right)}}$$

Expand using $E_k=\dfrac{\hbar^2k^2}{2m^*}$, $E_F=\dfrac{\hbar^2k_F^2}{2m^*}$, $E=\dfrac{\hbar^2k'^2}{2m^*}$, and $dE=\dfrac{\hbar^2k'dk'}{m^*}$

$$\boxed{\frac{1}{1+e^{\frac{\hbar^2(k^2-k_F^2)}{2m^*k_BT}}}=\frac{\hbar^2}{m^*}\int_0^\infty \frac{\theta\left(k'^2-k^2\right)k'dk'}{4k_BT\cosh^2\left(\frac{\hbar^2\left(k'^2-k_F^2\right)}{4m^*k_BT}\right)}}$$

This is a general mathematical identity. We now apply this identity to the two exponential terms in the general polarizability expression:

$$\Pi_{ii}(q)=\frac{4}{(2\pi)^2}\int_0^\infty dk\int_0^{2\pi}kd\theta\left(\frac{1}{q^2+2kq\cos(\theta)}\right)\int_0^\infty \left[\theta\left(k'^2-k^2-q^2-2kq\cos\theta\right)-\theta\left(k'^2-k^2\right)\right]\frac{k'dk'}{4k_BT\cosh^2\left(\frac{\hbar^2\left(k'^2-k_F^2\right)}{4m^*k_BT}\right)}$$

$$\Pi_{ii}(q)=\frac{4}{(2\pi)^2}\int_0^\infty dk'\frac{k'}{4k_BT\cosh^2\left(\frac{\hbar^2\left(k'^2-k_F^2\right)}{4m^*k_BT}\right)}\left[\int_0^\infty dk\int_0^{2\pi}kd\theta\left(\frac{1}{q^2+2kq\cos(\theta)}\right)\left(\theta\left(k'^2-k^2-q^2-2kq\cos\theta\right)-\theta\left(k'^2-k^2\right)\right)\right]$$

Comparing the factor in brackets to the $T=0$ expression, we find they match except for one important difference. This factor is a function of the integration variable k'.

$$\Pi_{ii}(q) = \frac{\hbar^2}{m^*} \int_0^\infty dk' \frac{k' \Pi_{ii}(q, k', T=0)}{4 k_B T \cosh^2\left(\frac{\hbar^2(k'^2 - k_F^2)}{4 m^* k_B T}\right)}$$

5.0 Final Form of Screening

In summary, there is one screening constant used for all subbands and it is found using:

$$\epsilon_r(q) = 1 + \sum_i \frac{e^2}{2 \epsilon_s q} \Pi_{ii}(q) A_{iiii}(q)$$ where $$\Pi_{ii}(q) = \int_0^\infty dE \frac{\Pi_{ii}(q, E, T=0)}{4 k_B T \cosh^2\left(\frac{E - E_F}{2 k_B T}\right)}$$ and

$$\Pi_{ii}(q, k', T=0) = \frac{m^*}{\hbar^2 \pi}\left[1 - \theta(q - 2k')\sqrt{1 - 4 k'^2/q^2}\right]$$ and $$E = \frac{\hbar^2 k'^2}{2 m'}$$

The integral is done numerically over a uniform grid using standard methods such as Simpson's rule or the Bode (Boole) rule.

6.0 Comparison with Literature

This derivation is consistent with the one first put forth by Maldague[1].

Harrison[2] makes the assumption that $E = E_F$ in the zero-temperature polarizability and therefore takes it out of the integral, so that the integral can be evaluated analytically. Harrison finds:

$$\Pi_{ii}(q) = \frac{m^*}{2 \hbar^2 \pi}\left(1 + \tanh(E_F/2 k_B T)\right)\left[1 - \theta(q - 2 k_f)\sqrt{1 - 4 k_f^2/q^2}\right]$$

This form was found to lead to significant errors.

[1] Maldague, P., "Many-body corrections to the polarizability of the two-dimensional electron gas," Surface Science 73 (1978).

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