Chapter 3 problems

Problem 3.1

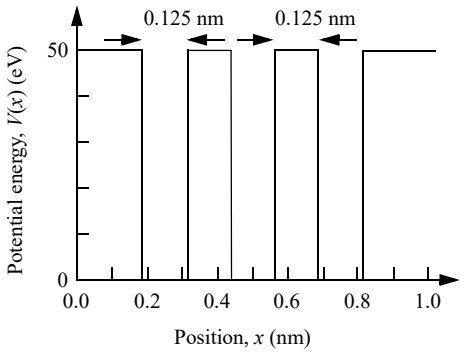
Write a computer program in MATLAB that uses the propagation matrix method to find the transmission resonances of a particle of mass $m = 0.07 \times m_0$ incident on a parabolic potential energy barrier with $V(x) = x^2/L^2$ eV for $|x| \le L = 5$ nm and $V(x) = 0$ eV for $|x| > L$. What happens to the resonant transmission energy levels if particle mass is $m = 0.14 \times m_0$?

The solution should include plots of transmission as a function of energy, a list of the resonant energy level values and associated spectral line widths, and a listing of the computer program used.

Problem 3.2

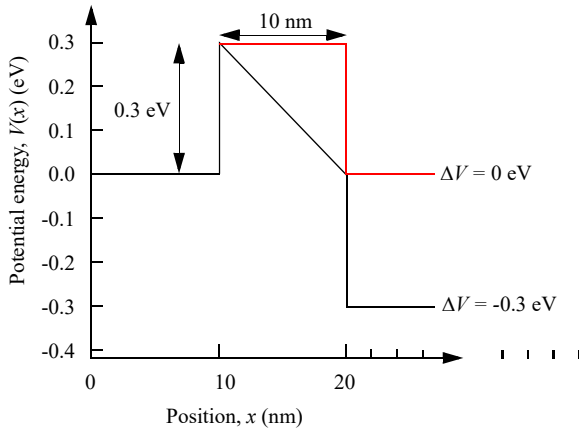
(a) Using the method outlined in 2.4, write a computer program to solve the Schrödinger wave equation for the first three eigenvalues and eigenstates of an electron of mass m_0 confined to a symmetric triple rectangular potential well sketched in the following figure. Each well is of thickness 0.125 nm and the barrier is of thickness 0.125 nm. The barrier potential energy is 50 eV. In the region $x \le 0$ nm and $x \ge 1$ nm the potential is infinite. Compare the energy eigenvalues with those obtained using the propagation method for the same potential except in the region $x \le 0$ nm and $x \ge 1$ 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?



The results should include: (i) a printout of the computer program 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 3.3



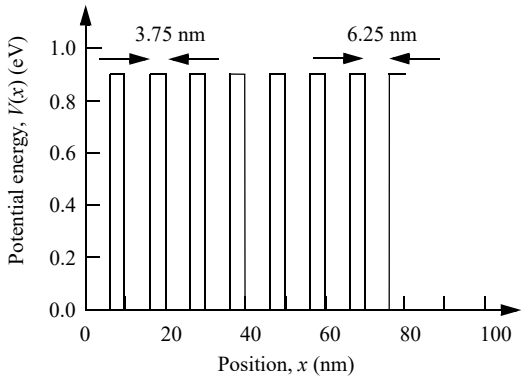
Write a program in MATLAB that uses the propagation matrix method to calculate transmission of an electron with effective mass $m_e^* = 0.07 \times m_0$ as a function of potential energy drop

$-2\ \text{eV} < \Delta V < 0\ \text{eV}$ caused by the application of a uniform electric field across a single potential barrier structure as shown in the above figure. 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 obtained.

Problem 3.4

(a) 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 following figure *with periodic boundary conditions*. Each of the eight quantum wells is of thickness 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.

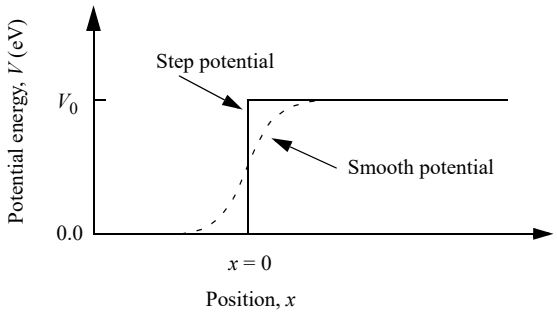
(b) How does dispersion in (a) change if quantum well thickness is changed to 8.75 nm and potential barrier thickness to 1.25 nm?



Problem 3.5

Use the results of Problem 3.4 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 thickness 0.25 nm. Plot the lowest and highest energy eigenfunction of the first band. Explain the difference in the wave functions obtained.

Problem 3.6



(a) Explain why an *abrupt* step change in potential by an amount V_0 at position $x = 0$ *always* causes quantum mechanical reflection for a particle mass m and energy $E > V_0$ and so *can never* give the classical result of no reflection when $E > V_0$.

(b) Quantum mechanical reflection in (a) can be reduced to zero if, as illustrated in the above figure, the step change in potential is replaced by a smoothly varying potential to ensure an adia-

batic transition near position $x = 0$. A suitable potential (which becomes a step potential in the limit $\alpha \to \infty$) is

$$V(x) = \frac{V_0}{e^{-\alpha x} + 1}$$

Using this potential, find an expression for the reflection coefficient when $E > V_0$ and show that the reflection coefficient is zero in the limit $\hbar \to 0$ for finite positive α.

Problem 3.7

What value (in eV) of the overlap integral $t_{\text{hop,1}}$ should be used 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 with lattice constant $L = 0.565$ nm ?

Problem 3.8

Explain why energy bandwidth of allowed electron states in a crystal to decrease as the lattice spacing between atoms increases.

Problem 3.9

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 3.10

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. 3.11(b) for an electron incident from the left on the potential shown in Fig. 3.11(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 magnitude 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 the results.

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

Problem 3.11

Starting with the same potential as Problem 3.10, 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. 3.11(b)? Explain the results. It can be helpful to plot the real and imaginary parts of the wave function on resonance.

(c) What objections are there to the use of complex potentials in quantum mechanics?

Problem 3.12

(a) Write a computer program in MATLAB that reproduces Fig. 3.19(a) of the text using the propagation matrix method. Use an electron effective mass $m^* = 0.07 \times m_0$, 1.5 nm barrier thickness, 1 eV barrier energy, and 2 nm well thickness. Consider electron energy in the range of 0 eV to 1 eV and vary the central barrier thickness from 0 nm to 6 nm. Include a three-dimensional plot of the transmission coefficient versus the injection energy and central barrier thickness. Describe why energy splitting occurs. Plot the logarithm of maximum transmission as a function of central barrier thickness on a linear scale and determine the approximate value of barrier thickness beyond which unity resonant electron transmission no longer occurs.

(b) Modify the code from (a) to include calculation of the wave function given a specific central barrier thickness and injection energy. Plot electron probability density at the transmission maxima for central barrier thicknesses of 0 nm and 6 nm. Because the propagation matrix is used 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 thickness is 3.5 nm. Explain the result and compare with the expected probability density when the central barrier thickness is less than 3 nm.

Problem 3.13

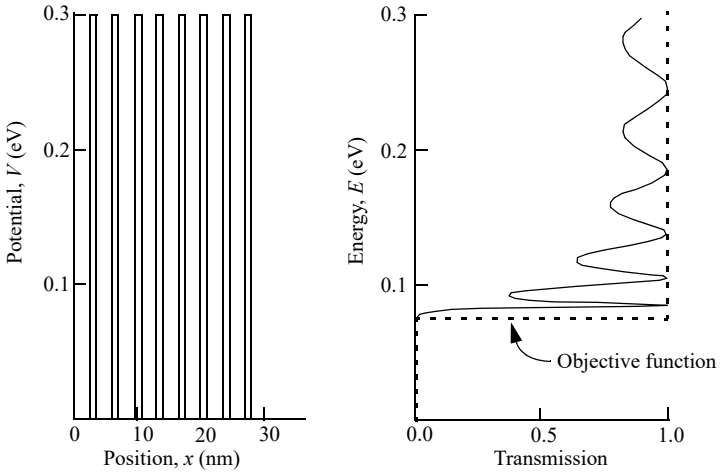
(a) Using the method outlined in Exercise 2.6 as a starting point, write a computer program that will numerically evaluate the time-evolution of both $|\psi(x, t)|^2$ and the current density of a superposition of states for an electron confined within a constant potential well with infinite potential barriers. 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 thick containing a 1 nm thick, 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 printout of the computer program. Describe how the superposition state evolves in time.

(b) Repeat part (a) using a potential well that is 30 nm thick containing a 20 nm thick 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 the results from parts (a) and (b) and explain their differences.

Problem 3.14

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) What physically limits finding a solution that *exactly* matches the objective function?

(c) 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 3.15

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 the solution for the first seven lowest-energy electron wave functions in the system.

Problem 3.16

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

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

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

Problem 3.17

Using the results of Problem 3.10 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) with peak position $x = 0$ at $t = 0$ and incident on a rectangular potential barrier of energy $V(25 \text{ nm} \le x \le 35 \text{ nm}) = 0.6$ eV. The electron has effective electron mass $m_{\text{eff}} = 0.07 \times m_0$, the standard deviation of the Gaussian wave packet is $\sigma_k = 3 \times 10^8 \text{ m}^{-1}$ and its central energy is 0.5 eV.

Problem 3.18
The Schrödinger equation describing the behavior of a single particle mass m incident on a potential barrier $V(x)$ is similar to the Helmholtz equation that describes the propagation of electromagnetic field incident on a lossless dielectric characterized by refractive index n_r.

(a) Consider a particle with positive 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 $|C|^2 \to 1$ as $\omega \to 0$. Make a 3D plot of $|C(k, \gamma)|^2$ using parameter values in the range $0 < k < 0.005$ and $-1 < \gamma < 2.5$.

(d) *If* group velocity $\upsilon_g = \dfrac{d\omega}{dk}$ in the dielectric in part (c) is limited to be less than or equal to the speed of light in vacuum, what further constraints are placed on allowed values of γ? Explain the limitations of the physical model used.

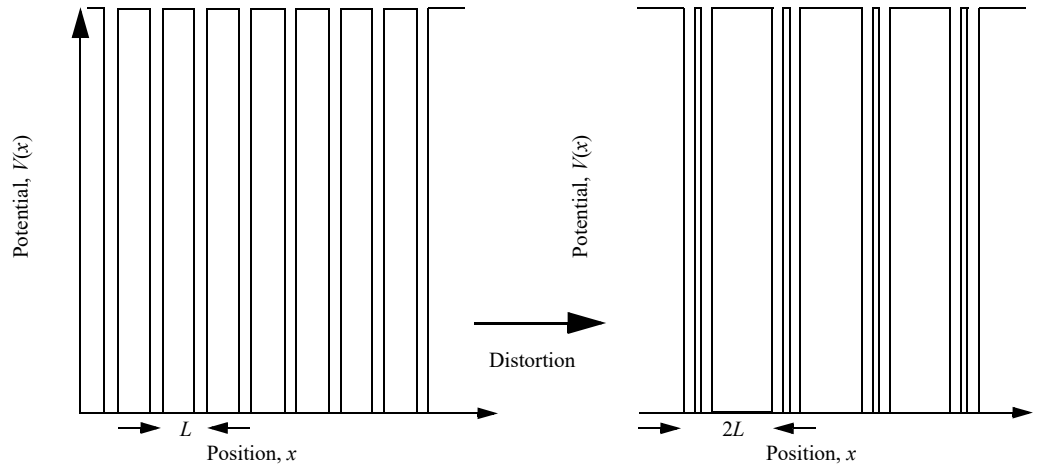
Problem 3.19
The wave function of an electron energy E_k constrained to motion in a one-dimensional periodic potential is a Bloch function $\psi_k(x) = U_k(x)e^{ikx}$

(a) Substitute $\psi_k(x)$ into the one-electron time-independent Schrödinger equation and show that the cell-periodic term $U_k(x)$ satisfies

$$\left(\frac{\hbar^2}{2m_0}\left(-i\frac{d}{dx}+k\right)^2 + V(x)\right)U_k(x) = E_k U_k(x)$$

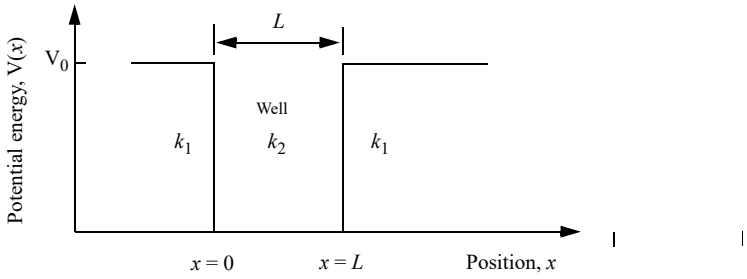
(b) Find $U_k(x)$ and E_k when the potential is a constant such that $V(x) = V_0$.

Problem 3.20
If the crystal structure of a simple one-dimensional metal with a potential periodic in L is deformed by a strain field such that the potential becomes periodic in $2L$ as illustrated in the following figure, what changes to the band structure and properties of the metal can be predicted?



Problem 3.21

The propagation matrix method can be used to find energy eigenvalues for bound states. To show this, consider a symmetric potential well of thickness L and energy V_0 illustrated in the following Fig. The wave function describing a particle mass m and energy E has wave vector $k_1 = \sqrt{2m(E - V_0)}/\hbar$ outside the potential well and $k_2 = \sqrt{2mE}/\hbar$ inside the well.



(a) The wave function at position $x = \pm\infty$ is connected via the propagation matrix such that

$$\begin{bmatrix} A \\ B \end{bmatrix}_{x=-\infty} = \mathbf{P} \begin{bmatrix} C \\ D \end{bmatrix}_{x=\infty} = \begin{bmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix}_{x=\infty}$$

Explain why bound-state solutions require $A = D = 0$.

(b) For the case when $L = 10$ nm, $m = 0.07 \times m_0$, and $V_0 = 0.5$ eV, plot P_{11} as a function of particle energy in the range $0 < E < V_0$ and find the bound-state energy eigenvalues.

(c) Explain the behavior of P_{11} when either $E < 0$ or $E > V_0$.

(d) Explain how to extend the propagation matrix method calculation of bound state energy eigenvalues and eigenfunctions to an arbitrary potential well.

Problem 3.22

An electron of energy E and mass m_e^* is incident at angle θ_1 from the normal of a planar rectangular potential barrier of energy V_0 and thickness L.

(a) For $m_e^* = 0.07 \times m_0$, $V_0 = 0.15$ eV, and $L = 15$ nm, calculate and plot electron transmission as a function of $0 \le \theta_1 < 60^\circ$ and $0 < E \le 0.35$ eV. Explain the results.

(b) Identify and plot the critical angle $\theta_{crit}(V_0 < E \le 0.35\ \text{eV})$. Why is transmission *not* zero for $\theta > \theta_{crit}$?

Problem 3.23

The dispersion relation of an electron moving in the conduction band of a one-dimensional periodic potential with lattice spacing $L = 0.5$ nm is described by a nearest neighbor tight-binding model.

(a) Find the value of the hopping integral $t_{hop,1}$ that results in an effective electron mass of $m_e^* = 0.07 \times m_0$ for an electron with energy $E = 50$ meV above the conduction band minimum.

(b) The dispersion relation in (a) is $\omega(k)$ with first derivative $d\omega/dk = \omega'(k)$ and second derivative $d^2\omega/dk^2 = \omega''(k)$.

A Gaussian electron wave function propagates in the band according to

$$\psi(x,t) = \left(\frac{\sigma_x^2}{2\pi}\right)^{\frac{1}{4}} \frac{e^{i(k_0(x-x_0)-\omega(k_0)t)}}{\sqrt{\sigma_x^2 + \frac{i\omega''(k_0)t}{2}}} e^{-(x-x_0-\omega'(k_0)t)^2/(4\sigma_x^2 + i2\omega''(k_0)t)}$$

where $\hbar\omega(k_0)$ is the central energy, x_0 is the initial mean position, and a measure of the initial spatial spread of the wave packet is the standard deviation σ_x. Plot $|\psi(x)|^2$ for the electron in (a) at time $t = 0$ and $t = 0.5$ ps with $\sigma_x = 10$ nm. How does the wave packet evolve in time if the central energy of the electron in the band is $E = 2 \times t_{hop,1}$?

Problem 3.24

(a) In the tight-binding nearest-neighbor approximation write down an expression for the energy of an electron s-orbital on the *n*-th site of a one-dimensional crystal with lattice constant *L* and nearest-neighbor hopping energy $t_{hop,1}$. Use the Bloch theorem to find an expression for electron energy dispersion $E(k)$ where *k* is the Bloch wave vector.

(b) The electron in (a) is subject to a static uniform longitudinal external electric field **E** in the *x*-direction. Find the time evolution of the Bloch wave vector in this system.

(c) If the lowest energy propagating state of the system is $E = 0$, find an expression for the group velocity, $\upsilon_g(k(t))$, of an electron with $k(t = 0) = 0$.

(d) Calculate the numerical value of the frequency and wavelength in free-space of Bloch oscillations for an electron in an electric field of strength $|\mathbf{E}| = 10^7\ \text{V m}^{-1}$ in the one-dimensional crystal with $L = 0.5$ nm.

Problem 3.25

Near the Γ-point of a direct band gap semiconductor, electron energy dispersion of propagating states in the conduction band may be written as

$$E_c - E_g \equiv \frac{\hbar^2 k^2}{2m_c^*} = E(1 + \alpha E)$$

where

$$\alpha = \frac{1}{E_g}\left(1 - \frac{m_c^*}{m_0}\right)^2$$

is the conduction band nonparabolicity factor and *E* is electron energy measured from the conduction band minimum, m_c^* is the effective electron mass at the conduction band minimum, E_g is the semiconductor band gap energy, and m_0 is the bare electron mass.

(a) Show that the group velocity of an electron propagating in the conduction band is

$$\upsilon_c = \frac{\sqrt{2E(1+\alpha E)/m_c^*}}{1+2\alpha E}.$$

(b) Using the GaAs band gap energy $E_g = 1.42$ eV and effective electron mass at the conduction band minimum $m_c^* = 0.07 \times m_0$, calculate the velocity of a conduction band electron of energy $E = 300$ meV and compare to the case when the value of the nonparabolicity factor is zero ($\alpha = 0$). Find the ratio of velocities.

Problem 3.26

The complex dispersion relation in the energy band *gap* of an ideal bulk crystalline semiconductor is a function $E(k) = \hbar\omega(k)$ in which wave vector k has an imaginary component, $\mathrm{Im}(k) = \mathrm{i}\kappa$.

(a) Explain why noninteracting electrons cannot occupy states with an energy eigenvalue that falls within the band gap energy of a perfect bulk crystal's static periodic potential.

(b) Why is complex band structure useful when considering finite-sized nanoscale semiconductor devices?

Problem 3.27

The Lippmann-Schwinger equation for the wave function $\psi(x)$ of a particle of energy E and mass m^* propagating in the x-direction from left to right positions x_L and x_R, respectively, in potential $V(x)$ may be written as

$$\psi(x) \approx \psi_0(x) + \int_{x_L}^{x_R} G(x, x'; E) V(x') \psi(x') \mathrm{d}x'$$

where the Green's function in the scattering integral is $G(x, x'; E) = \frac{m^*}{\hbar^2 \mathrm{i}k} \mathrm{e}^{\mathrm{i}k|x-x'|}$ and $\psi_0(x) = \mathrm{e}^{\mathrm{i}kx}$ is the wave function of the particle in free space.

(a) Using N uniformly spaced samples with $x_n = x$, $x_m = x'$, $\Delta x = x_{n+1} - x_n \approx \mathrm{d}x'$, $G_{n,m} = G(x_n, x_m)$, $V_m = V(x_m)$, and $n, m \in \{1, 2, \ldots, N\}$, express the scattering integral in the trapezoidal approximation and show that for sufficiently large N

$$\psi(x) \approx \psi_0(x) + \Delta x \sum_{m=1}^{N} G_{n,m} V_m \psi_m = \psi_0(x) + \sum_{m=1}^{N} K_{n,m} \psi_m$$

which may also be written in matrix form as $\psi = \psi_0 + \mathbf{K}\psi$.

(b) Defining a coefficient matrix $\mathbf{A} = \mathbf{1} - \mathbf{K}$, where $\mathbf{1}$ is the $N \times N$ identity matrix, show that $\psi = \mathbf{A}^{-1}\psi_0$.

(c) For $N = 4$ write down the matrix $\mathbf{A}^{-1}$. Calculate transmission as a function of energy $0 \le E \le 4$ eV for an electron of mass $m^* = m_0$ when $V_m = 0$ eV. Setting $N = 96$, calculate numerically and plot transmission for the case when the electron is incident on a domain of thickness 3 nm with a central potential barrier of thickness $L_b = 1$ nm, potential energy $V_0 = 1$ eV, and zero potential energy elsewhere. Compare and discuss your numerical results with the propagation matrix method.