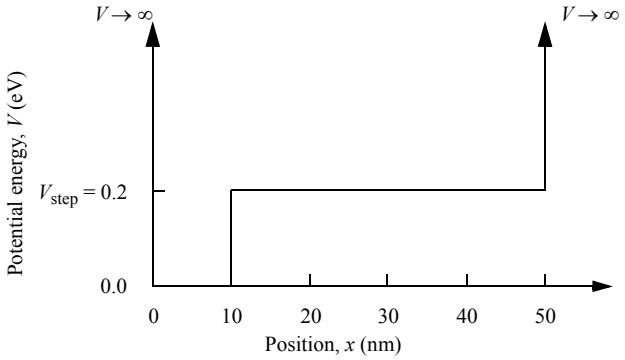
Chapter 3 problems

LAST NAME FIRST NAME

Problem 3.1

(a) Using the method outlined in Exercise 3.7 as a starting point, calculate numerically the first five energy eigenvalues and eigenfunctions for an electron with effective mass $m_e^* = 0.07 \times m_0$ confined to the asymmetric potential well sketched in the following figure and bounded by barriers of infinite energy at $x < 0$ nm and $x > 50$ nm. The value of the step change in potential energy in the figure is $V_{step} = 0.2$ eV.



Your solution should include plots of the eigenfunctions $\psi_n(x)$ and $|\psi_n(x)|^2$ along with a listing of the computer program you used to calculate the eigenfunctions and eigenvalues.

(b) Explain the change in shape of each wave function with increasing eigenenergy.

(c) If an eigenenergy coincides with the value of V_{step}, what is the shape of the eigenfunction?

Problem 3.2

(a) Use a Taylor expansion to show that the second derivative of a wave function $\psi(x)$ sampled at positions $x_j = jh_0$, where j is an integer and h_0 is a small fixed increment in position x, may be approximated as

$$\frac{d^2}{dx^2}\psi(x_j) = \frac{\psi(x_{j-1}) - 2\psi(x_j) + \psi(x_{j+1})}{h_0^2}$$

(b) By keeping additional terms to order h_0^4 in the expansion, show that a more accurate approximation of the second derivative is

$$\frac{d^2}{dx^2}\psi(x_j) = \frac{-\psi(x_{j-2}) + 16\psi(x_{j-1}) - 30\psi(x_j) + 16\psi(x_{j+1}) - \psi(x_{j+2})}{12h_0^2}$$

Problem 3.3

(a) Using the method outlined in Exercise 3.7 as a starting point, calculate numerically the first four energy eigenvalues and eigenfunctions for an electron with effective mass $m_e^* = 0.07 \times m_0$ confined to a potential $V(x) = 0$ of width $L = 10$ nm with *periodic* boundary conditions. Periodic boundary conditions require that the wave function at position $x = 0$ is connected (wrapped around) to position $x = L$. The eigenfunction and its first derivative are continuous and smooth at this connection.

Your solution should include plots of the eigenfunctions and a listing of the computer program you used to calculate the eigenfunctions and eigenvalues.

(b) Explain the change in shape of each eigenfunction with increasing eigenenergy.

Problem 3.4

(a) Using the method outlined in Exercise 3.7 as a starting point, calculate numerically the first six energy eigenvalues and eigenfunctions for an electron with effective mass $m_e^* = 0.07 \times m_0$ confined to a triangular potential well of width L = 20 nm bounded by barriers of infinite energy at $x \leq 0$ and $x \geq L$. The triangular potential well as a function of position x is given by $V(x) = V_0 \times x / L$ where V_0 = 1 eV.

Your solution should include plots of the eigenfunctions and a listing of the computer program you used to calculate the eigenfunctions and eigenvalues.

(b) Explain the change in shape of each eigenfunction with increasing eigenenergy.

Problem 3.5

Calculate the transmission and reflection flux coefficient for an electron of energy E, moving from left to right, impinging normal to the plane of a semiconductor heterojunction potential barrier of energy V_0, where the effective electron mass on the left-hand side is m_1 and the effective electron mass on the right-hand side is m_2.

If the potential barrier energy is V_0 = 1.5 eV and the ratio of effective electron mass on either side of the heterointerface is $m_1/m_2 = 3$, at what particle energy is the transmission flux coefficient unity? What is the transmission flux coefficient in the limit that particle energy $E \to \infty$?

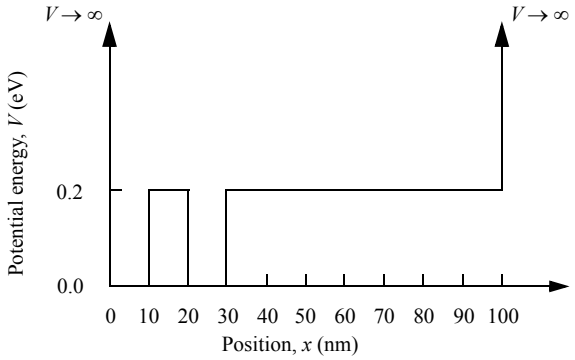
Problem 3.6

A particle mass m is confined to motion in one-dimension. The potential energy is $V(x) = 0$ for $0 < x < L$ and $V(x) = \infty$ elsewhere. Find the eigenenergies and normalized eigenfunctions $\psi(x, t)$ for the system.

You may find it helpful to make use of the relationship $2\sin(x)\sin(y) = \cos(x-y) - \cos(x+y)$.

Problem 3.7

Using the method outlined in Exercise 3.7 as a starting point, calculate numerically the first six energy eigenvalues and eigenfunctions for an electron with effective mass $m_e^* = 0.07 \times m_0$ confined to the double potential well sketched in the following figure and bounded by barriers of infinite energy for $x \leq 0$ nm and $x \geq 100$ nm.

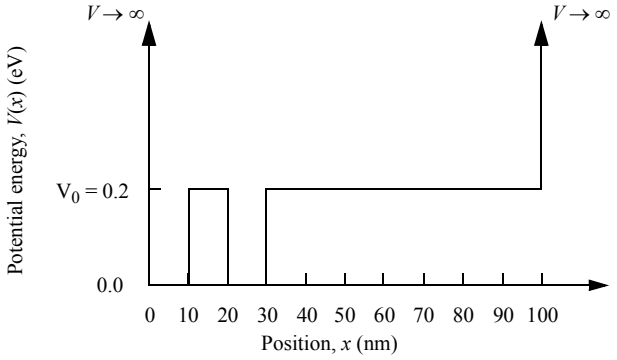


Your solution should include plots of the wave functions, wave functions squared, and a listing of the computer program you used for your calculations. Explain the shape of the ground state and

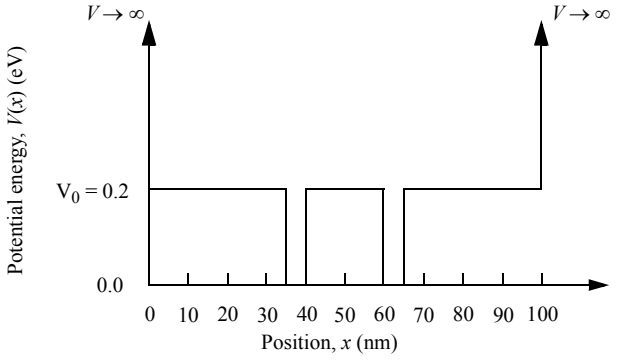
first excited state wave functions. Explain the change in shape of each higher excited state wave functions with increasing eigenenergy.

Problem 3.8

(a) A particle mass m_1 moves in the one-dimensional double barrier potential of energy $V_0 = 0.2$ eV sketched in the following figure and is bounded by barriers of infinite energy for $x \le 0$ nm and $x \ge 100$ nm . The ground state, first, and second excited state eigenenergies of the particle are $E_1 = 0.063$ eV , $E_2 = 0.098$ eV , and $E_3 = V_0 = 0.200$ eV respectively. Sketch and explain the shapes of the corresponding eigenfunctions.



(b) A particle mass m_2 moves in the symmetric one-dimensional double barrier potential of energy $V_0 = 0.2$ eV sketched in the following figure and is bounded by barriers of infinite energy for $x \le 0$ nm and $x \ge 100$ nm . The ground state, first, and second excited state eigenenergies of the particle are $E_1 = 0.06955$ eV , $E_2 = 0.06956$ eV , and $E_3 = V_0 = 0.200$ eV respectively. Sketch and explain the shapes of the corresponding eigenfunctions.



(c) Explain the differences between your results in part (a) and (b).

Problem 3.9

(a) Find the eigenfunctions $\psi_n(x, t)$ and energy eigenvalues E_n for a particle mass *m* moving in one-dimension and confined by the potential $V(x) = 0$ for $0 < x < L$ and $V(x) = \infty$ elsewhere.

(b) Repeat part (a) but now with constant *complex* potential $V(x) = V_1 + iV_2$, where $V_1 = 0$ eV and $V_2 \neq 0$ eV for $0 < x < L$ and $V(x) = \infty$ elsewhere. Explain your result.

(c) At time $t = 0$ ps the particle in (b) is in the ground state. What is the probability of finding the particle in the same state at time $t = 1$ ps if $V_2 = -0.001$ eV.

Problem 3.10

Six atoms are arranged symmetrically on the circumference of a ring of radius 0.15 nm.

(a) Using periodic boundary conditions, determine the wave vectors and eigenenergies for free electrons confined to the ring. If each atom contributes a single free electron to the ring, calculate the sum of the ground-state energies of these electrons.

(b) Repeat part (a) but with the atoms arranged in a linear chain, assuming an infinite potential outside of the chain.

(c) Obtain an estimate for the free-electron contribution to the energy required to break the ring of atoms into a linear chain.

Problem 3.11

An electron has wave function at time $t = 0$ that is

$$\Psi(x, t = 0) = \frac{1}{\sqrt{2}}(\psi_1(x) + \psi_2(x))$$

where ψ_1 is ground-state and ψ_2 is the first excited state of the particle in a one-dimensional potential well of width $L = 10$ nm and infinite barrier energy.

(a) What is the average energy of the particle at time $t = 0$?

(b) Find the state $\Psi(x, t)$ and average particle energy for time $t > 0$. Compare the result with the value obtained in (a).

Problem 3.12

Adiabatic quantum computing assumes it is possible to evolve a system from an initial to final configuration (potential) while remaining in the ground state. The adiabatic theorem guarantees this is possible if the system evolves slowly enough. The shortest evolution time between initial configuration, *A*, and final configuration, *B*, is normally achieved when the difference in energy, Δ, between the ground and first excited state is maximized over the complete path. Efficient adiabatic quantum computing is enabled by finding the optimal path. In this problem we wish to show that paths exist with different minimum energy gap, $\Delta_{\min}$.

Consider a system that consists of a particle mass $m = 0.07 \times m_0$ confined to motion in one dimension in a potential whose initial configuration is $V_0(x) = 0$ for $0 < x < L = 25$ nm and is infinite elsewhere and the final configuration is a potential consisting of two Gaussian peaks such that $V(x) = V_0 + V_1 e^{-((x-x_1)/\sigma_1)^2} + V_2 e^{-((x-x_2)/\sigma_2)^2}$ where $0 \le V_1 \le 0.35$ eV and $0 \le V_2 \le 0.35$ eV.

(a) Plot the energy gap Δ as a function of V_1 and V_2 for the case when $\sigma_1 = \sigma_2 = 2.5$ nm, $x_1 = 0.3 \times L$, and $x_2 = 0.7 \times L$. Explain the features of the Δ landscape. Show that an optimal path exists from initial configuration $A(V_1 = V_2 = 0)$ to any final configuration $B(V_1 \ge 0, V_2 \ge 0)$.

(b) Repeat (a) only now for the case when $\sigma_1 = 4.5$ nm and $\sigma_2 = 1.5$ nm. Explain the change in the features of the Δ landscape.

Problem 3.13

One may numerically integrate the Schrödinger equation in real-space and real-time using the finite-difference time-domain (FDTD) method. To illustrate this, consider the motion of an electron, mass m_0, moving in the x-direction such that

$$\frac{\partial}{\partial t}\psi(x, t) = \left(\frac{i\hbar}{2m_0}\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{i}{\hbar}V(x)\right)\psi(x, t)$$

(a) Rewrite the wave function in terms of real and imaginary components so that

$$\psi(x, t) = \psi_{\mathrm{Re}}(x, t) + i\psi_{\mathrm{Im}}(x, t)$$

and show that one obtains two coupled equations

$$\frac{\partial}{\partial t}\psi_{\mathrm{Re}}(x, t) = \left(\frac{-\hbar}{2m_0}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{\hbar}V(x)\right)\psi_{\mathrm{Im}}(x, t)$$

and

$$\frac{\partial}{\partial t}\psi_{\mathrm{Im}}(x, t) = \left(\frac{\hbar}{2m_0}\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{1}{\hbar}V(x)\right)\psi_{\mathrm{Re}}(x, t)$$

(b) Assuming time steps increment by t_0 and space steps increment by h_0, find the simplest finite-difference expression for the time and spatial derivatives appearing in (a).

(c) The j-th position in space is $x_j = j \times h_0$ where j is an integer. The real part of the wave function increments in time as $t_n = n \times t_0$ where n is an integer and the imaginary part of the wave function increments in time in half-integer steps. Show that this gives two equations

$$\psi_{\mathrm{Re}}(x_j, t_{n+1}) = \psi_{\mathrm{Re}}(x_j, t_n) - \frac{\hbar t_0}{2m_0 h_0^2}(\psi_{\mathrm{Im}}(x_{j+1}, t_{n+1/2}) - 2\psi_{\mathrm{Im}}(x_j, t_{n+1/2}) + \psi_{\mathrm{Im}}(x_{j-1}, t_{n+1/2})) + \frac{t_0}{\hbar}V(x_j)\psi_{\mathrm{Im}}(x_j, t_{n+1/2})$$

and

$$\psi_{\mathrm{Im}}(x_j, t_{n+3/2}) = \psi_{\mathrm{Im}}(x_j, t_{n+1/2}) + \frac{\hbar t_0}{2m_0 h_0^2}(\psi_{\mathrm{Re}}(x_{j+1}, t_{n+1}) - 2\psi_{\mathrm{Re}}(x_j, t_{n+1}) + \psi_{\mathrm{Re}}(x_{j-1}, t_{n+1})) - \frac{t_0}{\hbar}V(x_j)\psi_{\mathrm{Re}}(x_j, t_{n+1})$$

(d) An electron is confined to a region of space $0 \le x \le 100$ nm in which $V(x) = 0$. Consider an initial wave function that is a sinusoid modulated by a Gaussian such that it has the form

$$\psi_{\mathrm{Re}}(x) = e^{-((x-x_0)/\sigma_x)^2}\cos(2\pi((x-x_0)/\lambda_0))$$

and

$$\psi_{\mathrm{Im}}(x) = e^{-((x-x_0)/\sigma_x)^2}\sin(2\pi((x-x_0)/\lambda_0))$$

with $x_0 = 10$ nm, $\lambda_0 = 5$ nm, and $\sigma_x = 5$ nm. Integrate the Schrödinger equation to find the subsequent electron motion using the FDTD method with $t_0 = 0.01$ fs and $h_0 = 0.1$ nm. Plot $\psi_{\mathrm{Re}}(x)$, $\psi_{\mathrm{Im}}(x)$, and $|\psi(x)|^2$ at time $t = 400$ fs and explain your results. What happens if you change electron wavelength to $\lambda_0 = 10$ nm? Explain what happens if you swap the sine and cosine in the definition of the initial wave function.

Problem 3.14

Symplectic finite-difference time-domain (SFDTD) integration can be more accurate than the FDTD(2,2) method described in Problem 3.13. For SFDTD(3,4) the explicit equation for the real part of the wave function in one dimension is

$$\psi_{\mathrm{Re}}(x_j, t_{n+\ell,m}) = \psi_{\mathrm{Re}}(x_j, t_{n+(\ell-1),m}) + \frac{t_0}{\hbar} V(x_j)\psi_{\mathrm{Im}}(x_j, t_{n+\ell,m})$$
$$- \frac{\hbar t_0}{2m_0 h_0^2}\left\{\frac{4}{3} c_\ell(\psi_{\mathrm{Im}}(x_{j+1}, t_{n+\ell,m}) - 2\psi_{\mathrm{Im}}(x_j, t_{n+\ell,m}) + \psi_{\mathrm{Im}}(x_{j-1}, t_{n+\ell,m}))\right\}$$
$$+ \frac{\hbar t_0}{2m_0 h_0^2}\left\{\frac{1}{12} c_\ell(\psi_{\mathrm{Im}}(x_{j+2}, t_{n+\ell,m}) - 2\psi_{\mathrm{Im}}(x_j, t_{n+\ell,m}) + \psi_{\mathrm{Im}}(x_{j-2}, t_{n+\ell,m}))\right\}$$

where j, n, ℓ, and m are integers, $(n + \ell, m)$ denotes the ℓ-th time stage after n time steps, and m is the total number of 'time stages'. j and n have the same meaning as in Problem 3.13. We choose $m = 3$ so there are three time stages and $1 \le \ell \le 3$. The coupled set of equations is integrated in three ($m = 3$) stages per time step. The set of numbers c_ℓ weight the symplectic numerical integration of the real part of the wave function. The corresponding set of weights for the imaginary component of the wave function is d_ℓ and $d_\ell = c_{m-\ell+1}$. SFDTD(3,4) yields c_1 = 0.26833010, c_2 = -0.18799162, and c_3 = 0.91966152.

(a) Write down the corresponding equation for the imaginary component of the wave function.

(b) Modify the FDTD code in Problem 3.13 to incorporate the higher-order integrator. Introduce the higher-order accuracy in time by embedding a time stage loop within the time integration loop. Your code structure should resemble the following:

```
for t=1:tsteps
for time_stage=1:3
for x=1:xsteps
[code for real component]
end
for x=1:xsteps
[code for imaginary component]
end
end
end
```

Run the code and verify that for short times the same results are achieved as with the conventional FDTD(2,2) scheme. Take care to properly modify the various spatial loop limits for the higher-order method, and run your code to propagate the Gaussian wave packet up to time t = 400 fs.

(c) Integrate the probability distribution in space to calculate the total probability for time t_n,

$$P(t_n) = |\psi(t_n)|^2 = \sum_{j=1}^{xsteps} (\psi_{\mathrm{Re}}^2(x_j, t_n) + \psi_{\mathrm{Im}}^2(x_j, t_n))$$

Using $P(t_1)$ as the normalization for the probability distribution over the lattice, calculate the relative probability error, E_P, and error accumulation, $S(E_P)$, as functions of time,

$$E_P(t_n) = 10\log\left|\frac{P(t_1) - P(t_n)}{P(t_1)}\right|$$

$$S(t_n) = \log\left(\sum_{i=1}^{n}\left|\frac{P(t_1) - P(t_n)}{P(t_1)}\right|\right)$$

Do this for FDTD(2,2) and SFDTD(3,4) up to time t = 2000 fs and demonstrate the dramatic difference in conservation of total probability. Repeat for larger space and time increments and demonstrate that the SFDTD(3,4) method remains more accurate than the FDTD(2,2) method for coarser space-time grids.

Problem 3.15

The finite difference approximation used to obtain the second spatial derivative in the Schrödinger equation in Problem 3.13 does not use all the information available in the uniformly-sampled real-space wave function. An alternative approach, called the split-operator method, does this by exploiting the properties of Fourier transforms. To see how this works, consider a particle mass m_0 constrained to motion in the x-direction and moving in real potential $V(x)$ such that

$$\frac{\partial}{\partial t}\psi(x, t) = \left(\frac{i\hbar}{2m_0}\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{i}{\hbar}V(x)\right)\psi(x, t)$$

The wave function and potential are discretized uniformly so that the j-th position in space is $x_j = j \times h_0$ where j is an integer and h_0 is a constant spatial increment. The wave function increments in time as $t_n = n \times t_0$ where n is an integer and t_0 is a constant time step.

(a) Show that the time derivative in the Schrödinger equation may be approximated to second order as

$$\frac{\partial}{\partial t}\psi(x_j, t_n) = \frac{\psi(x_j, t_{n+1}) - \psi(x_j, t_{n-1})}{2t_0}$$

(b) Show that the second spatial derivative of the real-space wave function in the Schrödinger equation can be obtained by taking the inverse Fourier transform of the wave function in k-space multiplied by $-k^2$.

(c) Describe the functional elements of a numerical algorithm that increments the solution of the Schrödinger equation from wave function $\psi(t_n)$ to $\psi(t_{n+1})$. Comment on what you learn.