Chapt8Exercise7b.m

Thomas-Fermi vs RPA Screening at Low Density

Breakdown of Thomas-Fermi Approximation

Semiconductor Physics Documentation

Abstract

This document analyzes `Chapt8Exercise7b.m`, which compares Thomas-Fermi and RPA scattering rates at a low carrier density of $n = 10^{14}$ cm^{-3}. At this density, the Thomas-Fermi approximation breaks down, revealing the importance of non-local screening effects captured by RPA.

Contents

1 Theoretical Foundation

1.1 Validity Conditions for Thomas-Fermi Screening

Theorem 1 (Thomas-Fermi Validity). *The Thomas-Fermi approximation is valid when:*

$$q \ll k_F \quad \textit{and} \quad q_{TF} \sim k_F \tag{1}$$

This requires the electron gas to be sufficiently dense (degenerate).

Definition 1 (Degeneracy Criterion). *An electron gas is degenerate when:*

$$E_F \gg k_B T \tag{2}$$

where the Fermi energy is $E_F = \hbar^2 k_F^2/(2m^*)$.

1.2 Low-Density Regime

At $n = 10^{14}$ cm^{-3}:

$$k_F = (3\pi^2 n)^{1/3} = (3\pi^2 \times 10^{20})^{1/3} \approx 1.43 \times 10^7 \text{ m}^{-1} \tag{3}$$

Compare to $n = 10^{18}$ cm^{-3}:

$$k_F = 3.09 \times 10^8 \text{ m}^{-1} \tag{4}$$

The Fermi wavevector decreases by a factor of ~ 20.

1.3 Consequences for Screening

Theorem 2 (Weak Screening Limit). *At low density:*

$$q_{TF} \propto \sqrt{k_F} \propto n^{1/6} \tag{5}$$

The screening length increases, making screening less effective.

Corollary 1 (RPA Corrections). *When $q \gtrsim k_F$, the RPA dielectric function deviates significantly from Thomas-Fermi:*

$$\varepsilon_{RPA}(q) \neq \varepsilon_{TF}(q) \quad \textit{for } q \gtrsim k_F \tag{6}$$

2 Line-by-Line Code Analysis

2.1 Key Parameter: Low Carrier Density

```
clear;clf;
n=1e14;
n=n*1e6;
```

$$n = 10^{14} \text{ cm}^{-3} = 10^{20} \text{ m}^{-3} \tag{7}$$

Critical difference: carrier density is 10^4 times lower than Chapt8Exercise7a.

2.2 Physical Constants (Same as 7a)

```
m0=9.109382e-31;
echarge=1.6021764e-19;
epsilon0=8.85419e-12;
hbar=1.05457159e-34;
hbar3=hbar^3;
m=0.07*m0;
epsilonr0=13.2;
epsilon=epsilon0*epsilonr0;
```

Material parameters for GaAs remain unchanged.

2.3 Fermi Wavevector

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

$$k_F = (3\pi^2 \times 10^{20})^{1/3} \approx 1.43 \times 10^7 \text{ m}^{-1} \tag{8}$$

Much smaller than at high density, indicating weak degeneracy.

2.4 Energy Loop

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

$$E \in \{0.1, 0.3\} \text{ eV}, \quad k = \frac{\sqrt{2m^*E}}{\hbar} \tag{9}$$

Same electron energies as Chapt8Exercise7a for comparison.

2.5 RPA Constants

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

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

At low density, r_s is larger, indicating stronger electron-electron correlations.

2.6 Thomas-Fermi Wavevector

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

$$q_{\text{TF}} = \sqrt{\frac{k_F m^* e^2}{\varepsilon\pi^2\hbar^2}} \tag{11}$$

Smaller k_F leads to smaller q_{TF}, weaker screening.

2.7 Angular Discretization

```
theta=[pi/1800:pi/1800:pi];
        q=2*k*sin(theta/2);
   eta=sin(theta/2);
   deta=pi*cos(theta/2)./2/180;
   eta3=eta.^3;
```

Same angular grid as Chapt8Exercise7a.

2.8 RPA Dielectric Function

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

$$x = q/k_F \quad \text{(now larger values since } k_F \text{ is smaller)} \tag{12}$$

At low density, $x = q/k_F$ can be $\gg 1$, where TF fails.

2.9 Thomas-Fermi Dielectric Function

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

$$\varepsilon_{\mathrm{TF}} = \varepsilon \left(1 + \frac{q_{\mathrm{TF}}^2}{q^2}\right) \tag{13}$$

With smaller q_{TF}, the screening term is less effective.

2.10 Scattering Rates

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

$$\frac{1}{\tau} = \frac{2\pi m^*}{\hbar^3 k^3} n \left(\frac{e^2}{4\pi}\right)^2 \frac{d\eta}{\varepsilon(q)^2 \eta^3} \tag{14}$$

Same formula, but n is lower and screening is weaker.

2.11 Plotting with Restricted Axis

```
plot(theta*180/pi, TFrate,'r');
axis([0,35,0,9e9]);
...
plot(theta*180/pi, RPArate,'b');
```

Axis restricted to $\theta \in [0, 35]$ to focus on the forward-scattering region where differences are largest.

3 Physical Interpretation

3.1 Why TF Fails at Low Density

The Thomas-Fermi approximation assumes:

1. Local response: Perturbation at $\mathbf{r}$ only affects density at $\mathbf{r}$
2. Degenerate limit: All states up to E_F are filled
3. Slow spatial variation: $q \ll k_F$

At $n = 10^{14}$ cm^{-3}:

- Fermi energy: $E_F \approx 0.1$ meV (non-degenerate at room temperature)
- Typical scattering wavevector: $q \sim k \gg k_F$
- TF assumption $q \ll k_F$ is violated

3.2 RPA Captures the Correct Physics

The RPA (Lindhard) function includes:

$$\varepsilon(q) = 1 + \frac{q_{\mathrm{TF}}^2}{q^2} \cdot g(q/k_F) \tag{15}$$

where $g(x)$ is a correction factor that:

- Equals 1 for $x \ll 1$ (recovers TF)
- Decreases for $x \gtrsim 1$ (weakens screening)
- Vanishes for $x \gg 1$ (bare Coulomb restored)

3.3 Expected Results

- TF (red curve): Underestimates scattering at large angles
- RPA (blue curve): Shows stronger scattering due to weaker screening
- Difference is most pronounced at large q (large angles)

4 Comparison with Chapt8Exercise7a

Parameter	Chapt8Exercise7a	Chapt8Exercise7b
Carrier density n	10^{18} cm^{-3}	10^{14} cm^{-3}
Fermi wavevector k_F	3.09×10^8 m^{-1}	1.43×10^7 m^{-1}
Screening	Strong	Weak
TF validity	Good	Poor
TF-RPA agreement	Good	Poor

Table 1: Comparison of the two exercises

5 Summary

This code demonstrates the breakdown of the Thomas-Fermi approximation at low carrier densities. When the electron gas is non-degenerate and the typical scattering wavevector exceeds the Fermi wavevector, the local Thomas-Fermi approximation fails, and the full RPA treatment becomes necessary. The restricted angular range in the plot highlights the region where differences between TF and RPA are most pronounced.