Chapt7Fig6b.m

Fermi-Dirac Distribution at Lower Carrier Density

Non-Degenerate Semiconductor Regime

Semiconductor Physics Documentation

Abstract

This document analyzes `Chapt7Fig6b.m`, which plots the Fermi-Dirac distribution function at a carrier density of $n = 10^{17}$ cm^{-3}, one order of magnitude lower than `Chapt7Fig6a.m`. This lower density places the system closer to the non-degenerate (Maxwell-Boltzmann) regime, providing insight into the classical-quantum transition.

Contents

1 Theoretical Foundation

1.1 Fermi-Dirac Statistics Review

Theorem 1 (Fermi-Dirac Distribution)**.** *The probability of occupation of a quantum state with energy E is:*

$$f(E) = \frac{1}{e^{(E-\mu)/k_B T} + 1} \tag{1}$$

where μ is the chemical potential (Fermi level) and T is the temperature.

1.2 Degeneracy Parameter

Definition 1 (Degeneracy Parameter)**.** *The degeneracy of an electron gas is characterized by:*

$$\eta = \frac{\mu}{k_B T} \tag{2}$$

- $\eta \gg 1$*: Degenerate regime (quantum statistics essential)*
- $\eta \ll -1$*: Non-degenerate regime (classical approximation valid)*
- $|\eta| \lesssim 1$*: Transition regime*

1.3 Non-Degenerate Limit: Maxwell-Boltzmann Approximation

Theorem 2 (Maxwell-Boltzmann Limit)**.** *When $E - \mu \gg k_B T$ for all occupied states, the Fermi-Dirac distribution reduces to:*

$$f(E) \approx e^{-(E-\mu)/k_B T} \tag{3}$$

Proof. When $(E - \mu)/k_B T \gg 1$, we have $e^{(E-\mu)/k_B T} \gg 1$, so:

$$f(E) = \frac{1}{e^{(E-\mu)/k_B T} + 1} \approx \frac{1}{e^{(E-\mu)/k_B T}} = e^{-(E-\mu)/k_B T} \tag{4}$$

□

1.4 Chemical Potential Dependence on Carrier Density

Theorem 3 (Non-Degenerate Carrier Density)**.** *In the non-degenerate limit, the carrier density is:*

$$n = N_c \exp\left(\frac{\mu}{k_B T}\right) \tag{5}$$

where $N_c = 2\left(\frac{m^* k_B T}{2\pi\hbar^2}\right)^{3/2}$ is the effective density of states.

Corollary 1 (Chemical Potential in Non-Degenerate Regime)**.**

$$\mu = k_B T \ln\left(\frac{n}{N_c}\right) \tag{6}$$

When $n < N_c$, the chemical potential is negative (below the band edge).

1.5 Effective Density of States for GaAs

For GaAs with $m^* = 0.07m_0$:

$$N_c = 2\left(\frac{0.07m_0k_BT}{2\pi\hbar^2}\right)^{3/2} \tag{7}$$

At $T = 300$ K:

$$N_c \approx 4.7 \times 10^{17}\ \text{cm}^{-3} \tag{8}$$

Since $n = 10^{17}\ \text{cm}^{-3} < N_c$, the system is near the non-degenerate regime at room temperature.

2 Line-by-Line Code Analysis

2.1 Key Parameter Difference

```
n=1.e17
```

$$n = 1 \times 10^{17}\ \text{cm}^{-3} \tag{9}$$

This is the critical difference from Chapt7Fig6a.m. The carrier density is 10 times lower, pushing the system toward the non-degenerate regime.

2.2 Physical Constants (Identical to Chapt7Fig6a)

```
m0=9.109382;
```

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

Bare electron mass.

```
m1=0.07;
```

$$m^* = 0.07\, m_0 \tag{11}$$

Effective mass for GaAs conduction band electrons.

```
echarge=1.6021764;
```

$$e = 1.6021764 \times 10^{-19}\ \text{C} \tag{12}$$

Elementary charge.

```
hbar=1.05457159;
```

$$\hbar = 1.05457159 \times 10^{-34}\ \text{J} \cdot \text{s} \tag{13}$$

Reduced Planck constant.

```
kB=8.61734e-5;
```

$$k_B = 8.61734 \times 10^{-5}\ \text{eV/K} \tag{14}$$

Boltzmann constant in convenient units.

```
rerr=1.e-3;
```

$$\epsilon_{\text{rel}} = 10^{-3} \tag{15}$$

Relative error tolerance for chemical potential calculation.

2.3 Temperature Array

```
Temperature=[0.1,100,200,300,400];
```

$$T \in \{0.1, 100, 200, 300, 400\} \text{ K} \tag{16}$$

Same temperature range as Chapt7Fig6a for direct comparison.

```
nTemp=length(Temperature)
```

$$N_{\text{temp}} = 5 \tag{17}$$

Number of temperature curves to plot.

2.4 Energy Grid Setup

```
nplotpoints=300;
Emin=0;
Emax=200;
Estep=(Emax-Emin)/nplotpoints;
```

$$E_k = k \cdot \frac{200 \text{ meV}}{300} \quad \text{for } k = 0, 1, \ldots, 300 \tag{18}$$

Energy discretization from 0 to 200 meV.

2.5 Main Computation Loop

```
for j=1:1:nTemp
   kelvin=Temperature(j);
   kBT=1000.*kelvin*kB;
   beta=1./kBT;
```

$$\beta = \frac{1}{k_B T} \quad [\text{meV}^{-1}] \tag{19}$$

Compute inverse thermal energy for each temperature.

```
   mu1=chempot(kelvin,m1,n,rerr);
```

$$\mu = \mu(T, m^* = 0.07 m_0, n = 10^{17} \text{ cm}^{-3}) \tag{20}$$

At lower carrier density, μ will be smaller (possibly negative at high T).

2.6 Fermi Function Evaluation Loop

```
  for k = 1:1:nplotpoints+1
     energy=((k-1)*Estep)+Emin;
     E(k)=energy;
     Prob=fermi(beta,energy,mu1);
     FD(k)=Prob;
  end;
```

$$f(E_k) = \frac{1}{\exp[\beta(E_k - \mu)] + 1} \tag{21}$$

Evaluate Fermi-Dirac distribution at each energy point.

2.7 Plotting

```
    hold on;figure(1);plot(E,log(FD));axis([0 Emax -10 0]);
end
xlabel('Energy, E (meV)');
ylabel('ln(occupation factor)');
ttl=sprintf('Chapt7Fig6b, m* = %4.2f m0, Tmax = %4.1f K, n = %7.2e cm-3
    ',m1,kelvin,n);
title(ttl);
```

$$\ln f(E) \text{ vs } E \tag{22}$$

Logarithmic plot showing the exponential tail behavior more prominently.

3 Physical Interpretation and Comparison

3.1 Effect of Lower Carrier Density

Comparing $n = 10^{17}$ cm^{-3} (this code) with $n = 10^{18}$ cm^{-3} (Chapt7Fig6a):

Property	$n = 10^{17}$ cm^{-3}	$n = 10^{18}$ cm^{-3}
Chemical potential μ	Lower	Higher
Degeneracy $\eta = \mu/k_BT$	Smaller	Larger
Regime	Non-degenerate	Degenerate

Table 1: Comparison of regimes

3.2 Chemical Potential Estimates

At $T = 300$ K with $N_c \approx 4.7 \times 10^{17}$ cm^{-3}:

For $n = 10^{17}$ cm^{-3}:

$$\mu \approx k_BT \ln\left(\frac{10^{17}}{4.7 \times 10^{17}}\right) \approx k_BT \ln(0.21) \approx -1.56\, k_BT \approx -40 \text{ meV} \tag{23}$$

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

$$\mu \approx k_BT \ln\left(\frac{10^{18}}{4.7 \times 10^{17}}\right) \approx k_BT \ln(2.13) \approx 0.76\, k_BT \approx 20 \text{ meV} \tag{24}$$

3.3 Implications for the Plot

With lower carrier density:

- The chemical potential is lower (possibly negative at high T)
- The Fermi function drops off more steeply at low energies
- The system more closely follows Maxwell-Boltzmann statistics
- The logarithmic plot shows nearly linear behavior over a wider range

3.4 Temperature Dependence

At very low temperature ($T = 0.1$ K):

$$k_B T \approx 8.6 \times 10^{-6} \text{ eV} = 8.6 \times 10^{-3} \text{ meV} \tag{25}$$

Even at low carrier density, the thermal energy is so small that the distribution still shows sharp step-like behavior, with all electrons in states below the Fermi energy.

At $T = 400$ K:

$$k_B T \approx 34.5 \text{ meV} \tag{26}$$

The distribution is significantly broadened, and with $\mu < 0$, the occupation probability at $E = 0$ is already less than 0.5.

4 Numerical Considerations

4.1 The chempot Function

The function `chempot(kelvin, m1, n, rerr)` solves:

$$n = \frac{1}{2\pi^2} \left(\frac{2m^*}{\hbar^2} \right)^{3/2} \int_0^\infty \frac{\sqrt{E}}{e^{(E-\mu)/k_B T} + 1} dE \tag{27}$$

This is typically done using:

1. Initial guess based on non-degenerate approximation: $\mu_0 = k_B T \ln(n/N_c)$
2. Newton-Raphson iteration to refine
3. Convergence criterion: $|\mu_{i+1} - \mu_i| < \epsilon_{\text{rel}} \cdot |\mu_i|$

4.2 The fermi Function

The function `fermi(beta, E, mu)` computes:

$$f = \frac{1}{e^{\beta(E-\mu)} + 1} \tag{28}$$

Numerical care is needed for large arguments:

- If $\beta(E - \mu) > 700$: $f \approx 0$
- If $\beta(E - \mu) < -700$: $f \approx 1$

5 Summary

This code demonstrates the Fermi-Dirac distribution in the non-degenerate regime, where the carrier density is comparable to or less than the effective density of states. The key physical insight is that reducing the carrier density by a factor of 10 shifts the chemical potential significantly lower, bringing the system closer to classical (Maxwell-Boltzmann) behavior while still retaining quantum effects at low temperatures.