Chapt7Fig6a.m
Fermi-Dirac Distribution Function for Semiconductors
A Complete Mathematical Framework

Semiconductor Physics Documentation

Abstract

This document provides a comprehensive mathematical derivation and code explanation for `Chapt7Fig6a.m`, which plots the Fermi-Dirac distribution function for electrons in a semiconductor at various temperatures. We develop the theoretical framework from fundamental statistical mechanics axioms through to the numerical implementation.

Contents

1 Theoretical Foundation: From Axioms to Fermi-Dirac Statistics

1.1 Fundamental Axioms of Quantum Statistical Mechanics

Axiom 1 (Indistinguishability of Identical Particles). *In quantum mechanics, identical particles (such as electrons) are fundamentally indistinguishable. The state of a system is described by occupation numbers rather than individual particle trajectories.*

Axiom 2 (Pauli Exclusion Principle). *For fermions (particles with half-integer spin, including electrons), no two particles can occupy the same quantum state simultaneously. Mathematically, for occupation number n_i of state i:*

$$n_i \in \{0, 1\} \tag{1}$$

Axiom 3 (Principle of Equal A Priori Probabilities). *In thermal equilibrium, all accessible microstates of an isolated system are equally probable.*

Axiom 4 (Boltzmann Entropy Hypothesis). *The entropy S of a system is related to the number of microstates Ω by:*

$$S = k_B \ln \Omega \tag{2}$$

where k_B is Boltzmann's constant.

1.2 Derivation of the Fermi-Dirac Distribution

Definition 1 (Grand Canonical Ensemble). *For a system in thermal and chemical equilibrium with a reservoir at temperature T and chemical potential μ, the probability of a microstate with energy E and particle number N is:*

$$P(E, N) = \frac{1}{\mathcal{Z}} e^{-\beta(E - \mu N)} \tag{3}$$

where $\beta = 1/(k_B T)$ and $\mathcal{Z}$ is the grand partition function.

Theorem 1 (Fermi-Dirac Distribution Function). *For a system of non-interacting fermions in thermal equilibrium, the average occupation number of a single-particle state with energy E is:*

$$f(E) = \frac{1}{e^{\beta(E - \mu)} + 1} \tag{4}$$

Proof. Consider a single quantum state with energy ϵ. Due to the Pauli exclusion principle, the occupation number can only be $n = 0$ or $n = 1$.

The grand partition function for this single state is:

$$\mathcal{Z}_1 = \sum_{n=0}^{1} e^{-\beta(\epsilon - \mu)n} = 1 + e^{-\beta(\epsilon - \mu)} \tag{5}$$

The average occupation is:

$$\langle n \rangle = \frac{\sum_{n=0}^{1} n \cdot e^{-\beta(\epsilon - \mu)n}}{\mathcal{Z}_1} \tag{6}$$

$$= \frac{0 \cdot 1 + 1 \cdot e^{-\beta(\epsilon - \mu)}}{1 + e^{-\beta(\epsilon - \mu)}} \tag{7}$$

$$= \frac{e^{-\beta(\epsilon - \mu)}}{1 + e^{-\beta(\epsilon - \mu)}} \tag{8}$$

$$= \frac{1}{e^{\beta(\epsilon - \mu)} + 1} \tag{9}$$

$\square$

1.3 Chemical Potential in Semiconductors

Definition 2 (Density of States in 3D). *For a parabolic band with effective mass m^*, the density of states per unit volume is:*

$$g(E) = \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\sqrt{E} \tag{10}$$

Theorem 2 (Carrier Density Integral). *The electron concentration in the conduction band is given by:*

$$n = \int_0^\infty g(E)f(E)\,dE = \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\int_0^\infty \frac{\sqrt{E}}{e^{\beta(E-\mu)}+1}\,dE \tag{11}$$

Definition 3 (Fermi Integral of Order 1/2). *The Fermi integral of order j is defined as:*

$$\mathcal{F}_j(\eta) = \frac{1}{\Gamma(j+1)}\int_0^\infty \frac{x^j}{e^{x-\eta}+1}\,dx \tag{12}$$

where $\eta = \mu/(k_B T)$ is the reduced chemical potential.

Theorem 3 (Carrier Density in Terms of Fermi Integral).

$$n = N_c \mathcal{F}_{1/2}(\eta) \tag{13}$$

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

1.4 Numerical Method: Newton-Raphson for Chemical Potential

The code uses a helper function `chempot.m` to find μ given n. This requires solving the implicit equation:

$$n = N_c \mathcal{F}_{1/2}\left(\frac{\mu}{k_B T}\right) \tag{14}$$

Theorem 4 (Newton-Raphson Method). *To find the root of $f(x) = 0$, the Newton-Raphson iteration is:*

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \tag{15}$$

For finding chemical potential, we solve:

$$F(\mu) = n - N_c \mathcal{F}_{1/2}\left(\frac{\mu}{k_B T}\right) = 0 \tag{16}$$

The derivative uses the relation:

$$\frac{d\mathcal{F}_j}{d\eta} = \mathcal{F}_{j-1}(\eta) \tag{17}$$

2 Line-by-Line Code Analysis

2.1 Initialization and Physical Constants

```
clear;clf;
```

Clears workspace variables and current figure.

```
n=1.e18
```

$$n = 1 \times 10^{18} \text{ cm}^{-3} \tag{18}$$

Sets the carrier density. This is a typical doping concentration for heavily doped semiconductors.

```
m0=9.109382;
```

$$m_0 = 9.109382 \times 10^{-31} \text{ kg} \tag{19}$$

Bare electron mass (stored as coefficient, actual value includes $\times 10^{-31}$).

```
m1=0.07;
```

$$m^* = 0.07 \, m_0 \tag{20}$$

Effective electron mass for GaAs conduction band.

```
echarge=1.6021764;
```

$$e = 1.6021764 \times 10^{-19} \text{ C} \tag{21}$$

Elementary charge (coefficient form).

```
hbar=1.05457159;
```

$$\hbar = 1.05457159 \times 10^{-34} \text{ J} \cdot \text{s} \tag{22}$$

Reduced Planck constant (coefficient form).

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

$$k_B = 8.61734 \times 10^{-5} \text{ eV/K} \tag{23}$$

Boltzmann constant in eV/K for convenient energy calculations.

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

$$\epsilon_{\text{rel}} = 10^{-3} \tag{24}$$

Relative error tolerance for numerical calculation of chemical potential.

2.2 Temperature Array and Loop Parameters

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

$$T \in \{0.1, 100, 200, 300, 400\} \text{ K} \tag{25}$$

Array of temperatures spanning near-zero to elevated temperatures.

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

$$N_{\text{temp}} = 5 \tag{26}$$

Number of temperature values to iterate over.

```
nplotpoints=300;
```

Number of energy points for plotting the distribution.

```
Emin=0;
Emax=200;
```

$$E \in [0, 200] \text{ meV} \tag{27}$$

Energy range for the plot in millielectronvolts.

```
1  Estep=(Emax-Emin)/nplotpoints;
```

$$\Delta E = \frac{E_{\max} - E_{\min}}{N_{\text{points}}} = \frac{200}{300} \approx 0.667 \text{ meV} \tag{28}$$

Energy step size for discretization.

2.3 Main Computation Loop

```
1  for j=1:1:nTemp
2      kelvin=Temperature(j);
```

Iterate over each temperature value.

```
1      kBT=1000.*kelvin*kB;
```

$$k_B T = 1000 \times T \times k_B \text{ [meV]} \tag{29}$$

Thermal energy in meV (factor of 1000 converts eV to meV).

```
1      beta=1./kBT;
```

$$\beta = \frac{1}{k_B T} \text{ [meV}^{-1}] \tag{30}$$

Inverse thermal energy, the fundamental temperature parameter in statistical mechanics.

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

$$\mu = \mu(T, m^*, n) \text{ [meV]} \tag{31}$$

Calls external function to compute chemical potential by inverting the carrier density integral numerically.

2.4 Fermi Function Evaluation

```
1      for k = 1:1:nplotpoints+1
2          energy=((k-1)*Estep)+Emin;
3          E(k)=energy;
```

$$E_k = (k - 1) \cdot \Delta E + E_{\min} \tag{32}$$

Compute energy value for each grid point.

```
1          Prob=fermi(beta,energy,mu1);
```

$$f(E) = \frac{1}{e^{\beta(E-\mu)} + 1} \tag{33}$$

Evaluate Fermi-Dirac distribution at energy E with chemical potential μ.

```
1          FD(k)=Prob;
2      end;
```

Store the probability in array for plotting.

2.5 Plotting

```
1      hold on;figure(1);plot(E,log(FD));axis([0 Emax -10 0]);
2 end
```

$$\text{Plot: } \ln[f(E)] \text{ vs } E \tag{34}$$

Logarithmic plot reveals the exponential tail of the distribution.

At high energies ($E \gg \mu$), the Fermi function approaches:

$$f(E) \approx e^{-\beta(E-\mu)} \implies \ln f(E) \approx -\beta(E-\mu) \tag{35}$$

This explains why the logarithmic plot shows linear behavior in the tail region, with slope $-\beta = -1/(k_B T)$.

```
1 xlabel('Energy,␣E␣(meV)');
2 ylabel('ln(occupation␣factor)');
3 ttl=sprintf('Chapt7Fig6a,␣m*␣=␣%4.2f␣m0,␣Tmax␣=␣%4.1f␣K,␣n␣=␣%7.2e␣cm-3
    ',m1,kelvin,n);
4 title(ttl);
```

Add axis labels and title with parameter values.

3 Physical Interpretation

3.1 Temperature Dependence

- At $T \to 0$: The Fermi function becomes a step function

$$f(E) = \begin{cases} 1 & E < \mu \\ 0 & E > \mu \end{cases} \tag{36}$$

- At finite T: The step is "smeared" over an energy range $\sim k_B T$

- The slope of $\ln f(E)$ in the tail region is $-1/(k_B T)$

3.2 Significance of Parameters

- $n = 10^{18}$ cm^{-3}: Heavy doping, chemical potential likely positive (degenerate regime)

- $m^* = 0.07m_0$: Light effective mass typical of III-V semiconductors (GaAs)

- Temperature range 0.1–400 K spans quantum to classical regimes

4 Summary

This code visualizes the fundamental Fermi-Dirac distribution that governs electron statistics in semiconductors. The logarithmic plot clearly shows the transition from the plateau region ($f \approx 1$ for $E < \mu$) to the exponential tail ($f \propto e^{-E/k_B T}$ for $E \gg \mu$), with the transition width controlled by temperature.