

ECE 462 - Homework #7

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1 Problem 5.2.5

The number of states up to k_{max} is defined as:

$$N = \frac{a^2}{\pi} \int_0^{k_{max}} k \cdot dk$$

The number of states is $N = J \cdot a^2$:

$$J \cdot a^2 = \frac{a^2}{\pi} \int_0^{k_{max}} k \cdot dk$$

$$J = \frac{1}{\pi} \int_0^{k_{max}} k \cdot dk$$

$$J = \frac{1}{2\pi} k^2 \Big|_0^{k_{max}}$$

$$J = \frac{k_{max}^2}{2\pi}$$

From here, the k_{max} can be found, which is analogous to the fermi-energy (as it is the maximum state available):

$$k_{max} = \sqrt{2 \cdot J \cdot \pi}$$

2 Problem 5.2.6

The eigenenergies of a two-dimensional well are:

$$E_{n,m} = \frac{\hbar^2}{2m} \left(\frac{n^2}{a^2} + \frac{m^2}{b^2} \right)$$

Therefore the density of these states are simply $\rho = \frac{E_{n,m}}{a \cdot b}$:

$$\rho = \frac{\hbar^2}{2mab} \left(\frac{n^2}{a^2} + \frac{m^2}{b^2} \right)$$

3 Problem 5.3.1

$$n_C(E) = g_C(E)f_F(E)$$

$$n_C(E) = \frac{4\pi(2m_n^*)^{3/2}\sqrt{E-E_c}}{h^3} \cdot \frac{1}{1 + e^{\frac{E-E_F}{k_B T}}}$$

Where the problem states $E_c - E_f = 0.5$ and $E - E_c = 0.2$, which means the two required energy statements can be evaluated as:

$$E - E_c = 0.2eV$$

$$E_c - E_f = 0.5eV \rightarrow E - 0.2 - E_f = 0.5 \rightarrow E - E_f = 0.7eV$$

These can be substituted into the equal for $n_C(E)$ as follows:

3.1 Part (a)

For a temperature of 300 K:

$$n_C(E) = \frac{4\pi \cdot (2 \cdot 1.08 \cdot 9.109 \cdot 10^{-31})^{3/2} \sqrt{0.2}}{(4.135 \cdot 10^{-15})^3} \cdot \frac{1}{1 + e^{\frac{0.7}{8.62 \cdot 10^{-5} \cdot 300}}}$$
$$n_C(E) = P(E) = 3.85 \cdot 10^{-13}$$

3.2 Part (b)

For a temperature of 310 K:

$$n_C(E) = \frac{4\pi \cdot (2 \cdot 1.08 \cdot 9.109 \cdot 10^{-31})^{3/2} \sqrt{0.2}}{(4.135 \cdot 10^{-15})^3} \cdot \frac{1}{1 + e^{\frac{0.7}{8.62 \cdot 10^{-5} \cdot 310}}}$$
$$n_c(E) = P(E) = 9.216 \cdot 10^{-13}$$

4 Problem 5.4.1

```
In [2]: import numpy as np
        from numpy import linalg as la
        import matplotlib.pyplot as plt
        from pylab import rcParams
        import seaborn as sns

        NN = 100
        hbar = 1.054e-34
        m0 = 9.11e-31
        melec = m0
        ecoul = 1.6e-19
        eV2J = 1.6e-19
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J2eV = 1/eV2J
hbar_ev = hbar * J2eV

del_x = .1e-9
DX = del_x * 1e9
XX = np.arange(0, DX * NN, DX)

chi0 = hbar ** 2 / (2 * melec * del_x ** 2)

# Create H matrix
V = np.zeros((NN))
H = np.zeros((NN, NN))
for diag in range(NN):
    H[diag, diag] = 2 * chi0 + V[diag] # Assign diagonals
    try:
        H[diag, diag + 1] = -chi0      # Assign col+1
    except IndexError:
        pass
    try:
        H[diag, diag - 1] = -chi0      # Assign col-1
    except IndexError:
        pass
H[0, NN-1] = 0

# Get eigenfunctions
eps, phi = la.eig(H)
indices = np.argsort(eps)

E = [J2eV * eps[indices][m] for m in range(NN)]

# Calculate particle density
kB = 8.62e-5; EF = 0.01; F = np.zeros((NN)); rho = np.zeros((NN)); ndens = np.zeros((NN))
temps = [20, 100]

sns.set(style='whitegrid')
f, axes = plt.subplots(len(temps), 2, figsize=(15, 12), sharey='col', sharex='col')
[ax[0].set_xlim((0, 0.1)) for ax in axes]
sns.despine(left=True, right=True, top=True, bottom=True)
for i, (T, ax) in enumerate(zip(temps, axes)):

    for n in range(NN):
        F[n] = 1.0 / (1 + np.exp((E[n] - EF) / (kB * T)))
        n_elec += 2 * F[n]
        for k in range(NN):
            rho[k] += 2 * F[n] * phi[k, n] * np.conj(phi[k, n])
            ndens[k] += 2 * F[n] * phi[k, n] * np.conj(phi[k, n])

    sns.lineplot(E, F, ax=ax[0], lw=3).set_title('Probability of Occupation of States -

```

```
sns.lineplot(XX, ndens, ax=ax[1], lw=3).set_title('Probability of Occupation of States - T = 20 K')
```

