# Chapt8Fig15.m

## Screened vs Unscreened Coulomb Scattering

Demonstrating the Effect of Thomas-Fermi Screening

Semiconductor Physics Documentation


**Abstract**

This document analyzes `Chapt8Fig15.m`, which compares the angular distribution of scattering rates with and without Thomas-Fermi screening. This comparison vividly demonstrates how screening regularizes the divergent bare Coulomb scattering at small angles.


# Contents

# 1 Theoretical Foundation

## 1.1 Bare Coulomb Scattering

**Theorem 1** (Rutherford Scattering Rate)**.** *For bare Coulomb scattering (no screening):*

$$\frac{d(1/\tau)}{d\theta} = \frac{2\pi m^*}{\hbar^3 k^3} n_i \left(\frac{e^2}{4\pi\varepsilon_0\varepsilon_r}\right)^2 \frac{\sin\theta}{q^4} \tag{1}$$

*where* $q = 2k\sin(\theta/2)$*.*

**Corollary 1** (Small-Angle Divergence)**.** *As* $\theta \to 0$*:*

$$\frac{d(1/\tau)}{d\theta} \propto \frac{\theta}{(k\theta)^4} = \frac{1}{k^4\theta^3} \to \infty \tag{2}$$

*This divergence is unphysical and leads to an infinite total scattering rate.*

## 1.2 Screened Coulomb Scattering

**Theorem 2** (Thomas-Fermi Screened Rate)**.** *With Thomas-Fermi screening:*

$$\frac{d(1/\tau)}{d\theta} = \frac{2\pi m^*}{\hbar^3 k^3} n_i \left(\frac{e^2}{4\pi\varepsilon_0}\right)^2 \frac{\sin\theta}{\varepsilon_{TF}^2(q)\cdot q^4} \tag{3}$$

*where:*

$$\varepsilon_{TF}(q) = \varepsilon_r\left(1 + \frac{q_{TF}^2}{q^2}\right) \tag{4}$$

**Corollary 2** (Regularization)**.** *As* $\theta \to 0$ *with screening:*

$$\frac{d(1/\tau)}{d\theta} \propto \frac{\theta}{(q_{TF}^2)^2} = \mathit{finite} \tag{5}$$

*The screening wavevector* $q_{TF}$ *provides a natural cutoff.*

## 1.3 Physical Origin of Screening

**Definition 1** (Debye-Hückel/Thomas-Fermi Picture)**.** *Mobile electrons redistribute around a charged impurity:*

$$\delta n(r) \propto e^{-q_{TF}r} \tag{6}$$

*This creates a screening cloud that reduces the effective range of the Coulomb potential.*

The screened potential in real space:

$$V(r) = \frac{Ze^2}{4\pi\varepsilon_0\varepsilon_r r} e^{-q_{\mathrm{TF}}r} \tag{7}$$

This Yukawa-type potential has a finite range $\sim 1/q_{\mathrm{TF}}$.

# 2 Line-by-Line Code Analysis

## 2.1 Initialization

```
clear;clf;
n=1e18;
n=n*1e6;
```

$$n = 10^{18}\ \mathrm{cm}^{-3} = 10^{24}\ \mathrm{m}^{-3} \tag{8}$$

*High carrier density for strong screening.*

### 2.2 Physical Constants

```
m0=9.109382e-31;
eharge=1.6021764e-19;
epsilon0=8.8541878e-12;
hbar=1.05457159e-34;
hbar3=hbar^3;
```

*Note: Variable name is "eharge" (typo for "echarge").*

```
m=0.07*m0;
epsilonr0=13.2;
epsilon=epsilon0*epsilonr0;
```

$$m^* = 0.07m_0, \quad \varepsilon = 13.2\varepsilon_0 \tag{9}$$

*GaAs parameters.*

### 2.3 Fermi Wavevector

```
kF=(3*(pi^2)*n)^(1/3)
```

$$k_F = (3\pi^2 \times 10^{24})^{1/3} \approx 3.09 \times 10^8 \text{ m}^{-1} \tag{10}$$

*Fermi wavevector for degenerate electron gas.*

### 2.4 Energy Loop

```
E=-0.1*eharge;
for j=1:1:2
E=E+0.2*eharge
    k=sqrt(2*m*E)/hbar;
k3=k^3;
```

$$E \in \{0.1, 0.3\} \text{ eV} \tag{11}$$

*Two electron energies (note: E is in Joules since multiplied by "eharge").*

### 2.5 RPA Constants (Unused in Final Calculation)

```
    rs0=((3/(4*pi*n))^(1/3))*(m*(eharge^2)/(4*pi*epsilon0*(hbar^2)));
    xi=((32*(pi^2)/9)^(1/3))/(pi^2);
```

*These RPA constants are calculated but not used in the plotted rates.*

### 2.6 Thomas-Fermi Wavevector

```
  qTF=sqrt(kF*m*eharge^2/(epsilon*(pi^2)*(hbar^2)));
```

$$q_{\text{TF}} = \sqrt{\frac{k_F m^* e^2}{\varepsilon \pi^2 \hbar^2}} \tag{12}$$

*Thomas-Fermi screening wavevector.*

### 2.7 Angular Grid

```
theta=[pi/180:pi/180:pi];
        q=2*k*sin(theta/2);
   eta=sin(theta/2);
   deta=pi*cos(theta/2)./2/180;
   eta3=eta.^3;
```

$$\theta \in [1, 180], \quad q = 2k\sin(\theta/2) \tag{13}$$

*Standard angular discretization.*

### 2.8 Thomas-Fermi Dielectric Function

```
   TFepsilon=epsilon*(1+qTF^2./q.^2);
```

$$\varepsilon_{\mathrm{TF}}(q) = \varepsilon\left(1 + \frac{q_{\mathrm{TF}}^2}{q^2}\right) \tag{14}$$

*Screened dielectric function.*

### 2.9 Unscreened (Bare Coulomb) Rate

```
   NoScreenRate=2*pi*m/hbar3/k3*n*(eharge^2/4/pi)^2.*deta./epsilon.^2./
      eta3;
```

$$\left(\frac{1}{\tau}\right)_{\mathrm{bare}} = \frac{2\pi m^*}{\hbar^3 k^3} n \left(\frac{e^2}{4\pi}\right)^2 \frac{d\eta}{\varepsilon^2\eta^3} \tag{15}$$

*Bare Coulomb scattering rate (no screening, only background dielectric constant).*

### 2.10 Thomas-Fermi Screened Rate

```
   TFrate =2*pi*m/hbar3/k3*n*(eharge^2/4/pi)^2.*deta./TFepsilon.^2./
      eta3;
```

$$\left(\frac{1}{\tau}\right)_{\mathrm{TF}} = \frac{2\pi m^*}{\hbar^3 k^3} n \left(\frac{e^2}{4\pi}\right)^2 \frac{d\eta}{\varepsilon_{\mathrm{TF}}^2\eta^3} \tag{16}$$

*Thomas-Fermi screened scattering rate.*

### 2.11 Plotting Both Curves

```
  plot(theta*180/pi, TFrate,'r');
  axis([0 180 0 0.3e12]);
  ...
  plot(theta*180/pi, NoScreenRate,'b');
```

*Red: Thomas-Fermi screened; Blue: Bare Coulomb (unscreened).*

## 3 Physical Interpretation

### 3.1 Comparison of Curves

- **Blue curve (unscreened)**: Diverges at small angles
- **Red curve (TF screened)**: Finite at all angles
- At large angles ($\theta \gtrsim 90$): Both curves similar
- At small angles ($\theta \lesssim 30$): Dramatic difference

### 3.2 Crossover Angle

The screening becomes important when $q \sim q_{\rm TF}$:

$$2k \sin(\theta_c/2) \approx q_{\rm TF} \tag{17}$$

$$\theta_c \approx 2 \arcsin\left(\frac{q_{\rm TF}}{2k}\right) \tag{18}$$

For small angles:

$$\theta_c \approx \frac{q_{\rm TF}}{k} \tag{19}$$

### 3.3 Total Scattering Rate

Without screening:

$$\frac{1}{\tau_{\rm bare}} = \int_0^\pi \frac{d(1/\tau)}{d\theta} d\theta = \infty \tag{20}$$

With Thomas-Fermi screening:

$$\frac{1}{\tau_{\rm TF}} = \int_0^\pi \frac{d(1/\tau)}{d\theta} d\theta = \text{finite} \tag{21}$$

### 3.4 Practical Implications

- Bare Coulomb formula (Rutherford) cannot be used for transport calculations
- Screening is essential for finite mobility in doped semiconductors
- Higher doping $\Rightarrow$ stronger screening $\Rightarrow$ can partially compensate for more scatterers

## 4 Summary

This code provides a direct visual comparison between screened and unscreened Coulomb scattering, demonstrating:

1. The bare Coulomb potential leads to divergent scattering at small angles
2. Thomas-Fermi screening regularizes this divergence
3. The crossover occurs at angle $\theta_c \sim q_{\rm TF}/k$
4. At large angles, screening effects are minimal

This is a fundamental result in semiconductor transport theory, explaining why heavily doped semiconductors can still have finite (though reduced) mobility.