Chapter 4 problems

LAST NAME FIRST NAME

Problem 4.1

(a) Write a computer program in MATLAB that uses the propagation matrix method to find transmission as a function of energy for a particle mass m_0 through 12 identical one-dimensional potential barriers each of energy 1 eV, width 0.1 nm, sequentially placed every 0.5 nm (so that the potential well between each barrier has width 0.4 nm). Particle mass m_0 is the bare electron mass. What are the allowed (band) and disallowed (band gap) ranges of energy for particle transmission through the structure? How do you expect the velocity of the transmitted particle to vary as a function of energy?

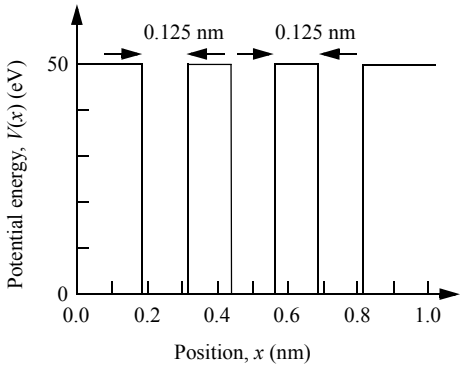
(b) How do these bands compare with the situation in which there are only three barriers, each with 1 eV barrier energy, 0.1 nm barrier width, and 0.4 nm well width?

Your solution should include plots of transmission as a function of energy and a listing of the computer program you used.

Problem 4.2

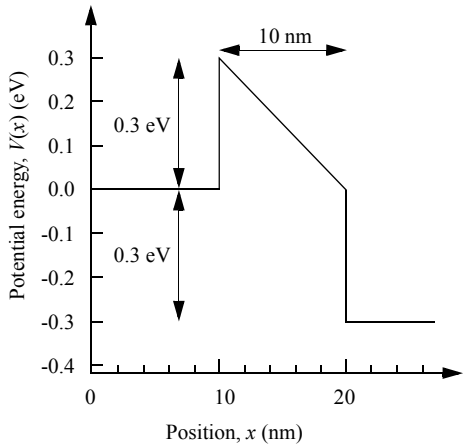
(a) Using the method outlined in 3.4, write a computer program to solve the Schrödinger wave equation for the first three eigenvalues and eigenstates of an electron of mass m_0 confined to a triple rectangular potential well sketched in the figure below. Each well is of width 0.125 nm and the barrier is of width 0.125 nm. The barrier potential energy is 50 eV. In the region $x \leq 0$ nm and $x \geq 1$ nm the potential is infinite. Compare the energy eigenvalues with those you may infer using the propagation method for the same potential except in the region $x \leq 0$ nm and $x \geq 1$ nm where the potential is zero.

(b) If (a) models an electron in a linear molecule, which state is likely to bond the molecule together?



Your results should include: (i) a printout of the computer program you used; (ii) a computer-generated plot of the potential; (iii) a list of the energy eigenvalues; (iv) a computer-generated plot of the eigenfunctions.

Problem 4.3



Write a computer program in MATLAB that uses the propagation matrix method to calculate transmission of an electron with effective mass $m_e^* = 0.07 \times m_0$ for the following one-dimensional potentials.

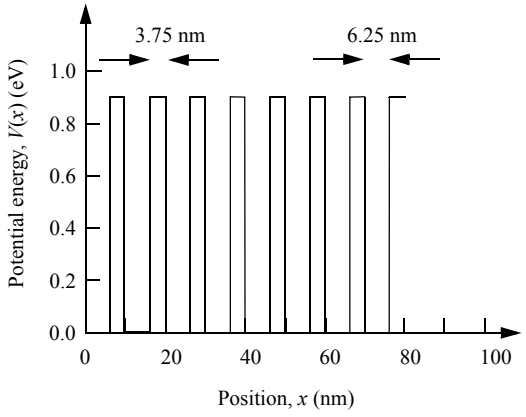
(a) A uniform electric field applied across a single potential barrier structure as shown in the above figure. The right-hand edge of the 10-nm-thick barrier with energy 0.3 eV is at a potential energy $\Delta V = -0.3$ eV below the left-hand edge of the barrier. Comment on the changes in transmission you observe as a function of incident particle energy $-0.3 < E < 1$ eV.

(b) Rewrite your program to calculate transmission of the particle as a function of potential energy drop $0 < \Delta V < -2$ eV caused by the application of an electric field across the barrier. Calculate the specific case of initial particle energy $E = 0.025$ eV with the particle incident on the structure from the left-hand side. Explain the results you obtain.

Your solution should include a printout of the computer program you used.

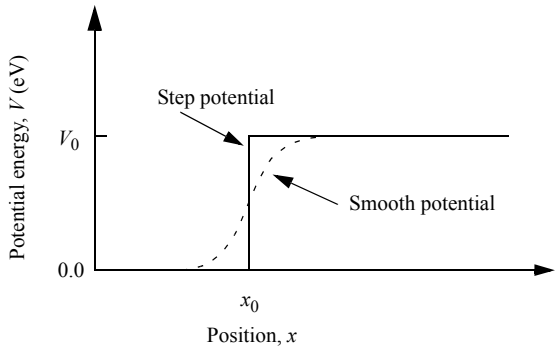
Problem 4.4

Write a computer program to solve the Schrödinger wave equation for the first 17 eigenvalues of an electron with effective mass $m_e^* = 0.07 \times m_0$ confined to the periodic potential sketched in the figure below *with periodic boundary conditions*. Each of the eight quantum wells is of width 6.25 nm. Each quantum well is separated by a potential barrier of thickness 3.75 nm. The barrier potential energy is 0.9 eV. How many energy band gaps are present in the first 17 eigenvalues and what are their values? Plot the highest energy eigenfunction of the first band and the lowest energy eigenfunction of the second band.



Problem 4.5
Use the results of Problem 4.4 with periodic boundary conditions to approximate a periodic one-dimensional delta function potential with period 10 nm by considering 8 potential barriers with energy 20 eV and width 0.25 nm. Plot the lowest and highest energy eigenfunction of the first band. Explain the difference in the wave functions you obtain.

Problem 4.6



A step change in potential by an amount V_0 at position $x = x_0$ causes quantum mechanical reflection for a particle mass m and energy $E > V_0$. This is in contrast to the classical result for which reflection is zero. Quantum mechanical reflection can be reduced if, as illustrated in the above figure, the step change in potential is replaced by a smoothly varying potential. Write down and equation that may be used for modeling the smoothly varying potential and indicate the parameter(s) in your model that quantify the smoothness. How slowly varying does a potential barrier have to be for reflection to approach the classical result?

Problem 4.7
What value (in eV) of the overlap integral t should you use in the nearest neighbor tight binding model to reproduce the effective electron mass $m^* = 0.07 \times m_0$ near the conduction band minimum of GaAs?

Use the fact that the lattice constant of GaAs is $L = 0.565$ nm.

Problem 4.8
Explain why you expect the energy band width of allowed electron states in a crystal to decrease as the lattice spacing between atoms increases.

Problem 4.9
A crystal with identical atoms at lattice sites $x_n = nL$, where n is an integer and L is the nearest neighbor atom spacing, has wave function $\psi_{k_x}(x)$ that can be expressed as a direct lattice sum of Wannier functions $\phi(x)$ localized around each lattice site x_n. Show that

$$\psi_{k_x}(x) = \sum_n e^{ik_x x_n} \phi(x - x_n)$$

satisfies the Bloch condition

$$\psi_{k_x}(x + L) = \psi_{k_x}(x) e^{ik_x L}$$

Problem 4.10

The propagation matrix method we have used divides a one-dimensional potential $V(x)$ into N potential steps and then solves the Schrödinger equation for a particle of energy E in a piece-wise constant fashion. The wave function across the j-th step is

$$\psi_j(x) = A_j e^{ik_j x} + B_j e^{-ik_j x}$$

and because we can calculate A_j and B_j it is possible to obtain $\psi_j(x)$.

(a) Use the propagation matrix method to reproduce the transmission characteristics shown in Fig. 4.11(b) for an electron incident from the left on the potential shown in Fig. 4.11(a). Verify the FWHM of the two lowest energy resonant transmission peaks.

(b) Calculate and plot the real and imaginary part of the wave function and the modulus of the wave function squared, $|\psi(x)|^2$, for the cases when the electron has energy $E = 321.6$ meV and energy $E = 401.5$ meV. Comment on your results.

(c) Plot $|\psi(x)|^2$ as a function of position and energy. Explain the features you see on your 3D plot or contour plot.

Your solution should include a printout of the computer program you used.

Problem 4.11

Starting with the same potential as Problem 4.10, plot the transmission, reflection, and probability density at the first two resonances for the cases when the potential in the *wells* is of the complex form $V = V_1 + iV_2$ such that

(a) $V_1 = 0$ eV and $V_2 = 0.01$ eV

(b) $V_1 = 0$ eV and $V_2 = -0.01$ eV

How do the FWHM of the resonances change compared to those of Fig. 4.11(b)? Explain your results. You may find it helpful to plot the real and imaginary parts of the wave function on resonance.

Problem 4.12

(a) Write a computer program in MATLAB that reproduces Fig. 4.14(a) of the text using the propagation matrix method. Use an electron effective mass $m^* = 0.07 \times m_0$, 1.5 nm barrier width, 1 eV barrier energy, and 2 nm well width. Consider electron energy in the range of 0 eV to 1 eV and vary the central barrier width from 0 nm to 6 nm. Include a 3-dimensional plot of the transmission coefficient versus the injection energy and central barrier width. Describe why energy splitting occurs. At approximately what barrier width does electron localization occur?

(b) Modify your code from (a) to include calculation of the wave function given a specific central barrier width and injection energy. Plot electron probability density at the transmission maxima for central barrier widths of 0 nm and 6 nm. Because you are using the propagation matrix to calculate the wave functions with a right-propagating wave initial condition, only one of the degenerate wave functions is calculated for the localized electron. Sketch by hand the other degenerate probability density.

(c) Plot the probability density at the transmission maximum when the central barrier width is 3.5 nm thick. Explain your result and compare with what you would expect the probability density to be just on the other side of the localization threshold.

Problem 4.13

(a) Using the method outlined in Exercise 3.7 as a starting point, write a computer program that will numerically evaluate the time-evolution of both $|\psi(x, t)|^2$ and the current density of a superposition of states for an electron confined within a constant potential well with infinite potential barri-

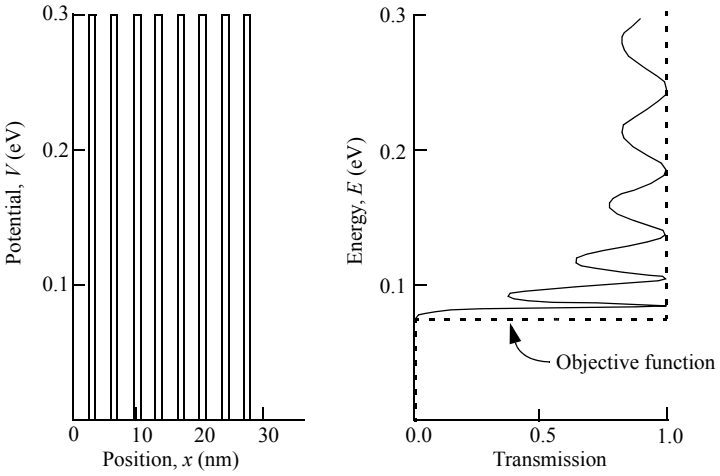
ers. Use this program to generate a movie of $|\psi(x, t)|^2$ and the current density of a superposition of the first and second excited states of an infinite potential well that is 11 nm wide containing a 1 nm wide, 0.6 eV energy barrier centered within the well. Use an effective electron mass of $m^* = 0.07 \times m_0$. Submit snapshots of $|\psi(x, t)|^2$ and current density at times $t = 0$, $t = 3$ fs, and $t = 7.5$ fs along with a computer printout of your program. Describe how the superposition state evolves in time.

(b) Repeat part (a) using a potential well that is 30 nm wide containing a 20 nm wide barrier of potential energy 0.6 eV centered within the well. Submit snapshots of $|\psi(x, t)|^2$ and current density at times $t = 0$, $t = 2.5$ fs, and $t = 6.5$ fs. Describe how the superposition state evolves in time.

(c) Compare your results from parts (a) and (b) and explain their differences.

Problem 4.14

Calculated transmission as a function of energy for an electron confined to motion in the x-direction and incident on an array of eight AlGaAs barriers is shown as a solid curve in the following figure. The conduction band electron has mass $m^* = 0.07 \times m_0$, each AlGaAs barrier is 1 nm thick and has barrier energy 0.3 eV relative to the GaAs wells, each of which are 2.5 nm thick.



(a) Keeping the total thickness of each barrier-well pair constant and by independently varying the relative thickness of each barrier-well pair, write a MATLAB program to find the optimal potential profile that minimizes transmission for electron energies less that 75 meV and maximizes electron transmission for energies in the range 75 meV to 300 meV. This step-function objective is shown as the dashed line in the figure.

(b) The optimization in (a) is formulated using a one-dimensional physical model (the electron is confined to motion in the x-direction). If the physical model allows surface roughness in the potential and electron scattering in the y and z-direction how does this change the optimization result in (a)?

Problem 4.15

Six atoms, each with a coulomb potential, form a ring with equal nearest-neighbor spacing between atoms. Treating this as a one-dimensional problem with spatial coordinate along the circumference of the ring, sketch and explain what you anticipate are the first seven lowest-energy electron wave functions in the system.

Problem 4.16

(a) Plot the first four real and first four imaginary bands $E_k(k)$ in the reduced zone for a Kronig-Penney model with $k_0 L = 8$.

(b) Explain the change in energy band width, energy band gap, and effective electron mass at the real and imaginary band extrema as a function of increasing energy, E_k.

(c) How do you expect the spatial extent of mid-gap states to change with increasing energy, E_k?

Problem 4.17

Using the results of Problem 4.10 write a MALAB program that demonstrates the propagation of a single-electron Gaussian wave packet superposition state $\psi(x, t)$ constrained to motion in the x-direction and initially moving left-to-right in (a) a constant potential $V(x) = 0$ eV and (b) incident on a rectangular potential barrier of energy $V_0 = 0.6$ eV and thickness $L = 5$ nm. The electron has effective electron mass $m_{\text{eff}} = 0.07 \times m_0$, the standard deviation of the Gaussian wave packet is $\sigma_k = 3 \times 10^8$ m^{-1} and its central energy is 0.5 eV. Comment on what you learn.

Problem 4.18

The Schrödinger equation describing the behavior of a single particle mass m in potential $V(x)$ is similar to the Helmholtz equation that describes the propagation of electromagnetic field through a lossless dielectric characterized by refractive index n_r.

(a) Consider a particle with energy $E = \hbar\omega$ and mass m moving in the x-direction that is incident on a rectangular potential barrier $V(x) = V_0$ for $0 < x < L$ and $V(x) = 0$ elsewhere. Show that the transmission probability $|C|^2 \to 0$ as $\omega \to 0$.

(b) Consider linearly polarized electromagnetic radiation of frequency ω and wave vector k normally incident on a lossless dielectric slab of thickness L and refractive index n_r. Show that the transmission probability $|C|^2 \to 1$ as $\omega \to 0$ and explain the difference in this result compared to (a).

(c) *If*, in the low frequency limit, the lossless dielectric slab in (b) has dispersion $\omega = ak^\gamma$ where a is a constant, find the values of γ for which $|C|^2 \to 0$ as $\omega \to 0$. Use MATLAB to make a 3D plot of $\omega = k^\gamma$ and a 3D plot of $|C(k, \gamma)|^2$ using parameter values in the range $0 < k < 2.5$ and $0 < \gamma < 2.5$. Explain anything you learn about the limitations of the physical model used.