TTT4120 Digital Signal Processing

Problem Set 1

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Contents

Part 1: Schrödingers Equation and the Kronig-Penney Model

Problem 1

(a) Start from the general, time-dependent Schrödinger equation

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t)$$

We assume that we can the solutions can be separated into spatial and time-dependent parts. Therefore we kan assume that $\Psi(\mathbf{x},t) = \psi(\mathbf{x})T(t)$, where $\psi(\mathbf{x})$ is the spatial part, and $T(t) = e^{(}-\frac{iEt}{\hbar})$ is the time-dependent part.

By replacing this in the Schrödinger equation

$$i\hbar\psi(\mathbf{x})\frac{dT}{dt} = -\frac{\hbar^2}{2m}T(t)\nabla^2\psi(\mathbf{x}) + V(\mathbf{x})\psi(\mathbf{x})T(t)$$

Divide both part with $\psi(\mathbf{x})T(t)$ to separate the variables:

$$i\hbar\frac{1}{T(t)}\frac{dT}{dt} = -\frac{\hbar^2}{2m}\frac{1}{\psi(\mathbf{x})}\nabla^2\psi(\mathbf{x}) + V(\mathbf{x})$$

The right side of this equation only depend on spatial variables, while the left side are only dependent og time. Therefore both side must be constant to sattisfy the equation for all $\mathbf{x}$ and t. we call this konstant for energy E, which gives us two equations:

$$i\hbar\frac{1}{T(t)}\frac{dT}{dt} = E$$

$$-\frac{\hbar^2}{2m}\frac{1}{\psi(\mathbf{x})}\nabla^2\psi(\mathbf{x}) + V(\mathbf{x}) = E$$

After reorganising the other equation we get the time independent Schrödinger equartion:

$$E\psi(\mathbf{x}) = -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{x}) + V(\mathbf{x})\psi(\mathbf{x})$$

b) Consider the infinite quantum well, described by the potential

$$V(x) = \begin{cases} \infty & x \leq 0 \\ 0 & 0 < x < L \\ \infty & x \geq 0 \end{cases}$$

This is a infinite quantum well in one dimension, therefore the particle can only move along the x-axis where $0 < x < L$. Since the potential is infinitely high outside the well, the wave function must me zero outside the well. Inside the well the wave function and its second derivative must be continlus. The wave equation only can exist inside the well, this implies that the wave equation is also normalizable.

In the area $0 < x < L$, the potential energy $V(x) = 0$, this gives us:

$$\frac{\partial^2}{\partial x^2}\phi = -\frac{2m}{\hbar^2}E\phi$$

We copy Faststoff project part one:

$$k^2 = \frac{2mE}{\hbar^2}$$

$$\frac{\partial^2}{\partial x^2}\phi = -k^2\phi$$

The general solution must be:E

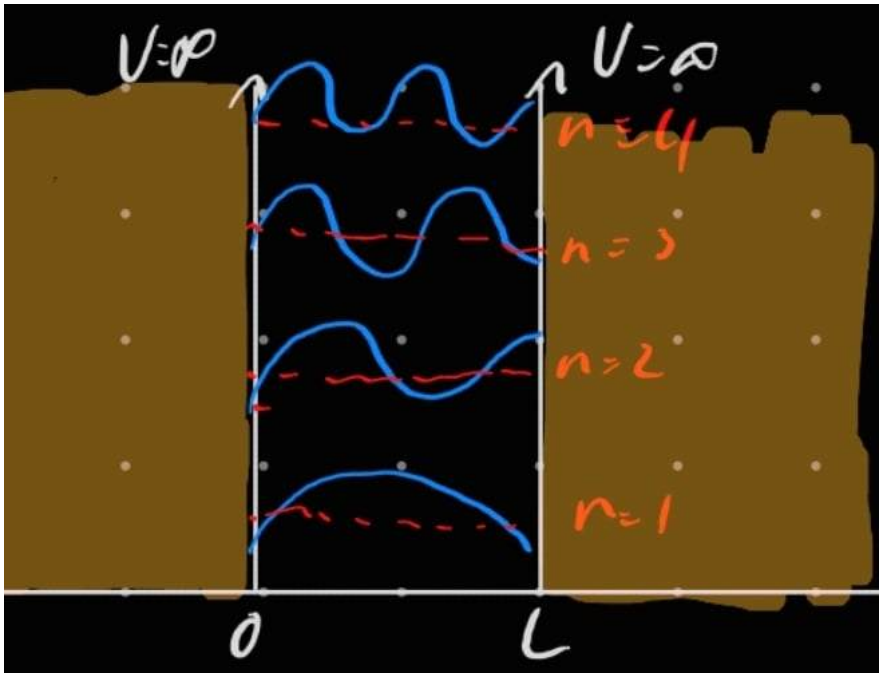
$$\phi(x) = A\sin(kx) + B\cos(kx)$$

For the function to be normalizable B must equal to 0. This does also imply that $\phi(L) = A\sin(kL) = 0$

This gives us the equation

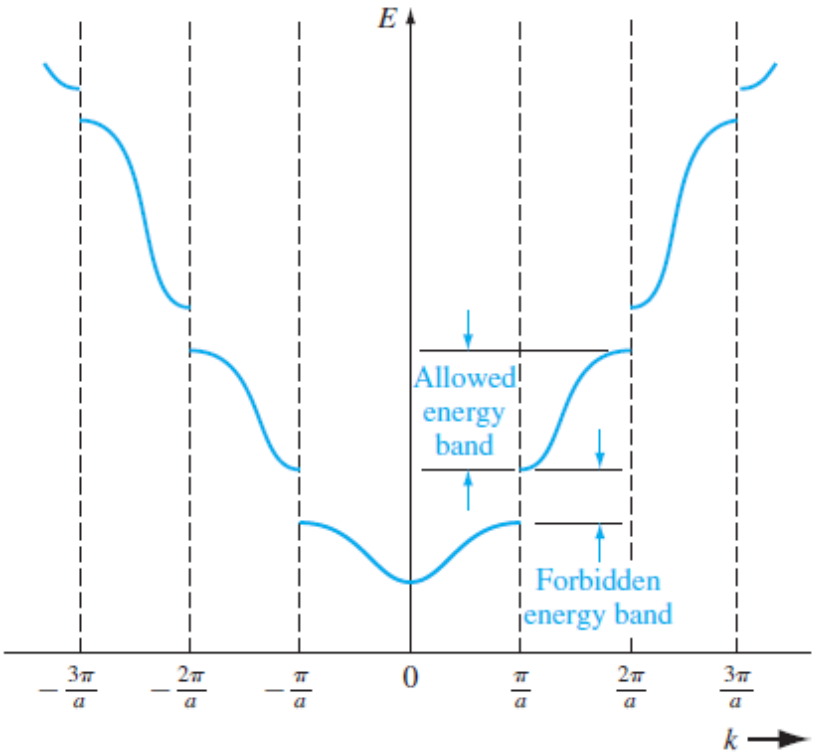
$$\phi(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$$

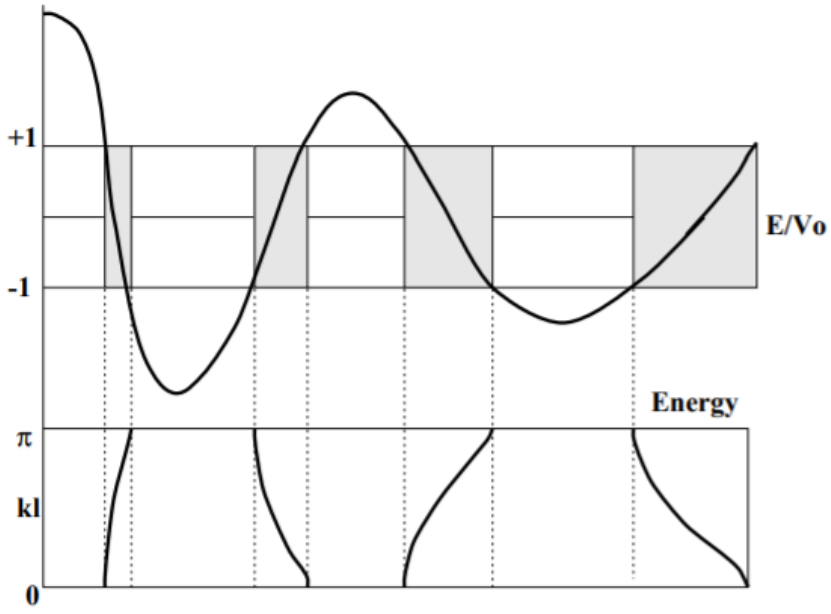
where the integral over the function from 0 to $L = 1$



(c) Kronig-Penney Model

By solving the Kronig-Penney model, we can calculate the dispersion relation by finding the energy levels for diffrent values of the wavevector k. This gives us a function $E(k)$ that describes how the energy of a electron changes with the wave equation mentioned in the previous problem.


E
Allowed energy band
Forbidden energy band
$-\frac{3\pi}{a}$
$-\frac{2\pi}{a}$
$-\frac{\pi}{a}$
0
$\frac{\pi}{a}$
$\frac{2\pi}{a}$
$\frac{3\pi}{a}$
k


+1
-1
E/Vo
Energy
π
kl
0

Part 2: Effective Mass

Problem 2

I expect to find the electrons with the highest mobility in the conduction band minima Γ as it has the highest curvature. This will give us tha least effective mass as

$$m* = \hbar^2 \frac{\partial^E (k)}{\partial k^2}$$

Problem 3

You cannot find information about the effective mass mass the effective mass are affected by the medium in which the electron it is traveling thru as well as the direction og the velovity in the medium as well.

Part 3: Carrier Concentrations

Problem 4

a) State the fermi-dirac distribution and explain what it describes.

The fermi-dirac distribution describes the probability for if a given energy state is occupied by a electron at a given temperature. It is given by the equation:

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

Where $f(E)$ is the probability for if a given energy state with the energy E is occupied by a electron. E_F is the Fermi-energy, k_B is Boltzmanns constant, and T is the temperature.

b) The general expression for calculating the concentration of electrons in the conduction band is

$$n_0 = \int_{E_c}^{\infty} f(E)N(E)dE$$

Explain the terms and parameters in the equation above and use it to derive the simplified expression

$$n_0 = N_c e^{-(E_c - E_F)/k_B T}$$

In this equation, the following terms are present:

1. n_0 is the total number of electrons in the conduction band per unit volume.
2. E_c is the minimum energy required for an electron to be in the conduction band.
3. $\int_{E_c}^{\infty}$ is an integral over all the energy states starting from E_c up to infinity. This integral sums up the probability of occupation times the number of available states at that energy.
4. $f(E)$ is the Fermi-Dirac distribution function, which gives the probability of occupation of an energy state E at a given temperature.
5. $N(E)$ is the density of available states at a given energy E

In this case we have that

$$N_C(E) = 4\pi \left(\frac{2m^*}{h^2}\right)^{\frac{3}{2}} \cdot E^{1/2}$$

and

$$f(E) = \frac{1}{1 + e^{(E-E_F)/k_BT}}$$

We aim to derive the simplified expression for n_0:

$$n_0 = N_c e^{-(E_c - E_F)/k_BT}$$

To proceed, we insert the expressions for $f(E)$ and $N(E)$ into the original equation and simplify:

$$\begin{aligned} n_0 &= \int_{E_c}^{\infty} \frac{N_c}{1 + e^{(E-E_F)/(k_BT)}}\, dE \\ &= N_c \int_{E_c}^{\infty} \frac{1}{1 + e^{(E-E_F)/(k_BT)}}\, dE \end{aligned}$$

We perform the integral by making the substitution $u = (E - E_F)/(k_BT)$ which implies $dE = k_BT\, du$:

$$\begin{aligned} n_0 &= N_c k_B T \int_{(E_c-E_F)/(k_BT)}^{\infty} \frac{1}{1 + e^u}\, du \\ &\approx N_c k_B T \int_{-\infty}^{0} e^u\, du \\ &= N_c k_B T [-e^u]_{-\infty}^{0} \\ &= N_c(1) \\ &= N_c e^{-(E_c-E_F)/(k_BT)} \end{aligned}$$

Note: The approximation step where the integral limits change assumes that E_c is sufficiently greater than E_F such that the Fermi-Dirac distribution is almost zero beyond E_c.

Thus, we have derived the simplified expression:

$$n_0 = N_c e^{-(E_c-E_F)/(k_BT)}$$

c) Show that the equation above may be written as

$$n_0 = n_i e^{(E_F - E_i)/k_B T}$$

where n_i and E_i are the intrinsic electron concentration and intrinsic fermi-level, respectively.

First, let's define the intrinsic electron concentration n_i in terms of N_c and E_c:

$$n_i = N_c e^{-(E_c - E_i)/k_B T}$$

Now, substitute this definition into the original equation for n_0:

$$n_0 = N_c e^{-(E_c - E_F)/k_B T}$$

Divide both sides by n_i:

$$\frac{n_0}{n_i} = \frac{N_c e^{-(E_c - E_F)/k_B T}}{N_c e^{-(E_c - E_i)/k_B T}}$$

Simplifying, we get:

$$\frac{n_0}{n_i} = e^{(E_i - E_F)/k_B T}$$

Multiply both sides by n_i:

$$n_0 = n_i e^{(E_F - E_i)/k_B T}$$

Thus, we have shown that the original equation can be rewritten in the desired form.

d) Show that the intrinsic fermi level E_i is in the middle of the bandgap if and only if the effective densities of states N_c and N_v are equal

We know the expressions for the intrinsic carrier concentrations for electrons n_i and holes p_i as:

$$n_i = N_c e^{-(E_c - E_i)/k_B T}$$

$$p_i = N_v e^{-(E_i - E_v)/k_B T}$$

For intrinsic semiconductors, $n_i = p_i$. Setting these equal gives:

$$N_c e^{-(E_c - E_i)/k_B T} = N_v e^{-(E_i - E_v)/k_B T}$$

Taking the logarithm of both sides yields:

$$-(E_c - E_i)/k_B T + \ln N_c = -(E_i - E_v)/k_B T + \ln N_v$$

Simplifying, we find:

$$(E_c - E_i) - (E_i - E_v) = k_B T(\ln N_c - \ln N_v)$$

Further simplifying:

$$E_c - E_v = k_B T \ln\left(\frac{N_c}{N_v}\right)$$

For E_i to be in the middle of the bandgap, $E_c - E_i = E_i - E_v$ or $E_i = (E_c + E_v)/2$.

This condition is met if $\ln(N_c/N_v) = 0$ or $N_c = N_v$.

Thus, E_i is in the middle of the bandgap if and only if $N_c = N_v$.

e) Use

$$N_C = 2\left(\frac{2\pi m_n^* k_B T}{h^2}\right)^{\frac{3}{2}}$$
$$N_V = 2\left(\frac{2\pi m_p^* k_B T}{h^2}\right)^{\frac{3}{2}}$$

to show that the intrinsic Fermi level E_i is positioned below the middle of the bandgap by

$$\Delta E = k_B T \ln\left(\frac{m_n^*}{m_p^*}\right)^{\frac{3}{4}}$$

We previously derived that:

$$E_c - E_v = k_B T \ln\left(\frac{N_c}{N_v}\right)$$

Substitute the expressions for N_C and N_V:

$$E_c - E_v = k_B T \ln\left(\frac{2\left(\frac{2\pi m_n^* k_B T}{h^2}\right)^{\frac{3}{2}}}{2\left(\frac{2\pi m_p^* k_B T}{h^2}\right)^{\frac{3}{2}}}\right)$$

Simplifying, we get:

$$E_c - E_v = k_B T \ln\left(\left(\frac{m_n^*}{m_p^*}\right)^{\frac{3}{2}}\right)$$

$$E_c - E_v = \frac{3}{2} k_B T \ln\left(\frac{m_n^*}{m_p^*}\right)$$

For E_i to be at the middle of the bandgap, we would have:

$$E_i = \frac{E_c + E_v}{2}$$

Due to the effective mass difference, E_i will actually be shifted by ΔE below the middle:

$$E_i = \frac{E_c + E_v}{2} - \Delta E$$

Where ΔE is:

$$\Delta E = \frac{1}{2} \times \frac{3}{2} k_B T \ln\left(\frac{m_n^*}{m_p^*}\right)$$

$$\Delta E = k_B T \ln\left(\frac{m_n^*}{m_p^*}\right)^{\frac{3}{4}}$$

Thus, we have shown that ΔE is the amount by which the intrinsic Fermi level is positioned below the middle of the bandgap.

f) Calculate this deviation (from the midgap energy) for Ge and GaAs.

Effective masses for Ge: $m_n^* = 0.56m_0; m_p^* = 0.29m_0$
Effective masses for GaAs: $m_n^* = 0.067m_0; m_p^* = 0.48m_0$

o calculate the deviation ΔE for Ge and GaAs, we use the formula:

$$\Delta E = k_B T \ln \left(\frac{m_n^*}{m_p^*} \right)^{\frac{3}{4}}$$

Here $k_B = 8.617 \times 10^{-5}\,\text{eV/K}$ is the Boltzmann constant, and we assume room temperature $T = 300\,\text{K}$.

For Ge:

Effective masses for Ge are $m_n^* = 0.56m_0$ and $m_p^* = 0.29m_0$.

$$\Delta E_{\text{Ge}} = 8.617 \times 10^{-5} \times 300 \ln \left(\frac{0.56}{0.29} \right)^{\frac{3}{4}}$$

After calculations, we find $\Delta E_{\text{Ge}} \approx 0.010\,\text{eV}$.

For GaAs:

Effective masses for GaAs are $m_n^* = 0.067m_0$ and $m_p^* = 0.48m_0$.

$$\Delta E_{\text{GaAs}} = 8.617 \times 10^{-5} \times 300 \ln \left(\frac{0.067}{0.48} \right)^{\frac{3}{4}}$$

After calculations, we find $\Delta E_{\text{GaAs}} \approx -0.029\,\text{eV}$.

Thus, we have calculated the deviations ΔE from the midgap energy for Ge and GaAs.