Chapt8Exercise7a.m
Thomas-Fermi vs RPA Screening
Ionized Impurity Scattering in Semiconductors

Semiconductor Physics Documentation

Abstract

This document provides a complete theoretical framework and code analysis for `Chapt8Exercise7a.m`, which compares ionized impurity scattering rates calculated using Thomas-Fermi (TF) screening with the more accurate Random Phase Approximation (RPA). The carrier density is $n = 10^{18}$ cm^{-3}, representing a heavily doped semiconductor.

Contents

1 Theoretical Foundation

1.1 Fundamental Axioms of Scattering Theory

Axiom 1 (Fermi's Golden Rule). *The transition rate from initial state $|i\rangle$ to final state $|f\rangle$ due to a perturbation V is:*

$$W_{i\to f} = \frac{2\pi}{\hbar}|\langle f|V|i\rangle|^2\delta(E_f - E_i) \tag{1}$$

Axiom 2 (Born Approximation). *For weak scattering potentials, the scattering amplitude is proportional to the Fourier transform of the potential:*

$$f(\theta) \propto \int V(\mathbf{r})e^{i\mathbf{q}\cdot\mathbf{r}}d^3r \tag{2}$$

where $\mathbf{q} = \mathbf{k}' - \mathbf{k}$ is the momentum transfer.

Axiom 3 (Linear Response Theory). *The response of an electron gas to an external perturbation is characterized by the dielectric function $\varepsilon(\mathbf{q}, \omega)$.*

1.2 Coulomb Scattering by Ionized Impurities

Definition 1 (Bare Coulomb Potential). *An ionized impurity of charge Ze creates a potential:*

$$V_{bare}(r) = \frac{Ze^2}{4\pi\varepsilon_0\varepsilon_r r} \tag{3}$$

Theorem 1 (Fourier Transform of Coulomb Potential).

$$V_{bare}(q) = \frac{Ze^2}{\varepsilon_0\varepsilon_r q^2} \tag{4}$$

1.3 Screening in an Electron Gas

Definition 2 (Screened Potential). *In the presence of mobile carriers, the effective potential is:*

$$V_{scr}(q) = \frac{V_{bare}(q)}{\varepsilon(q)} \tag{5}$$

where $\varepsilon(q)$ is the static dielectric function.

1.4 Thomas-Fermi Screening

Theorem 2 (Thomas-Fermi Dielectric Function). *In the Thomas-Fermi approximation:*

$$\varepsilon_{TF}(q) = \varepsilon_r\left(1 + \frac{q_{TF}^2}{q^2}\right) \tag{6}$$

where the Thomas-Fermi screening wavevector is:

$$q_{TF} = \sqrt{\frac{k_F m^* e^2}{\pi^2\hbar^2\varepsilon_0\varepsilon_r}} \tag{7}$$

Definition 3 (Fermi Wavevector). *For a 3D electron gas with density n:*

$$k_F = (3\pi^2 n)^{1/3} \tag{8}$$

1.5 Random Phase Approximation (RPA)

Theorem 3 (Lindhard Dielectric Function). *The RPA (Lindhard) dielectric function is:*

$$\varepsilon_{RPA}(q) = \varepsilon_r + \frac{r_s}{\xi} \left[\frac{1}{x} + \frac{1 - x^2/4}{2x^2} \ln \left| \frac{x+2}{x-2} \right| \right] \tag{9}$$

where $x = q/k_F$ is the dimensionless wavevector.

Definition 4 (Wigner-Seitz Radius). *The dimensionless density parameter is:*

$$r_s = \left(\frac{3}{4\pi n} \right)^{1/3} \frac{m^* e^2}{4\pi \varepsilon_0 \hbar^2} \tag{10}$$

1.6 Scattering Rate Formula

Theorem 4 (Differential Scattering Rate). *The angular-dependent scattering rate is:*

$$\frac{1}{\tau(\theta)} = \frac{2\pi m^*}{\hbar^3 k^3} n_i \left(\frac{e^2}{4\pi \varepsilon_0} \right)^2 \frac{1}{\varepsilon(q)^2} \cdot \frac{d\eta}{\eta^3} \tag{11}$$

where:

- $\eta = \sin(\theta/2)$

- $q = 2k \sin(\theta/2)$ *is the momentum transfer*

- n_i *is the impurity density*

2 Line-by-Line Code Analysis

2.1 Physical Constants

```
1  clear;clf;
2  n=1e18;
```

$$n = 10^{18} \text{ cm}^{-3} \tag{12}$$

Carrier density (heavily doped regime).

```
1  n=n*1e6;
```

$$n = 10^{24} \text{ m}^{-3} \tag{13}$$

Convert to SI units.

```
1  m0=9.109382e-31;
```

$$m_0 = 9.109382 \times 10^{-31} \text{ kg} \tag{14}$$

Bare electron mass.

```
1  echarge=1.6021764e-19;
```

$$e = 1.6021764 \times 10^{-19} \text{ C} \tag{15}$$

Elementary charge.

```
1  epsilon0=8.85419e-12;
```

3

$$\varepsilon_0 = 8.85419 \times 10^{-12} \text{ F/m} \tag{16}$$

Permittivity of free space.

```
hbar=1.05457159e-34;
hbar3=hbar^3;
```

$$\hbar = 1.05457159 \times 10^{-34} \text{ J} \cdot \text{s}, \quad \hbar^3 = 1.174 \times 10^{-102} \text{ J}^3\text{s}^3 \tag{17}$$

Reduced Planck constant and its cube.

```
m=0.07*m0;
```

$$m^* = 0.07\,m_0 = 6.377 \times 10^{-32} \text{ kg} \tag{18}$$

Effective electron mass for GaAs.

```
epsilonr0=13.2;
epsilon=epsilon0*epsilonr0;
```

$$\varepsilon_r = 13.2, \quad \varepsilon = \varepsilon_0\varepsilon_r = 1.169 \times 10^{-10} \text{ F/m} \tag{19}$$

GaAs low-frequency dielectric constant.

2.2 Fermi Wavevector Calculation

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

$$k_F = (3\pi^2 n)^{1/3} = (3\pi^2 \times 10^{24})^{1/3} \approx 3.09 \times 10^8 \text{ m}^{-1} \tag{20}$$

Fermi wavevector for the degenerate electron gas.

2.3 Energy Loop

```
E=-0.1*echarge;
for j=1:1:2
E=E+0.2*echarge;
```

$$E \in \{0.1, 0.3\} \text{ eV} \tag{21}$$

Loop over two electron energies: 0.1 eV and 0.3 eV.

```
    k=sqrt(2*m*E)/hbar;
```

$$k = \frac{\sqrt{2m^*E}}{\hbar} \tag{22}$$

Electron wavevector from the dispersion relation $E = \hbar^2 k^2/(2m^*)$.

```
k3=k^3;
```

$$k^3 = k^3 \text{ [m}^{-3}] \tag{23}$$

Cube of wavevector for rate formula.

2.4 RPA Model Constants

```
1    rs0=((3/(4*pi*n))^(1/3))*(m*(echarge^2)/(4*pi*epsilon0*(hbar^2)));
```

$$r_s = \left(\frac{3}{4\pi n}\right)^{1/3} \cdot \frac{m^* e^2}{4\pi \varepsilon_0 \hbar^2} \tag{24}$$

Wigner-Seitz radius (dimensionless density parameter).

```
1    xi=((32*(pi^2)/9)^(1/3))/(pi^2);
```

$$\xi = \frac{(32\pi^2/9)^{1/3}}{\pi^2} \tag{25}$$

Numerical constant in Lindhard function.

2.5 Thomas-Fermi Screening Wavevector

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

$$q_{\text{TF}} = \sqrt{\frac{k_F m^* e^2}{\varepsilon \pi^2 \hbar^2}} \tag{26}$$

Thomas-Fermi screening wavevector.

2.6 Angular Grid

```
1  theta=[pi/1800:pi/1800:pi];
```

$$\theta \in [0.1°, 180°] \text{ with step } 0.1° \tag{27}$$

Scattering angle array (in radians).

```
1        q=2*k*sin(theta/2);
```

$$q = 2k\sin(\theta/2) \tag{28}$$

Momentum transfer magnitude for elastic scattering.

```
1    eta=sin(theta/2);
2    deta=pi*cos(theta/2)./2/180;
3    eta3=eta.^3;
```

$$\eta = \sin(\theta/2), \quad d\eta = \frac{\pi}{360}\cos(\theta/2), \quad \eta^3 \tag{29}$$

Angular transformation variable and its differential.

2.7 RPA Dielectric Function

```
1    x=q/kF;
2    absx=abs(x+2)./abs(x-2);
3    RPAepsilonr=epsilonr0+((rs0./x.^3)*xi.*(x+((1-((x.^2)/4)).*log(absx)
         )));
```

$$\varepsilon_{\text{RPA}}(x) = \varepsilon_r + \frac{r_s \xi}{x^3}\left[x + \left(1 - \frac{x^2}{4}\right)\ln\left|\frac{x+2}{x-2}\right|\right] \tag{30}$$

Lindhard (RPA) dielectric function where $x = q/k_F$.

2.8 Thomas-Fermi Dielectric Function

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

$$\varepsilon_{\text{TF}}(q) = \varepsilon \left(1 + \frac{q_{\text{TF}}^2}{q^2} \right) \tag{31}$$

Thomas-Fermi dielectric function.

2.9 Scattering Rates

```
1    RPArate=2*pi*m/hbar3/k3*n*(echarge^2/4/pi/epsilon0)^2.*deta./
        RPAepsilonr.^2./eta3;
```

$$\frac{1}{\tau_{\text{RPA}}} = \frac{2\pi m^*}{\hbar^3 k^3} n \left(\frac{e^2}{4\pi\varepsilon_0} \right)^2 \frac{d\eta}{\varepsilon_{\text{RPA}}^2 \eta^3} \tag{32}$$

RPA scattering rate.

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

$$\frac{1}{\tau_{\text{TF}}} = \frac{2\pi m^*}{\hbar^3 k^3} n \left(\frac{e^2}{4\pi} \right)^2 \frac{d\eta}{\varepsilon_{\text{TF}}^2 \eta^3} \tag{33}$$

Thomas-Fermi scattering rate.

2.10 Plotting

```
1    plot(theta*180/pi, TFrate,'r');
2    ...
3    plot(theta*180/pi, RPArate,'b');
```

Plot both rates vs angle: TF in red, RPA in blue.

3 Numerical Method Details

3.1 Discretization Scheme

The angular integration is discretized uniformly:

$$\theta_j = \frac{\pi j}{1800}, \quad j = 1, 2, \dots, 1800 \tag{34}$$

This gives 0.1° resolution, sufficient to capture the sharp forward-scattering peak.

3.2 Lindhard Function Evaluation

The logarithmic term in the Lindhard function requires care:

$$\ln \left| \frac{x+2}{x-2} \right| \tag{35}$$

- For $x < 2$ (small-angle scattering): Regular evaluation
- At $x = 2$ (backscattering at $\theta = 180$): Singularity (pole)
- For $x > 2$: Argument becomes negative inside, hence absolute value

4 Physical Interpretation

4.1 TF vs RPA Comparison

- **Thomas-Fermi**: Local approximation, accurate for $q \ll k_F$

- **RPA**: Includes non-local response, accurate for all q

At high carrier density ($n = 10^{18}$ cm^{-3}), both models should agree reasonably well because:

$$q_{\mathrm{TF}} \sim k_F \quad \text{(strong screening)} \tag{36}$$

4.2 Angular Dependence

The scattering rate diverges at small angles:

$$\frac{1}{\tau} \propto \frac{1}{\sin^3(\theta/2)} \tag{37}$$

This is regularized by screening (the q_{TF}^2 or RPA terms in the denominator).

5 Summary

This code compares two models for ionized impurity scattering:

1. Thomas-Fermi: Simple analytical model assuming local screening

2. RPA (Lindhard): More accurate model including the full wavevector-dependent response

At $n = 10^{18}$ cm^{-3}, the system is degenerate and strongly screened, so both models give similar results with the characteristic forward-scattering peak regularized by screening.