# Chapt9Exercise3.m

## Lorentzian Line Broadening in Semiconductor Lasers

### Homogeneous Broadening of Optical Gain and Spontaneous Emission

Semiconductor Physics Documentation

**Abstract**

This document provides a comprehensive analysis of `Chapt9Exercise3.m`, which calculates the optical gain and spontaneous emission spectra with and without Lorentzian (homogeneous) broadening. The code demonstrates how finite carrier lifetimes and scattering processes broaden the idealized delta-function transitions into Lorentzian lineshapes, significantly affecting the gain spectrum near the band edge.

## Contents

# 1 Theoretical Foundation

## 1.1 Fundamental Axioms of Line Broadening

**Axiom 1** (Heisenberg Uncertainty Principle)**.** *The energy-time uncertainty relation imposes a fundamental limit on spectral linewidth:*

$$\Delta E \cdot \tau \geq \frac{\hbar}{2} \tag{1}$$

*where $\tau$ is the characteristic lifetime of the excited state. Any finite lifetime leads to energy broadening.*

**Axiom 2** (Fermi's Golden Rule with Broadening)**.** *The transition rate between states includes a lineshape function $L(E)$:*

$$W_{fi} = \frac{2\pi}{\hbar}|M_{fi}|^2 L(E_f - E_i - \hbar\omega) \tag{2}$$

*where $L(E)$ replaces the ideal delta function $\delta(E)$.*

**Axiom 3** (Causality and Kramers-Kronig Relations)**.** *Physical response functions must satisfy causality, leading to:*

$$\chi'(\omega) = \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} \frac{\chi''(\omega')}{\omega' - \omega} d\omega' \tag{3}$$

$$\chi''(\omega) = -\frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} \frac{\chi'(\omega')}{\omega' - \omega} d\omega' \tag{4}$$

*The Lorentzian lineshape naturally satisfies these relations.*

## 1.2 Lorentzian Line Shape Theory

**Definition 1** (Lorentzian Distribution)**.** *The normalized Lorentzian lineshape is:*

$$L(E - E_0) = \frac{1}{\pi}\frac{\gamma/2}{(E - E_0)^2 + (\gamma/2)^2} \tag{5}$$

*where:*

- *$E_0$ is the center energy*
- *$\gamma$ is the full-width at half-maximum (FWHM)*
- *Normalization: $\int_{-\infty}^{\infty} L(E - E_0)\, dE = 1$*

**Theorem 1** (Lorentzian from Exponential Decay)**.** *For a state with exponential decay $\psi(t) \propto e^{-t/2\tau}e^{-iE_0 t/\hbar}$, the Fourier transform yields the Lorentzian:*

$$|\tilde{\psi}(E)|^2 \propto \frac{1}{(E - E_0)^2 + (\hbar/2\tau)^2} \tag{6}$$

*Thus $\gamma = \hbar/\tau$ relates the broadening to the lifetime.*

*Proof.* The Fourier transform of the damped oscillator is:

$$\tilde{\psi}(E) = \int_0^{\infty} e^{-t/2\tau}e^{-iE_0 t/\hbar}e^{iEt/\hbar}dt \tag{7}$$

$$= \int_0^{\infty} e^{-t/2\tau}e^{i(E-E_0)t/\hbar}dt \tag{8}$$

$$= \frac{1}{1/2\tau - i(E - E_0)/\hbar} \tag{9}$$

Taking the modulus squared:

$$|\tilde{\psi}(E)|^2 = \frac{1}{(1/2\tau)^2 + (E - E_0)^2/\hbar^2} \propto \frac{1}{(E - E_0)^2 + (\gamma/2)^2} \tag{10}$$

□

## 1.3 Broadened Optical Gain

**Definition 2** (Unbroadened Gain Spectrum). *Without broadening, the optical gain is:*

$$g_0(\hbar\omega) = C\sqrt{\hbar\omega - E_g}(f_e + f_h - 1)\Theta(\hbar\omega - E_g) \tag{11}$$

*where $\Theta$ is the Heaviside step function (gain is zero below bandgap).*

**Theorem 2** (Broadened Gain by Convolution). *The broadened gain spectrum is obtained by convolving with the Lorentzian:*

$$g(\hbar\omega) = \int_0^\infty g_0(E)L(\hbar\omega - E_g - E)\,dE \tag{12}$$

*Explicitly:*

$$g(\hbar\omega) = \int_0^\infty C\sqrt{E}(f_e(E) + f_h(E) - 1) \cdot \frac{\gamma/2\pi}{(\hbar\omega - E_g - E)^2 + (\gamma/2)^2}\,dE \tag{13}$$

**Corollary 1** (Sub-Bandgap Absorption). *Lorentzian broadening allows non-zero gain/absorption below the nominal bandgap ($\hbar\omega < E_g$), as the Lorentzian tail extends into this region.*

## 1.4 Broadened Spontaneous Emission

**Theorem 3** (Broadened Spontaneous Emission Rate). *The broadened spontaneous emission spectrum is:*

$$r_{sp}(\hbar\omega) = \int_0^\infty C\sqrt{E} \cdot f_e(E_e) \cdot f_h(E_h) \cdot \frac{\gamma/2\pi}{(\hbar\omega - E_g - E)^2 + (\gamma/2)^2}\,dE \tag{14}$$

## 1.5 Gain-Spontaneous Emission Relationship

**Theorem 4** (Fundamental Relationship). *The gain and spontaneous emission are related by:*

$$g(\hbar\omega) = r_{sp}(\hbar\omega) \cdot \left(1 - e^{(\hbar\omega - \Delta\mu)/k_BT}\right) \tag{15}$$

*where $\Delta\mu = \mu_e + \mu_h$ is the quasi-Fermi level separation.*

*Proof.* Starting from the Fermi factors:

$$\begin{aligned} f_e + f_h - 1 &= f_e(1 - f_h) - (1 - f_e)f_h + f_ef_h \qquad (16)\\ &= f_ef_h\left(\frac{1 - f_h}{f_h} - \frac{1 - f_e}{f_e} + 1\right) \qquad (17)\end{aligned}$$

Using $\frac{1-f}{f} = e^{(E-\mu)/k_BT}$:

$$f_e + f_h - 1 = f_ef_h\left(1 - e^{(E_e - \mu_e + E_h - \mu_h)/k_BT}\right) \tag{18}$$

Since $E_e + E_h = \hbar\omega - E_g$ and energy conservation:

$$f_e + f_h - 1 = f_ef_h\left(1 - e^{(\hbar\omega - E_g - \Delta\mu)/k_BT}\right) \tag{19}$$

□

## 2 Numerical Methods: Convolution Integration

### 2.1 Riemann Sum Approximation

The convolution integral is computed numerically using a Riemann sum:

$$\int_0^{E_{max}} f(E)\,dE \approx \sum_{k=1}^{N} f(E_k)\cdot \Delta E \tag{20}$$

For the broadened spontaneous emission:

$$r_{sp}^{brd}(\hbar\omega_j) = C\sum_{k=1}^{1400} \sqrt{E_k}\cdot f_e(E_k^e)\cdot f_h(E_k^h)\cdot L(\hbar\omega_j - E_g - E_k)\cdot \Delta E \tag{21}$$

### 2.2 Discretization Parameters

- Energy step: $\Delta E = 0.001$ eV $= 1$ meV
- Integration range: $E \in [0, 1.4]$ eV (1400 points)
- Photon energy range: $E_g - 0.1$ to $E_g + 0.3$ eV
- Critical requirement: $\Delta E \ll \gamma$ for accurate Lorentzian sampling

### 2.3 Lorentzian Sampling Criterion

**Theorem 5** (Sampling Requirement)**.** *To accurately represent the Lorentzian, the energy step must satisfy:*

$$\Delta E \leq \frac{\gamma}{5} \tag{22}$$

*With $\gamma = 0.015$ eV, we need $\Delta E \leq 3$ meV. The code uses $\Delta E = 1$ meV, satisfying this criterion.*

## 3 Line-by-Line Code Analysis

### 3.1 Physical Constants and Material Parameters

```
clear
clf
    echarge=1.6021764e-19;
    hbar=1.05457159e-34;
    c = 2.99792458e8;
    kB=8.61734e-5;
    epsilon0=8.8541878e-12;
```

$$e = 1.602\times 10^{-19}\,\mathrm{C},\quad \hbar,\quad c,\quad k_B = 8.617\times 10^{-5}\,\mathrm{eV/K} \tag{23}$$

*Standard physical constants. Note $k_B$ is in eV/K for direct energy calculations.*

```
    m0=9.109382e-31;
    me=0.07*m0;
    mhh=0.5*m0;
    mr=1/(1/me+1/mhh);
    rerr=1e-3;
```

$$m_e^* = 0.07m_0,\quad m_{hh}^* = 0.5m_0,\quad m_r = \frac{m_e^* m_{hh}^*}{m_e^* + m_{hh}^*} \tag{24}$$

*GaAs effective masses. The reduced mass $m_r$ determines joint density of states.*

```
nr=3.3;
Eg=1.4
```

$$n_r = 3.3, \quad E_g = 1.4\,\text{eV} \tag{25}$$

*GaAs refractive index and bandgap energy.*

### 3.2 Operating Conditions

```
    n=2.0e18;
ncarrier=n*1e6;
```

$$n = 2 \times 10^{18}\,\text{cm}^{-3} = 2 \times 10^{24}\,\text{m}^{-3} \tag{26}$$

*Carrier density chosen to produce significant optical gain.*

```
kelvin=300.0;
kBT=kB*kelvin;
beta=1/kBT;
gamma=0.015
```

$$T = 300\,\text{K}, \quad k_B T = 0.0259\,\text{eV}, \quad \beta = 38.7\,\text{eV}^{-1}, \quad \gamma = 15\,\text{meV} \tag{27}$$

*Room temperature operation. The broadening parameter $\gamma = 15$ meV is typical for GaAs lasers.*

### 3.3 Gain Constant and Chemical Potentials

```
const=2.64e4;
```

$$C = 2.64 \times 10^4\,\text{cm}^{-1}\text{eV}^{-1/2} \tag{28}$$

*Empirical constant calibrated to give $g \approx 330$ $cm^{-1}$ at $n = 2 \times 10^{18}$ $cm^{-3}$.*

```
muhh=mu(mhh,ncarrier,kelvin,rerr);
mue =mu(me, ncarrier,kelvin,rerr);
deltamu=mue+muhh
```

$$\mu_h = \mu(m_{hh}^*, n, T), \quad \mu_e = \mu(m_e^*, n, T), \quad \Delta\mu = \mu_e + \mu_h \tag{29}$$

*Chemical potentials computed via Newton-Raphson iteration on Fermi integrals.*

### 3.4 Energy Grid Setup

```
deltae=0.001;
for m=1:400
   Energy(m)=0;
   rspon(m)=0;
   gain1(m)=0;
end
```

$$\Delta E = 1\,\text{meV}, \quad \text{Arrays initialized to 400 points} \tag{30}$$

*Energy step and array preallocation.*

### 3.5 Unbroadened Calculation

```
for j=100:1:400
    Energy(j)=(j*deltae)-0.1;
    Ehh=(Energy(j))/(1+mhh/me);
    Ee=(Energy(j))/(1+me/mhh);
```

$$E = j \cdot \Delta E - 0.1, \quad E_h = \frac{E}{1 + m_{hh}/m_e}, \quad E_e = \frac{E}{1 + m_e/m_{hh}} \tag{31}$$

*Energy partitioning: lighter carriers get more kinetic energy. Loop starts at $j = 100$ to give $E = 0$ (bandgap).*

```
    fhh=fermi(beta,Ehh,muhh);
    fe=fermi(beta,Ee,mue);
    rspon(j)=(const)*(Energy(j)^0.5)*(fe*fhh);
    gain1(j)=rspon(j)*(1-exp((Energy(j)-deltamu)*beta));
end
```

$$f_h = \frac{1}{1 + e^{\beta(E_h - \mu_h)}}, \quad f_e = \frac{1}{1 + e^{\beta(E_e - \mu_e)}} \tag{32}$$

$$r_{sp}^{(0)}(E) = C\sqrt{E} \cdot f_e \cdot f_h \tag{33}$$

$$g^{(0)}(E) = r_{sp}^{(0)}(E) \cdot \left(1 - e^{(E - \Delta\mu)/k_B T}\right) \tag{34}$$

*Unbroadened spontaneous emission and gain using the fundamental relationship.*

### 3.6 Broadened Calculation with Lorentzian Convolution

```
for j=1:400
    Ephoton(j)=(Eg-0.1)+(j*deltae);
    rspint=0;
    E=0;
```

$$\hbar\omega_j = E_g - 0.1 + j \cdot \Delta E \tag{35}$$

*Photon energy array, starting 100 meV below bandgap to capture tail absorption.*

```
    for k=1:1400
        E=E+deltae;
        Ehh=E/(1+mhh/me);
        Ee=E/(1+me/mhh);
        fhh=fermi(beta,Ehh,muhh);
        fe=fermi(beta,Ee,mue);
```

$$E_k = k \cdot \Delta E, \quad E_h^{(k)}, E_e^{(k)}, f_h^{(k)}, f_e^{(k)} \tag{36}$$

*Inner loop over transition energies for convolution integration.*

```
        rspint=rspint+(sqrt(E))*fhh*fe*deltae*(gamma/2/pi)/((Eg+E-
            Ephoton(j))^2+(gamma/2)^2);
    end
```

$$r_{sp,int} \leftarrow r_{sp,int} + \sqrt{E_k} \cdot f_h^{(k)} \cdot f_e^{(k)} \cdot \Delta E \cdot \frac{\gamma/2\pi}{(E_g + E_k - \hbar\omega_j)^2 + (\gamma/2)^2} \tag{37}$$

*Riemann sum implementing the convolution integral with Lorentzian lineshape.*

```
    rsponbrd(j)=(const)*rspint;
    gain(j)=rsponbrd(j)*(1-exp(((Ephoton(j)-Eg)-deltamu)*beta));
end
```

$$r_{sp}^{brd}(\hbar\omega_j) = C \cdot r_{sp,int} \tag{38}$$

$$g^{brd}(\hbar\omega_j) = r_{sp}^{brd}(\hbar\omega_j) \cdot \left(1 - e^{(\hbar\omega_j - E_g - \Delta\mu)/k_B T}\right) \tag{39}$$

*Broadened spontaneous emission and gain spectra.*

### 3.7 Plotting

```
figure(1)
plot(Ephoton-Eg, rsponbrd,'b');
hold on;
plot(Energy, rspon,'r');
hold off
axis([-.1,.3,0,1000]);
xlabel('Photon energy, (eV)');
ylabel('Spontaneous emission, rspon (arb.)');
```

*Figure 1: Compares broadened (blue) vs unbroadened (red) spontaneous emission. Broadening smooths the sharp band-edge onset.*

```
figure(2)
plot(Ephoton-Eg, gain,'b');
hold on;
plot(Energy, gain1,'r');
hold off;
axis([-.1,.1,-500,500]);
xlabel('Photon energy, (eV)');
ylabel('gain, (cm^-^1)');
```

*Figure 2: Compares broadened vs unbroadened gain. Broadening reduces peak gain and extends absorption tail below bandgap.*

## 4 Physical Interpretation

### 4.1 Effect of Broadening on Gain

The Lorentzian broadening has several important effects:

1. **Peak gain reduction**: The convolution smooths the sharp peak, reducing maximum gain by $\sim 20 - 30\%$
2. **Spectral broadening**: The gain bandwidth increases
3. **Sub-bandgap absorption**: The Lorentzian tail allows transitions below $E_g$
4. **Transparency shift**: The energy where $g = 0$ shifts slightly

### 4.2 Physical Origins of Broadening

The broadening parameter $\gamma = 15$ meV arises from:

- Carrier-carrier scattering: $\tau_{cc} \sim 50$ fs
- Carrier-phonon scattering: $\tau_{LO} \sim 100$ fs
- Intraband relaxation: $\tau_{intra} \sim 100$ fs

The total scattering rate gives $\gamma = \hbar/\tau_{total} \approx 10 - 20$ meV.

### 4.3 Design Implications

For semiconductor laser design:

- Higher carrier density needed to achieve same peak gain
- Broader emission spectrum (affects single-mode operation)
- Absorption tail affects internal losses
- Temperature dependence through $\gamma(T)$

# 5 Summary

This code demonstrates Lorentzian line broadening in semiconductor gain media:

1. Unbroadened gain shows sharp band-edge with zero sub-bandgap response
2. Lorentzian convolution smooths spectra and enables sub-bandgap transitions
3. Broadening parameter $\gamma = 15$ meV typical for GaAs at room temperature
4. Numerical integration uses Riemann sums with $\Delta E \ll \gamma$
5. Gain-spontaneous emission relationship maintained under broadening