Problems and Solutions

for

Quantum Mechanics for Scientists and Engineers

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Introduction

All of the problems in the book *Quantum Mechanics for Scientists and Engineers* (Cambridge University Press, 2008) are collected here, section by section, together with all of their solutions, for easy reference by instructors. The problems are each individually linked to the solutions – clicking on the problem text will take you to the solution. Solutions to each problem start on separate pages for ease of use in homework solution sets.

Note that solutions to problems marked with an asterisk here and in the book itself are openly available on-line at www.cambridge.org/9780521897839 so that students have access to additional worked examples. Such problems should not, therefore, be used as graded assignments. For clarity in this document, we have also highlighted such problems in blue font.

Since this document contains solutions to all of the problems in the book, it should not be circulated or distributed, especially not in electronic form.

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Chapter 2

Waves and quantum mechanics – Schrödinger's equation

2.1 Rationalization of Schrödinger's equation

2.2 Probability densities

2.3 Diffraction by two slits

2.3.1 Suppose we have a screen that is opaque to electrons except for two thin slits separated by 5 nm. (We might imagine a plane of atoms with two missing rows of atoms, 5 nm apart, for example, as one way we might make such a structure.) We accelerate electrons, which are initially stationary, through 1 V of potential. These electrons arrive at the back of the screen perpendicular to the surface. A phosphorescent surface (e.g., like a cathode ray tube screen) is placed 10 cm away from the other side of the screen and parallel to it.

    (i) What is the spatial period of the bright and dark stripes seen on the phosphorescent surface (i.e., the distance between the centers of the bright stripes)?

    (ii) What is the period of the stripes if we use protons (hydrogen nuclei) instead of electrons? (The mass of a proton is $\sim 1.67 \times 10^{-27}$ kg.)

2.3.2 In an electron diffraction experiment, consider a screen with a single vertical slit of finite width, d, in the x direction, "illuminated" from behind by a plane monochromatic electron wave of wavelength λ, with the wave fronts parallel to the plane of the slit (i.e., the wave is propagating perpendicularly to the screen). Presume that we take the simple Huygens's principle model of diffraction and, as shown previously, model the slit as a source of a spherically expanding (complex) wave (and, hence, each vertical line in the slit is a source of a circularly expanding wave).

    (i)   Find an approximate analytic expression for the form of the wave amplitude (by "form," we mean here that you may neglect any constant factor multiplying the wave amplitude) at a plane a distance z_o from the screen (assuming $z_o \gg d$).

    (ii) For a slit of width $d = 1$ μm, with an electron wavelength of $\lambda = 50$ nm, plot the magnitude of the light intensity we would see on a phosphorescent screen placed 10 cm in front of the slit, as a function of the lateral distance in the x direction. Continue the plot sufficiently far in x to illustrate all of the characteristic behavior of this intensity.

    (iii) Consider now two such slits in the screen, positioned symmetrically a distance 5 μm apart in the x direction, but with all other parameters identical to part (ii). Plot the intensity pattern on the phosphorescent screen for this case.

(Notes: You may presume that, in the denominator, the distance r from a slit to a point on the screen is approximately constant at $r \simeq z_o$ [though you must not make this assumption for the numerator in

the calculation of the phase]. You may also presume that for all x of interest on the screen, $x << z_o$, a so-called paraxial approximation. You will probably want to use a computer program or high-level mathematical computer package to plot the required functions. With this particular problem, you may find that you want to avoid asking the program to calculate the amplitude or brightness at exactly $x = 0$ because there may be a formal [though not actual] problem with evaluating the function there.)

2.4 Linearity of quantum mechanics: multiplying by a constant

2.4.1 Which of the following differential equations is linear in the sense that, if some function $\psi(z)$ is a solution (and this may well be a different function for each equation), so also is the function $\phi(z) = a\psi(z)$, where a is an arbitrary constant? Justify your answers.

   (i) $z\dfrac{d\psi(z)}{dz} + g(z)\psi(z) = 0$, where $g(z)$ is some specific function

   (ii) $\psi(z)\dfrac{d\psi(z)}{dz} + \psi(z) = 0$

   (iii) $\dfrac{d^2\psi(z)}{dz^2} + b\dfrac{d\psi(z)}{dz} = c\psi(z)$, where b and c are constants

   (iv) $\dfrac{d^3\psi(z)}{dz^3} = 1$

   (v) $\dfrac{d^2\psi(z)}{dz^2} + \left(1 + \left|\psi(z)\right|^2\right)\dfrac{d\psi(z)}{dz} = g\psi(z)$, where g is a constant

(Note: You do not need to solve these equations for the function $\psi(z)$. Merely show that if $\psi(z)$ is a solution, then $a\psi(z)$ is or is not also a solution. Hint: Is the equation for $\phi(z)$ identical to the equation for $\psi(z)$, or does a unavoidably appear in the equation for $\phi(z)$, meaning $\phi(z)$ is necessarily a solution of a different equation if we insist on arbitrary a?)

2.5 Normalization of the wavefunction

2.6 Particle in an infinitely deep potential well ("particle in a box")

2.6.1* An electron is in a potential well of thickness 1 nm, with infinitely high potential barriers on either side. It is in the lowest possible energy state in this well. What would be the probability of finding the electron between 0.1 and 0.2 nm from one side of the well?

2.6.2 Which of the following functions have a definite parity relative to the point $x = 0$ (i.e., we are interested in their symmetry relative to $x = 0$)? For those that have a definite parity, state whether it is even or odd.

   (i) $\sin(x)$

   (ii) $\exp(ix)$

   (iii) $(x-a)(x+a)$

   (iv) $\exp(ix) + \exp(-ix)$

   (v) $x(x^2 - 1)$

2.6.3 Consider the problem of an electron in a one-dimensional "infinite" potential well of width L_z in the z direction (i.e., the potential energy is infinite for $z < 0$ and for $z > L_z$, and, for simplicity, zero

for other values of z). For each of the following functions, in exactly the form stated, is this function a solution of the time-independent Schrödinger equation?

   (i) $\sin(7\pi z/L_z)$

   (ii) $\cos(2\pi z/L_z)$

   (iii) $0.5\sin(3\pi z/L_z) + 0.2\sin(\pi z/L_z)$

   (iv) $\exp(-0.4i)\sin(2\pi z/L_z)$

2.6.4 Consider an electron in a three-dimensional cubic box of side length L_z. The walls of the box are presumed to correspond to infinitely high potentials.

   (i) Find an expression for the allowed energies of the electron in this box. Express the result in terms of the lowest allowed energy, E_1^∞, of a particle in a one-dimensional box.

   (ii) State the energies and describe the form of the wavefunctions for the four lowest energy states.

   (iii) Are any of these states degenerate? If so, say which, and also give the degeneracy associated with any of the eigenenergies you have found that are degenerate.

(Note: This problem can be formally separated into three uncoupled one-dimensional equations, one for each direction, with the resulting wavefunction being the product of the three solutions and the total energy being the sum of the three energies. This is easily verified by presuming this separation does work and finding that the product wavefunction is, indeed, a solution of the full three-dimensional equation.)

2.7 Properties of sets of eigenfunctions

2.7.1 Which of the following pairs of functions are orthogonal on the interval –1 to +1?
   (i) x, x^2
   (ii) x, x^3
   (iii) x, $\sin x$
   (iv) x, $\exp(i\pi x/2)$
   (v) $\exp(-2\pi ix)$, $\exp(2\pi ix)$

2.7.2 Suppose we wish to construct a set of orthonormal functions so that we can use them as a basis set. We wish to use them to represent any function of x on the interval between –1 and +1. We know that the functions $f_0(x)=1$, $f_1(x)=x$, $f_2(x)=x^2$, ..., $f_n(x)=x^n$, ... are all independent; that is, we cannot represent one as a combination of the others, and in this problem we will form combinations of them that can be used as this desired orthonormal basis.
   (i)   Show that not all of these functions are orthogonal on this interval. (You may prove this by finding a counter example.)
   (ii) Construct a set of orthogonal functions by the following procedure:
       (a) Choose $f_0(x)$ as the (unnormalized) first member of this set, and normalize it to obtain the resulting normalized first member, $g_0(x)$.
       (b) Find an (unnormalized) linear combination of $g_0(x)$ and $f_1(x)$ of the form $f_1(x)+a_{10}g_0(x)$ that is orthogonal to $g_0(x)$ on this interval (this is actually trivial for this particular case), and normalize it to give the second member, $g_1(x)$, of this set.
       (c) Find a linear combination of the form $f_2(x)+a_{20}g_0(x)+a_{21}g_1(x)$ that is orthogonal to $g_0(x)$, and $g_1(x)$ on this interval, and normalize it to obtain the third member, $g_2(x)$ of this set.
       (d) Write a general formula for the coefficient a_{ij} in the $i+1$ th unnormalized member of this set.
       (e) Find the normalized fourth member, $g_3(x)$, of this set, orthogonal to all the previous members.
       (f) Is this the only set of orthogonal functions for this interval that can be constructed from the powers of x? Justify your answer.

(Note: This kind of procedure is known as Gram–Schmidt orthogonalization, and you should succeed in constructing a version of the Legendre polynomials by this procedure.)

## 2.8 Particles and barriers of finite heights

2.8.1* An electron of energy 1 eV is incident perpendicularly from the left on an infinitely high potential barrier. Sketch the form of the probability density for the electron, calculating a value for any characteristic distance you find in your result.

2.8.2 An electron wave of energy 0.5 eV is incident on an infinitely thick potential barrier of height 1 eV. Is the electron more likely to be found (a) within the first 1 Å of the barrier, or (b) somewhere farther into the barrier?

2.8.3* Graph the (relative) probability density as a function of distance for an electron wave of energy 1.5 eV incident from the left on a barrier of height 1 eV. Continue your graph far enough in distance on both sides of the barrier to show the characteristic behavior of this probability density.

2.8.4 Consider the one-dimensional problem, in the z direction, of an infinitely thick barrier of height V_o, at $z = 0$, beside an infinitely thick region with potential $V = 0$. We are interested in the behavior of an electron wave with electron energy E, where $E > V_o$.

(i) For the case where the barrier is to the right (i.e., the barrier is for $z > 0$), as shown as follows
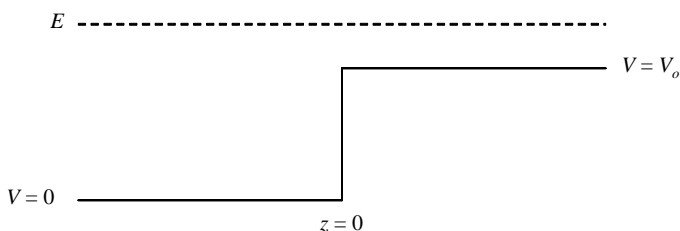
and the electron wave is incident from the left,

(a) solve for the wavefunction everywhere, within one arbitrary constant for the overall wavefunction amplitude, and

(b) sketch the resulting probability density, giving explicit expressions for any key distances in your sketch, and being explicit about the phase of any standing wave patterns you find.
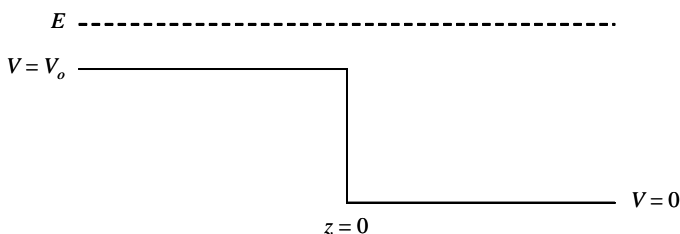
(ii) Repeat (i) but for the case where the barrier is on the left (i.e., for $z < 0$), the potential is V_o, and for $z > 0$ the potential is $V = 0$, as shown in the second figure. The electron is still "incident" from the left (i.e., from within the barrier region, in this case).

2.8.5 Electrons with energy E are incident, in the direction perpendicular to the barrier, on an infinitely thick potential barrier of height V_o, where $E > V_o$. Show that the fraction of electrons reflected from this barrier is

$$R = \left[(1-a)/(1+a)\right]^2$$

where $a = \sqrt{(E-V_o)/E}$.

2.8.6 An electron wave of unit amplitude is incident from the left on the potential structure shown in the following figure. In this structure, the potential barrier at $z = 0$ is infinitely high, and there is a

potential step of height V_o and width b just to the left of the infinite potential barrier. The potential may be taken to be zero elsewhere on the left. For the purposes of this problem, we only consider electron energies $E > V_o$.
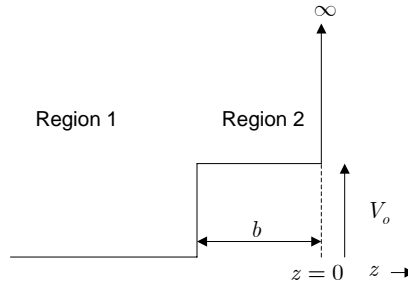
(i) Show that the wavefunction in Region 2 may be written in the form $\psi(z) = C\sin(fz)$, where C is a complex constant and f is a real constant.

(ii) What is the magnitude of the wave amplitude of the reflected wave (i.e., the wave propagating to the left)?

(iii) Find an expression for C in terms of E, V_o, and b.

(iv) Taking $V_o = 1$ eV and $b = 10$ Å, sketch $|C|^2$ as a function of energy from 1.1 to 3 eV.

(v) Sketch the (relative) probability density in the structure at $E = 1.356$ eV.

(vi) Provide an explanation for the form of the curve in part (iv).

2.8.7* Consider an electron in the infinitely deep one-dimensional "stepped" potential well shown in the following figure.
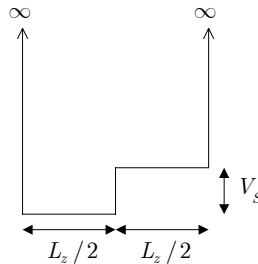
The potential step is of height V_S and is located in the middle of the well, which has total width L_z. V_S is substantially less than $(\hbar^2/2m_o)(\pi/L_z)^2$.

(i) Presuming that this problem can be solved and that it results in a solution for some specific eigenenergy E_S, state the functional form of the eigenfunction solutions in each half of the well, being explicit about the values of any propagation constants or decay constants in terms of the eigenenergy E_S, the step height V_S, and the well width L_z. (Note: Do not attempt a full solution of this problem – it does not have simple closed-form solutions for the eigenenergies. Merely state what the form of the solutions in each half would be if we had found an eigenenergy E_S.)

(ii) Sketch the form of the eigenfunctions (presuming we have chosen to make them real functions) for each of the first two states of this well. In your sketch, be explicit about whether any zeros in these functions are in the left half, the right half, or exactly in the middle. (For clarity, you may exaggerate differences between these wavefunctions and those of a simply infinitely deep well.)

(iii) State whether each of these first two eigenfunctions has definite parity with respect to the middle of the structure and, if so, whether that parity is even or odd.

(iv) Sketch the form of the probability density for each of the two states.

(v) State for each of these eigenfunctions whether the electron is more likely to be found in the left or the right half of the well.

2.9 Particle in a finite potential well

2.9.1* Consider a one-dimensional problem with a potential barrier as shown here. A particle wave is incident from the left, but no wave is incident from the right. The energy, E, of the particle is less than the height, V_o, of the barrier.

(i) Describe and sketch the form of the probability density in all three regions (i.e., on the left, in the barrier, and on the right). (Presume that the situation is one in which the transmission probability of the particle through the barrier is sufficiently large that the consequences of this finite transmission are obvious in the sketched probability density.)

(ii) Show qualitatively how the probability density on the right of the barrier can be increased without changing the energy of the particle or the amplitude of the incident wave, solely by *increasing* the potential in some region to the left of the barrier. (This may require some creative thought!)

2.9.2* A one-dimensional potential well has a barrier of height 1.5 eV (relative to the energy of the bottom of the well) on the right-hand side and a barrier higher than this on the left-hand side. We happen to know that this potential well has an energy eigenstate for an electron at 1.3 eV (also relative to the energy at the bottom of the well).

State the general form of the wavefunction solution (i.e., within a normalizing constant that you need not attempt to determine) in each of the following two cases, giving actual values for any wavevector magnitude k and/or decay constant κ in these wavefunctions

(a) within the well

(b) in the barrier on the right-hand side

2.9.3 Consider a barrier, 10 Å thick and 1 eV high. An electron wave is incident on this barrier from the left (perpendicular to the barrier).

(i) Plot the probability of the transmission of an electron from one side of this barrier to the other as a function of energy from 0 to 3 eV.

(ii) Plot the probability density for the electron from 1 Å to the left of the barrier to 1 Å to the right of the barrier at an energy corresponding to the first maximum in the transmission for energies above the barrier.

(iii) Attempt to provide a physical explanation for the form of the transmission as a function of energy for energies above the top of the barrier.

Hints:

(1) The probability of transmission of the electron can be taken to be $|\psi_{RF}|^2 / |\psi_{LF}|^2$, where $\psi_{LF}(z) \propto \exp(ikz)$ is the forward-going wave (i.e., the wave propagating to the right) on the left of the barrier, and $\psi_{RF}(z) \propto \exp(ikz)$ is the forward-going wave on the right of the barrier.

(2) Presume that there is a specific amplitude for the forward-going wave on the right and no backward-going wave on the right (there is no wave incident from the right). This enables you to work the problem mathematically "backward" from the right.

(3) You may wish to use a computer program or high-level mathematical programming package to deal with this problem, or, at least, a programmable calculator. This problem can be done by hand, though it is somewhat tedious to do that.

2.9.4 In semiconductors, it is possible to make actual potential wells, quite similar to the finite potential well discussed previously, by sandwiching a "well" layer of one semiconductor material (e.g., InGaAs) between two "barrier" layers of another semiconductor material (e.g., InP). In this structure, the electron has lower energy in the "well" material and sees some potential barrier height V_o at the

interface to the "barrier" materials. This kind of structure is used extensively in, for example, the lasers for telecommunications with optical fibers. In semiconductors, such potential wells are called *quantum wells*. In these semiconductors, the electrons in the conduction band behave as if they had an effective mass, m^*, that is different from the free electron mass, m_o, and this mass is different in the two materials (e.g., m_w^* in the well and m_b^* in the barrier). Because the electron effective mass differs in the two materials, the boundary condition that is used at the interface between the two materials for the derivative of the wavefunction is not continuity of the derivative $d\psi/dz$; instead, a common choice is continuity of $(1/m)(d\psi/dz)$, where m is different for the materials in the well and in the barrier. (Without such a change in boundary conditions, there would not be conservation of electrons in the system as they moved in and out of the regions of different mass.) The wavefunction itself is still taken to be continuous across the boundary.

(i)   Rederive the relations for the allowed energies of states in this potential well (treating it like the one-dimensional well analyzed previously) – i.e., relations like Eqs. (2.68) and (2.70) – using this different boundary condition.

(ii) InGaAs has a so-called bandgap energy of ~ 750 meV. The bandgap energy is approximately the photon energy of light that is emitted in a semiconductor laser. This energy corresponds to a wavelength that is too long for optimum use with optical fibers. (The relation between photon energy, E_{photon}, in electron-Volts and wavelength, λ, in meters is $E_{photon} = hc/e\lambda$, which becomes, for wavelengths in microns, $E_{photon} \cong 1.24/\lambda_{(microns)}$, a very useful relation to memorize.) For use with optical fibers, we would prefer light with wavelength ~ 1.55 microns. We wish to change the photon energy of emission from the InGaAs by making a quantum well structure with InGaAs between InP barriers. The confinement of electrons in this structure will raise the lowest possible energy for an electron in the conduction band by the "zero-point" energy of the electron (i.e., the energy of the first allowed state in the quantum well). Assuming for simplicity in this problem that the entire change in the bandgap is to come from this zero-point energy of the electron, what thickness should the InGaAs layer be made? (For InGaAs, the electron effective mass is $m_{InGaAs}^* \cong 0.041 m_o$, and for InP, it is $m_{InP}^* \cong 0.08 m_o$. The potential barrier seen by the electrons in the InGaAs at the interface with InP is $V_o \cong 260$ meV.)

2.10   Harmonic oscillator

2.10.1 Suppose we have a "half harmonic oscillator" potential, for example, exactly half of a parabolic potential on the right of the "center" and an infinitely high potential barrier to the left of the center. Compared to the normal harmonic oscillator, what are the (normalized) energy eigenfunctions and eigenvalues? (Hint: There is very little you have to solve here; this problem mostly requires thought, not mathematics.)

2.11   Particle in a linearly varying potential

2.11.1* Give actual energy levels in electron-Volts to three significant figures for the first three levels in the triangular well as in Fig. 2.13 (i.e., with a field of 1 V/Å).

2.11.2 Repeat the calculation of Problem 2.11.1 for electrons in the semiconductor GaAs, for specific electric fields of 1 V/µm and 10 V/µm. Instead of using the free electron mass, use the effective mass of an electron in GaAs, $m_{eff} \simeq 0.07 m_o$. Also, calculate the distance from the interface to the classical turning point in each case.

2.11.3 For the following two fields, calculate the first three energy levels (in electron-Volts) for an electron in a 100 Å GaAs potential well with infinitely high barriers, and plot the probability densities in units of Å^{-1} for each of the three states. State the energies relative to the energy of the center of the well (*not* relative to the lower corner). Presume that the electron can be treated as having an effective mass of $m_{eff} \simeq 0.07 m_o$. (For this problem, mathematical software will be required. You need to be able to find roots numerically, evaluate the Airy functions, and perform numerical integration for normalization.)

    (i)   zero field
    (ii)   20 V/µm

Chapter 3

The time-dependent Schrödinger equation

3.1 Rationalization of the time-dependent Schrödinger equation

3.1.1 Consider Schrödinger's time-dependent equation for an electron, with a potential that is uniform and constant at a value V_o, with a solution of the form $\exp[i(kz - \omega t)]$. Deduce the relationship giving k in terms of ω and V_o, and deduce under what conditions there is a solution for real k.

3.1.2* Presuming that the potential is constant in time and space and has a zero value, which of the following are possible solutions of the time-dependent Schrödinger equation for some positive (nonzero) real values of k and ω?

(i) $\sin(kz - \omega t)$

(ii) $\exp(ikz)$

(iii) $\exp\left[-i(\omega t + kz)\right]$

(iv) $\exp[i(\omega t - kz)]$

3.1.3 Consider the problem of an electron in a one-dimensional "infinite" potential well of width L_z in the z direction (i.e., the potential energy is infinite for $z < 0$ and for $z > L_z$ and, for simplicity, zero for other values of z). For each of the following functions, in exactly the form stated, state whether the function is a solution of the time-dependent Schrödinger equation (with time variable t).

(i) $\exp\left(-i\dfrac{\hbar\pi^2}{2m_o L_z^2}t\right)\sin\left(\dfrac{\pi z}{L_z}\right)$

(ii) $\exp\left(i\dfrac{4\hbar\pi^2}{2m_o L_z^2}t\right)\sin\left(\dfrac{2\pi z}{L_z}\right)$

(iii) $\exp\left(-i\left(\dfrac{\hbar\pi^2}{2m_o L_z^2}t + \dfrac{\pi}{2}\right)\right)\cos\left(\dfrac{\pi z}{L_z} + \dfrac{\pi}{2}\right)$

(iv) $2\exp\left(-i\dfrac{\hbar\pi^2}{2m_o L_z^2}t\right)\sin\left(\dfrac{\pi z}{L_z}\right) - i\exp\left(-i\dfrac{9\hbar\pi^2}{2m_o L_z^2}t\right)\sin\left(\dfrac{3\pi z}{L_z}\right)$

3.2 Relation to the time-independent Schrödinger equation

3.3 Solutions of the time-dependent Schrödinger equation

3.3.1 Consider the problem of an electron in a one-dimensional "infinite" potential well of width L_z in the
z direction (i.e., the potential energy is infinite for $z < 0$ and for $z > L_z$ and, for simplicity, zero for
other values of z). (In the functions below, t refers to time.)

(i) For each of the following functions, state whether it could be a solution to the time-*independent*
Schrödinger equation for this problem.

(a) $\sin\left(3\pi z / L_z\right)$

(b) $\exp\left(-i\dfrac{\left(7.5\right)^2 \hbar \pi^2}{2m_o L_z^2}t\right)\sin\left(7.5\pi z / L_z\right)$

(c) $A\sin\left(\pi z / L_z\right) + B\sin\left(4\pi z / L_z\right)$, where A and B are arbitrary complex constants.

(d) $A\exp\left(-i\dfrac{\hbar \pi^2}{2m_o L_z^2}t\right)\sin\left(\pi z / L_z\right) + B\exp\left(-i\dfrac{8\hbar \pi^2}{m_o L_z^2}t\right)\sin\left(4\pi z / L_z\right)$, where A and B are arbitrary
complex constants.

(ii) For each of these functions, state whether it could be a solution of the time-*dependent*
Schrödinger equation for this problem.

3.4 Linearity of quantum mechanics: linear superposition

3.5 Time dependence and expansion in the energy eigenstates

3.6 Time evolution of infinite potential well and harmonic oscillator

3.6.1 An electron in an infinitely deep potential well of thickness 4 Å is placed in a linear superposition
of the first and third states. What is the frequency of oscillation of the electron probability density?

3.6.2* A one-dimensional harmonic oscillator with a potential energy of the form $V\left(z\right) = az^2$ in its
classical limit (i.e., in a coherent state with a large expectation value of the energy) would have a
frequency of oscillation of *f* cycles per second.

(i)   What is the energy separation between the first and second energy eigenstates in this harmonic
oscillator?

(ii) If the potential energy was changed to $V\left(z\right) = 0.5az^2$, would the energy separation between
these states increase or decrease?

3.6.3 Consider an electron in an infinitely deep one-dimensional potential well of width $L_z = 1$ nm. This
electron is prepared in a state that is an equal linear superposition of the first three states. Presuming
that oscillations in the squared modulus of the wavefunction amplitude lead to oscillations at the
same frequency in the charge density, and that oscillations in the charge density at any point in the
structure give rise to emitted electromagnetic radiation at the same frequency, list all of frequencies
(in Hertz) of radiation that will be emitted by this system.

3.6.4 Consider an electron in a one-dimensional potential well of width L_z in the z direction, with infinitely high potential barriers on either side (i.e., at $z = 0$ and $z = L_z$). For simplicity, we assume the potential energy is zero inside the well. Suppose that at time $t = 0$, the electron is in an equal linear superposition of its lowest two energy eigenstates, with equal real amplitudes for those two components of the superposition.

(i)   Write down the wavefunction at time $t = 0$ such that it is normalized.
(ii) Starting with the normalized wavefunction at time $t = 0$, write down an expression for the wavefunction valid for all times t.
(iii) Show explicitly whether this wavefunction is normalized for all such times t.

3.7 Time evolution of wavepackets

3.7.1* Suppose that in some semiconductor material, the relation between the electron eigenenergies E and the effective wavevector k in the z direction is given by

$$E = -\frac{\hbar^2 k^2}{2b}$$

for some positive real constant b. If we consider a wavepacket made from waves with wavevectors in a small range around a given value of k, in what direction is the wavepacket moving
(i) for a positive value of k?
(ii) for a negative value of k?

3.7.2 In a crystalline solid material, the energy E of the electron energy eigenstates can be expressed as a function of an effective wavevector k_z for waves propagating in the z direction as shown in the following figure.
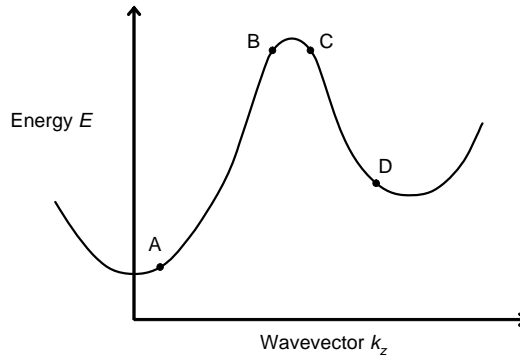
Consider now the motion of a wavepacket formed from states in the immediate vicinity of the particular points A, B, C, and D marked on the figure. State for each of these points
(i) the direction of the group velocity (i.e., is the electron moving in a positive or negative z direction?), and

(ii) the sign of the parameter, m_{eff}, known as the effective mass, where $\dfrac{1}{m_{eff}} = \dfrac{1}{\hbar^2}\dfrac{d^2E}{dk_z^2}$.

3.7.3 (This problem can be used as a substantial assignment.) (Notes: (i) See Section 2.11 before attempting this problem; (ii) some mathematical and/or numerical software will be required.) Consider the one-dimensional problem of an electron in a uniform electric field F, and in which there is an infinitely high potential barrier at $z = 0$ (i.e., the potential is infinite for all negative z) as sketched here, with the potential taken to be zero at $z = 0$ (or, at least, just to the right of $z = 0$).
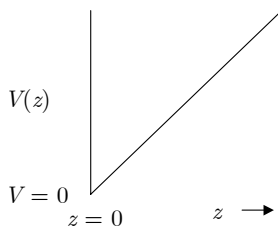
The field is in the +ve z direction and, consequently, the potential energy associated with the electron in that field is taken to be $V(z) = eFz$, for $z > 0$. (A positive field pushes the electron in the negative z direction, so the negative z direction is "downhill" for the electron; therefore, the electron has increasing potential energy in the positive z direction.)

(i) For an applied electric field of 10^{10} V/m, solve for the lowest twenty energy eigenvalues of the electron (in electron-Volts), and graph and state the explicit functional form of the first three energy eigenfunctions. (You need not normalize the eigenfunctions for this graph.)

(ii) Consider a wavepacket consisting of a linear superposition of such energy eigenfunctions. In particular, choose a wavepacket corresponding to an energy expectation value of about 17 eV, with a characteristic energy distribution width much less than 17 eV. (One convenient form is a wavepacket with a Gaussian distribution, in energy, of the weights of the [normalized] energy eigenfunctions.) Calculate and graph the time evolution of the resulting probability density, showing sufficiently many different times to show the characteristic behavior of this wavepacket. Also, describe in words the main features of the time evolution of this wavepacket. State explicitly whether the behavior of this system is exactly cyclic in time, and justify your answer.

(iii) Compare the quantum mechanical behavior to what one would expect classically, on the assumption that the electron would bounce perfectly off the barrier. In what ways is the behavior the same? In what ways is it different? (Note: Approximate numerical calculations and comparisons should be sufficient here.)

3.8 Quantum mechanical measurement and expectation values

3.8.1 As in Problem 3.6.4, consider an electron in a one-dimensional potential well of width L_z in the z direction, with infinitely high potential barriers on either side (i.e., at $z = 0$ and $z = L_z$). For simplicity, we assume the potential energy is zero inside the well. Suppose that, at time $t = 0$, the electron is in an equal linear superposition of its lowest two energy eigenstates, with equal real amplitudes for those two components of the superposition. What is the expectation value of the energy for an electron in this state? Does it depend on time t?

3.9 The Hamiltonian

3.10 Operators and expectation values

3.10.1 Using a system of units in which the electron mass $m = 1$ and $\hbar = 1$, an electron in a potential $V(z) = z^2/2$ has a wavefunction at a given instant in time

$$\psi(z) = \frac{1}{\sqrt{2\sqrt{\pi}}} \left(1 + \sqrt{2}\, z\right) \exp\left(-z^2/2\right)$$

What is the expectation value of the energy for the particle in this state? (You may use numerical integration to get a result, if you wish.)

3.11 Time evolution and the Hamiltonian operator

3.11.1 If the eigenenergies of the Hamiltonian $\hat{H}$ are E_n and the eigenfunctions are $\psi_n(\mathbf{r})$, what are the eigenvalues and eigenfunctions of the operator $\hat{H}^2 - \hat{H}$?

3.12 Momentum and position operators

3.12.1* Suppose that a particle of mass m is in a one-dimensional potential well with infinitely high barriers and thickness L_z in the z direction. Suppose also that it is in a state that is an equal linear superposition of the first and second states of the well.

(Note that $\int_0^\pi \sin(\theta)\cos(2\theta)d\theta = -2/3$, $\int_0^\pi \sin(2\theta)\cos(\theta)d\theta = 4/3$.)

(i) At what frequency is this system oscillating in time?

(ii) Evaluate the expectation value of the z component of the momentum (i.e., $\langle p_z(t) \rangle$) as a function of time.

(iii) Suppose instead that the particle is in an equal linear superposition of the first and third states of the well. Deduce what now is $\langle p_z(t) \rangle$. (Hint: This should not need much additional algebra and may involve consideration of the consequences of odd functions in integrals.)

3.12.2 We perform an experiment in which we prepare a particle in a given quantum mechanical state and then measure the momentum of the particle. We repeat this experiment many times and obtain an average result for the momentum $\langle \mathbf{p} \rangle$ (the expectation value of the momentum). For each of the following quantum mechanical states, give the (vector) value of $\langle \mathbf{p} \rangle$ or, if appropriate, $\langle \mathbf{p}(t) \rangle$, where t is the time after the preparation of the state.

(i) $\psi(\mathbf{r}) \propto \exp(i\mathbf{k} \cdot \mathbf{r})$

(ii) a particle of mass m in an infinitely deep potential well of thickness L_z (here you need only give $\langle p_z \rangle$ or $\langle p_z(t) \rangle$, the z-component of the value, where z is the direction perpendicular to the walls of the well), in the lowest energy state.

(iii) Offer an explanation for the result of part (ii) based on the result from part (i).

3.12.3 Consider the equal linear superposition of the first two states of an infinitely deep potential well.

(i) Show by explicit substitution that this state is a solution of the time-dependent Schrödinger equation for a particle in such a well.

(ii) For this state, what is the expectation value of the position?

(Note: Take the expectation value of position as being given by the expression $\langle z \rangle = \int \Psi^* z \Psi dz$.)

3.12.4 In an experiment, an electron is prepared in the state described by the wavefunction $\Psi(\mathbf{r}, t)$, where t is the time from the start of each run of the experiment. In this experiment, the momentum is measured at a specific time t_o after the start of the experiment. This experiment is then repeated multiple times. Give an expression, in terms of differential operators, fundamental constants, and this wavefunction, for the average value of momentum that would be measured in this set of experiments.

3.12.5 Suppose an electron is sitting in the lowest energy state of some potential, such as a one-dimensional potential well with finite potential depth (i.e., finite height of the potential barriers on either side). Suppose next we measure the momentum of the electron. What will have happened to the expectation value of the energy? That is, if we now measure the energy of the electron again, what will have happened to the average value of the result we now get? Has it increased, decreased, or stayed the same compared to what it was originally? Explain your answer.

3.13 Uncertainty principle

3.13.1 Suppose we have a 1g mass, whose position we know to a precision of 1 Å.

(i) What would be the minimum uncertainty in its velocity in a given direction?

(ii) What would be the corresponding uncertainty in velocity if the particle was an electron instead of a 1g mass?

3.14 Particle current

3.14.1 Suppose we have a particle in a wavepacket, where the spatial wavefunction at some time t is $\psi(\mathbf{r}) = A(\mathbf{r})\exp(i\mathbf{k} \cdot \mathbf{r})$. Here, $A(\mathbf{r})$ is a function that varies very slowly in space compared to the function $\exp(i\mathbf{k} \cdot \mathbf{r})$, describing the envelope of the wavepacket.

(i) Given that the particle current density is given by $\mathbf{j}_p = (i\hbar/2m)(\Psi\nabla\Psi^* - \Psi^*\nabla\Psi)$, show that $\mathbf{j}_p \cong |\psi(\mathbf{r})|^2 \mathbf{p}/m$, where $\mathbf{p}$ is the (vector) expectation value of the momentum.

(ii) With similar approximations, evaluate the expectation value of the energy on the assumption that the potential energy is constant in space.

(iii) Hence, show that the velocity of the probability density corresponds to the velocity we would expect classically.

3.14.2 There are situations in quantum mechanics in which the mass is not constant in space. This occurs specifically in analysis of semiconductor heterostructures where the effective mass is different in different materials. For the case where mass $m(z)$ varies with z, we can postulate the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2}\frac{d}{dz}\left(\frac{1}{m(z)}\frac{d}{dz}\right) + V(z)$$

(For the sake of simplicity, we consider here only a one-dimensional case.)

(i) Show that this Hamiltonian leads to conservation of particle density if we postulate that the particle current (for the z direction) is given by

$$j_{pz} = \frac{i\hbar}{2m(z)}\left[\psi\frac{d\psi^*}{dz} - \psi^*\frac{d\psi}{dz}\right]$$

(actually, the same expression as in the situation in which mass did not depend on position). (Hint: Follow through the preceding argument for the particle current but with the new form of the Hamiltonian given here.)

(ii) Show that the boundary conditions that should be used at a potential step with this new Hamiltonian are continuity of $\frac{1}{m}\frac{d\psi}{dz}$ and continuity of ψ. (These are commonly used boundary conditions for analyzing such problems.) (Hint: Follow through the argument leading up to Eqs. (2.38) and (2.39) with the new Hamiltonian.)

3.15 Quantum mechanics and Schrödinger's equation

Chapter 4

Functions and operators

Prerequisites: Chapters 2 and 3.

4.1 Functions as vectors

4.1.1 Suppose we adopt a notation

$$|n\rangle \equiv \sqrt{\frac{2}{L_z}} \sin\left(\frac{n\pi z}{L_z}\right)$$

to label the states of a particle in a one-dimensional potential well of thickness L_z. Write the bra-ket notation form that is equivalent to each of the following integrals (do not evaluate the integrals – just change the notation).

(i) $\dfrac{2}{L_z} \displaystyle\int_0^{L_z} \sin\left(\dfrac{3\pi z}{L_z}\right)\sin\left(\dfrac{5\pi z}{L_z}\right) dz$

(ii) $\dfrac{2G}{L_z} \displaystyle\int_0^{L_z} \sin\left(\dfrac{3\pi z}{L_z}\right)\sin\left(\dfrac{3\pi z}{L_z}\right) dz$, where G is some constant

(iii) $\displaystyle\int_0^{L_z} \sin\left(\dfrac{5\pi z}{L_z}\right)\sin\left(\dfrac{5\pi z}{L_z}\right) dz$

4.1.2 Suppose that there are two quantum mechanically measurable quantities, c with associated operator $\hat{C}$ and d with associated operator $\hat{D}$. In particular, operator $\hat{C}$ has two eigenvectors $|\phi_1\rangle$ and $|\phi_2\rangle$, and similarly operator $\hat{D}$ has two eigenvectors $|\psi_1\rangle$ and $|\psi_2\rangle$. The relation between the eigenvectors is

$$|\phi_1\rangle = \frac{1}{5}\left(3|\psi_1\rangle + 4|\psi_2\rangle\right)$$

$$|\phi_2\rangle = \frac{1}{5}\left(4|\psi_1\rangle - 3|\psi_2\rangle\right)$$

Suppose a measurement is made of the quantity c, and the system is measured to be in state $|\phi_1\rangle$. Then a measurement is made of quantity d and, following that, the quantity c is again measured. What is the probability (expressed as a fraction) that the system will be found in state $|\phi_1\rangle$ on this second measurement of c? (Note: This is really a problem in quantum mechanical measurement discussed in the previous chapter, but it is a good exercise in the use of the Dirac notation.)

4.2 Vector space

4.2.1 We consider the function space that corresponds to all linear functions of a single variable; that is, functions of the form

$$f(x) = ax + b$$

defined over the range $-1 < x < 1$.

(i) Show that the functions $\psi_1(x) = 1/\sqrt{2}$ and $\psi_2(x) = \sqrt{\dfrac{3}{2}}x$ are orthonormal.

(ii) By showing that any arbitrary function $f(x) = ax + b$ can be represented as the linear combination $f(x) = c_1\psi_1(x) + c_2\psi_2(x)$, show that the functions $\psi_1(x)$ and $\psi_2(x)$ constitute a complete basis set for representing such functions.

(iii) Represent the function $2x+3$ as a vector in a two-dimensional function space by drawing that vector in a two-dimensional diagram with orthogonal axes corresponding to the functions $\psi_1(x)$ and $\psi_2(x)$, stating the values of appropriate coefficients or components.

4.3 Operators

4.4 Linear operators

4.5 Evaluating the elements of the matrix associated with an operator

4.6 Bilinear expansion of linear operators

4.6.1 In the notation in which functions in a Hilbert space are expressed as vectors in that space and operators are expressed as matrices, for functions $|f\rangle$ and $|g\rangle$ and an operator $\hat{A}$, state where each of the following expressions corresponds to a column vector, a row vector, a matrix, or a complex number.

(i) $\langle f|g\rangle$

(ii) $\langle f|\hat{A}$

(iii) $|f\rangle\langle g|$

(iv) $\hat{A}|f\rangle\langle g|$

(v) $\hat{A}^{\dagger}|f\rangle(|f\rangle)^{\dagger}$

4.7 Specific important types of linear operators

4.8 Identity operator

4.8.1 Prove that the sum of the modulus squared of the matrix elements of a linear operator $\hat{A}$ is independent of the complete orthonormal basis used to represent the operator.

4.9 Inverse operator

4.10 Unitary operators

4.10.1* Consider the operator $\hat{M}_{old} = \begin{bmatrix} 0 & i \\ -i & 0 \end{bmatrix}$

  (i)   What are the eigenvalues and associated (normalized) eigenvectors of this operator?
  (ii) What is the unitary transformation operator that will diagonalize this operator (i.e., the matrix that will change the representation from the old basis to a new basis in which the operator is now represented by a diagonal matrix)? Presume that the eigenvectors in the new basis are $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$, respectively.
  (iii) What is the operator $\hat{M}_{new}$ in this new basis?

4.10.2 Evaluate the unitary matrix for transforming a vector in two-dimensional space to a representation in a new set of axes rotated by an angle θ in an anticlockwise direction.

4.10.3 Consider the orthonormal basis functions $\psi_1(x) = 1/\sqrt{2}$ and $\psi_2(x) = \sqrt{3/2}\,x$ that are capable of representing any function of the form $f(x) = ax + b$ defined over the range $-1 < x < 1$.

  (i)   Consider now the new basis functions $\phi_1(x) = \dfrac{\sqrt{3}x}{2} + \dfrac{1}{2}$ and $\phi_2(x) = \dfrac{\sqrt{3}x}{2} - \dfrac{1}{2}$.

        Represent the functions $\phi_1(x)$ and $\phi_2(x)$ in a two-dimensional diagram with orthogonal axes corresponding to the functions $\psi_1(x)$ and $\psi_2(x)$, respectively.
  (ii) Construct the matrix that will transform a function in the old representation as a vector

        $$\begin{bmatrix} c_1 \\ c_2 \end{bmatrix}$$

        into a new representation in terms of these new basis functions as a vector

        $$\begin{bmatrix} d_1 \\ d_2 \end{bmatrix}$$

        where an arbitrary function $f(x) = ax + b$ is represented as the linear combination

        $$f(x) = d_1\phi_1(x) + d_2\phi_2(x)$$

  (iii) Show that the matrix from part (ii) is unitary.

  (iv) Use the matrix of part (ii) to calculate the vector $\begin{bmatrix} d_1 \\ d_2 \end{bmatrix}$ for the specific example function $2x + 3$.

  (v)   Indicate the resulting vector on the same diagram as used for part (i).

4.10.4 Consider the so-called Pauli matrices

$$\hat{\sigma}_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \ \hat{\sigma}_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \ \hat{\sigma}_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

(which are used in quantum mechanics as the operators corresponding to the x, y, and z components of the spin of an electron, though for the purposes of this problem we can consider them simply as abstract operators represented by matrices). For this problem, find all the requested eigenvalues and eigenvectors by hand (i.e., not using a calculator or computer to find the eigenvalues and eigenvectors) and show your calculations.

  (i)   Find the eigenvalues and corresponding (normalized) eigenvectors $\left| \psi_{zi} \right\rangle$ of the operator $\hat{\sigma}_z$.
  (ii) Find the eigenvalues and corresponding (normalized) eigenvectors $\left| \psi_{xi} \right\rangle$ of the operator $\hat{\sigma}_x$.

(iii) Show by explicit calculation that $\sum_i |\psi_{xi}\rangle\langle\psi_{xi}| = \hat{I}$, where $\hat{I}$ is the identity matrix in this two-dimensional space.

(iv) These operators have been represented in a basis that is the set of eigenvectors of $\hat{\sigma}_z$. Transform all three of the Pauli matrices into a representation that uses the set of eigenvectors of $\hat{\sigma}_x$ as the basis.

4.10.5 Consider an operator $\hat{W} = \sum_{i,j} a_{ij} |\phi_i\rangle\langle\psi_j|$ where $|\phi_i\rangle$ and $|\psi_j\rangle$ are two different complete sets of functions. Show that if the columns of the matrix representation of the operator are orthogonal (i.e., if $\sum_i a_{iq}^* a_{ij} = \delta_{qj}$), then the operator $\hat{W}$ is unitary. (Note: When multiplying operators represented by expansions, use different indices in the expansion summations for the different operators.)

4.10.6 Prove that the time-evolution operator $\hat{A} = \exp(-i\hat{H}t/\hbar)$ is unitary.

See also Problem 13.4.2.

4.11 Hermitian operators

4.11.1 For each of the following matrices, state whether it is unitary and whether it is Hermitian.

(i) $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ (ii) $\begin{bmatrix} 1 & i \\ -i & 1 \end{bmatrix}$ (iii) $\begin{bmatrix} i & 0 \\ 0 & i \end{bmatrix}$ (iv) $\begin{bmatrix} 0 & 1 \\ i & 0 \end{bmatrix}$

4.11.2 Prove that for two square matrices A and B, $(AB)^\dagger = B^\dagger A^\dagger$.

(Hint: Consider a general element (e.g., the ijth element) of the resulting matrix and write the result of the matrix multiplication for that element as a summation over appropriate terms.)

4.11.3 Consider the Hermiticity of the following operators:

(i) Prove that the momentum operator is Hermitian. For simplicity, you may perform this proof for a one-dimensional system (i.e., only consider functions of x and consider only the $\hat{p}_x$ operator).

(Hints: Consider $\int_{-\infty}^{\infty} \psi_i^*(x)\hat{p}_x \psi_j(x)dx$, where the $\psi_n(x)$ are a complete orthonormal set. You may want to consider an integration by parts. Note that the $\psi_n(x)$ must vanish at $\pm\infty$ because otherwise they could not be normalized.)

(ii) Is the operator $\dfrac{d}{dx}$ Hermitian? Prove your answer.

(iii) Is the operator $\dfrac{d^2}{dx^2}$ Hermitian? Prove your answer.

(Hints: You may want to consider another integration by parts and you may presume that the derivatives $\dfrac{d\psi_n(x)}{dx}$ also vanish at $\pm\infty$.)

(iv) Is the operator $\hat{H} = -\dfrac{\hbar^2}{2m}\dfrac{d^2}{dx^2} + V(x)$ Hermitian if $V(x)$ is real? Prove your answer.

4.11.4* Prove by operator algebra that a Hermitian operator transformed to a new coordinate system by a unitary transformation is still Hermitian.

4.11.5 A Hermitian operator $\hat{A}$ has a complete orthonormal set of eigenfunctions $|\psi_n\rangle$ with associated eigenvalues α_n. Show that we can always write

$$\hat{A} = \sum_i \alpha_i |\psi_i\rangle\langle\psi_i|$$

(This is known as the expansion of $\hat{A}$ in its eigenfunctions and is a very useful expansion.)

Now find a similar, simple expression for the inverse, $\hat{A}^{-1}$.

(This is also a very useful result. This result shows that if we can find the eigenfunctions of an operator, also known as *diagonalizing* the operator, we have effectively found the inverse and usually, in practice, we have solved the quantum mechanical problem of interest.)

4.11.6 Considering the expansion of $\hat{A}$ in its eigenfunctions (see Problem 4.11.5), show that the trace, $Tr(\hat{A})$, is always equal to the sum of the eigenvalues.

4.11.7* Prove the integral form of the definition of the Hermiticity of the operator $\hat{M}$

$$\int g^*(x)\hat{M}f(x)dx = \int \left\{\hat{M}g(x)\right\}^* f(x)dx$$

by expanding the functions *f* and *g* in a complete basis $|\psi_n\rangle$ and using the matrix element definition of Hermiticity

$$M_{ij} = M_{ji}^*$$

where

$$M_{ij} = \int \psi_i^*(x)\hat{M}\psi_j(x)dx$$

4.11.8 Prove for any Hermitian operator $\hat{M}$ and any arbitrary function or state $|f\rangle$ that the quantity $\langle f|\hat{M}|f\rangle$ is real. (Hence, the expectation value of any quantity represented by a Hermitian operator is always real, which is one good reason for using Hermitian operators to represent measurable quantities.)

4.12 Matrix form of derivative operators

4.12.1 Given that $d^2/dx^2 \equiv \lim_{\delta x \to 0}\left[\left(f(x-\delta x) - 2f(x) + f(x+\delta x)\right)/(\delta x)^2\right]$, find an appropriate matrix that could represent such a derivative operator, in a form analogous to the first derivative operator matrix.

4.13 Matrix corresponding to multiplying by a function

Chapter 5

Operators and quantum mechanics

5.1 Commutation of operators

5.1.1 The Pauli spin matrices are quantum mechanical operators that operate in a two-dimensional Hilbert space and can be written as

$$\hat{\sigma}_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \ \hat{\sigma}_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \ \hat{\sigma}_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Find the commutation relations between each pair of these operators, proving your answer by explicit matrix multiplication and simplifying the answers as much as possible.

5.1.2* Show, for Hermitian operators $\hat{A}$ and $\hat{B}$ that the product $\hat{A}\hat{B}$ is a Hermitian operator if and only if $\hat{A}$ and $\hat{B}$ commute.

5.1.3 Prove that the operator that is the commutator $\left[\hat{A}, \hat{B}\right]$ of two Hermitian operators $\hat{A}$ and $\hat{B}$ is never Hermitian if it is nonzero.

5.2 General form of the uncertainty principle

5.2.1* Suppose that an operator $\hat{A}$ that does not depend on time (i.e., $\partial \hat{A}/\partial t = 0$ [where here we strictly mean the zero operator]) commutes with the Hamiltonian $\hat{H}$. Show that the expectation value of this operator, for an arbitrary state $|\psi\rangle$, does not depend on time (i.e., $\partial\langle A\rangle/\partial t = 0$). (Hint: Remember that $\hat{H} \equiv i\hbar\partial/\partial t$.)

5.2.2 Show that $\left\langle f \left|\left(\hat{A} - \bar{A}\right)^2\right| f\right\rangle = \left\langle f\left|\hat{A}^2 - \bar{A}^2\right| f\right\rangle$ for any (normalized) function $|f\rangle$ and any Hermitian operator $\hat{A}$.

5.2.3 Consider the "angular momentum" operators
$$\hat{L}_x = y\hat{p}_z - z\hat{p}_y, \ \hat{L}_y = z\hat{p}_x - x\hat{p}_z, \text{ and } \hat{L}_z = x\hat{p}_y - y\hat{p}_x$$
where $\hat{p}_x$, $\hat{p}_y$, and $\hat{p}_z$ are the usual momentum operators associated with the x, y, and z directions. (Note that these momentum operators are all Hermitian.)
 (i) Prove whether $\hat{L}_x$ is Hermitian.
 (ii) Construct an uncertainty principle for $\hat{L}_x$ and $\hat{L}_y$.

5.3 Transitioning from sums to integrals

5.4 Continuous eigenvalues and delta functions

5.4.1 Prove that the operator

$$\hat{U} \equiv (1/\sqrt{2\pi})\int \exp(-ikz)\,dz$$

with Hermitian adjoint

$$\hat{U}^\dagger \equiv (1/\sqrt{2\pi})\int \exp(ik'z)\,dz$$

is unitary.

5.4.2* Demonstrate explicitly that the commutator $[\hat{z}, \hat{p}_z]$ is identical, regardless of whether it is evaluated in the position or the momentum representation.

5.4.3 Formally transform the momentum operator $\hat{p}_z$ into the momentum basis using algebra similar to that for the transformation of the position operator into the momentum basis.

Chapter 6

Approximation methods in quantum mechanics

6.1 Example problem – potential well with an electric field

6.2 Use of finite matrices

6.2.1 Solve the problem of an electron in a potential well with three units of field using the first two energy eigenfunctions of the well without field as the finite basis subset. Give the energies (in the dimensionless units) and explicit formulae for the normalized eigenfunctions for the first two levels calculated by this method. Do the algebra of this problem by hand; that is, do not use mathematical software to evaluate matrix elements or to solve for the eigenvalues and eigenfunctions.
(Note: $\int_0^1 (\xi - 1/2)\sin(\pi\xi)\sin(2\pi\xi)d\xi = -(8/9\pi^2)$)

6.2.2 (This problem can be used as a substantial assignment.) Electrons in semiconductors can behave as if they had the charge of a normal electron but have a much different mass (the so-called effective mass). For GaAs, the electron effective mass is $\sim 0.07\, m_o$. We are interested in a semiconductor device that could be a tunable detector for infrared wavelengths. We make this device using a 100 Å thick layer of GaAs, surrounded on either side by materials considered to behave as if the electron sees an infinitely high potential barrier on either side of the GaAs layer (this is an approximation to the actual behavior of AlGaAs barriers).

The concept in this device is that there will be an electron initially in the lowest state in this infinitely deep potential well and we are interested in the optical absorption of light polarized in the z direction (i.e., the optical electric field is in the z direction) that takes the electron from this lower state to one or other of the higher states in the well. We presume that the energy of the photons that can be absorbed corresponds to the energy separations of the states being considered. Once into these higher states, we have some other mechanism that we need not consider in detail that extracts any electrons from these higher states to give a photocurrent in the device (in practice, with actual finite barrier heights, this can be either a thermal emission or a tunneling through the finite barrier), and we also presume that we have another mechanism that puts another electron in the lower state again after any such photocurrent "emission."

The optical electric field is at all times very small, so we can presume its only effect is to cause transitions between levels, not otherwise to perturb the levels themselves. To tune the strengths and wavelengths of the optical transitions in this device, however, we apply an electric field F along the positive z direction, with a practical range from 0 to 10 V/µm (use this range for calculations.)

Consider the first, second, and third electron levels as a function of field F.

    (i)   Calculate the energy separations between the first and second electron levels and between the first and third energy levels over the stated range of fields and plot these on a graph.

    (ii)   Consider the energy eigenfunctions for each of the first three levels as a function of field. Specifically, calculate the approximate amplitudes of the first four infinite well basis functions in the expansion of each of these eigenfunctions and plot these amplitudes as a function of field, for each of the first three levels.

    (iii)   Relative to the strength (i.e., transition rate for a given optical field amplitude) of the optical absorption between the first and second levels at zero applied field, plot the strength of the optical absorption between the first and second levels and between the first and third levels as a function of field. (Note: The transition rate between states $|\psi_j(z)\rangle$ and $|\psi_i(z)\rangle$ for a given optical field amplitude can be taken to be proportional to $|z_{ij}|^2$, where $z_{ij} = \langle \psi_i(z) | z | \psi_j(z) \rangle$.)

    (iv)   Given that we presume this device is useful as a tunable detector only for optical absorption strengths that are at least 1/10 of that of the optical absorption between the first and second levels at zero applied field, what are the tuning ranges, in wavelength, for which this detector is useful given the stated range of fields F?

6.3 Time-independent nondegenerate perturbation theory

6.3.1* Consider a one-dimensional potential well of thickness L_z in the z direction, with infinitely high potential barriers on either side. Suppose we apply a fixed electric field in the z direction of magnitude F.

    (i)   Write down an expression, valid to the lowest order in F for which there is a nonzero answer, for the shift of the second electron energy level in this potential well as a function of field.

    (ii)   Suppose that the potential well is 10 nm thick and is made of the semiconductor GaAs, in which we can treat the electron as having an effective mass of 0.07 of the normal electron mass. What, approximately, is the shift of this second level relative to the potential in the center of the well, in electron-Volts (or milli-electron-Volts), for an applied electric field of 10^5 V/cm? (A numerical answer that one would reasonably expect to be accurate to better than 10 percent is sufficient.) Be explicit about the sign of the shift: Is this energy increasing or decreasing?

Note: You may need the expression

$$\int_0^{\pi} \left(\zeta - \frac{\pi}{2} \right) \sin(q\zeta) \sin(n\zeta) \, d\zeta = -\frac{4qn}{(n-q)^2 (n+q)^2} \text{ for n + q odd}$$

$$= 0 \text{ for } n+q \text{ even}$$

6.3.2 Consider an electron in a one-dimensional potential well of width L_z, with infinitely high barriers on either side and in which the potential energy inside the potential well is parabolic, of the form

$$V(z) = u(z - L_z/2)^2$$

where u is a real constant. This potential is presumed to be small compared to the energy E_1 of the first confined state of a simple rectangular potential well of the same width L_z. (Note for interest: This kind of situation can arise in semiconductor structures, where the parabolic curvature comes from the electrostatic potential of uniform background doping of the material.)

Find an approximate expression, valid in the limit of small u, for the transition energy between the first and second allowed states of this well in terms of u, L_z, and fundamental constants.

6.3.3 The polarization P can be considered as the average position of the charge density, $\rho(z)$; that is, for a particle of charge q, relative to some position z_o

$$P = \int (z - z_o) \rho(z) dz$$

$$= q \int (z - z_o) |\phi(z)|^2 \, dz$$

$$= q \int \phi^*(z)(z - z_o) \phi(z) dz$$

$$= q \langle \phi | (z - z_o) | \phi \rangle$$

where $\phi(z)$ is the (normalized) wavefunction.

In the absence of applied electric field, the particle is presumed to be in the mth eigenstate, $\left|\psi_m\right\rangle$, of the unperturbed Hamiltonian. The symmetry of this unperturbed state is such that $\left\langle\psi_m\right|(z-z_o)\left|\psi_m\right\rangle=0$ (e.g., it is symmetric about the point z_o). A field F is applied along the z direction so that the perturbing Hamiltonian is

$$\hat{H}_p = -qF\left(z-z_o\right)$$

(i)   Evaluate P for the case $F = 0$.

(ii)   Find an expression for P for the case of finite F. (Retain only the lowest order nonzero terms.)

(iii) Find an expression for the change in energy ΔE of this mth state of the system for finite F, again retaining only the lowest order nonzero terms.

(iv)   Hence, show that, to lowest nonzero order

$$\Delta E \cong -\frac{1}{2}PF$$

6.4 Degenerate perturbation theory

6.4.1 Consider an ideal cubical quantum box for confining an electron. The cube has length L on all three sides, with edges along the x, y, and z directions, and the walls of the box are presumed to correspond to infinitely high potential barriers. The resulting energy eigenfunctions in this box are simply the products of the particle-in-a-box wavefunctions in each of the three coordinate directions, as can be verified by substitution into the Schrödinger wave equation. (Note: We presume here for simplicity that $(x, y, z) = (0,0,0)$ is the point in the center of the box and it may be more convenient to write the wavefunctions centered on this point rather than on, say, a corner of the box.)

(i) Write down the normalized wavefunctions for the first three excited states for an electron in this box. (Note: In these states, the electron will be in the second state in one direction and the lowest state in the other two directions.)

(ii) Now presume that there is a perturbation $\hat{H}_p = eFz$ applied (e.g., from an electric field F in the z direction). What happens to the three states as a result of this perturbation, according to first-order degenerate perturbation theory?

(iii) Now presume that a perturbation $\hat{H}_p = \alpha z^2$ is applied instead. (Such a perturbation could result, e.g., from a uniform fixed background charge density in the box.) Using first-order degenerate perturbation theory, what are the new eigenstates and eigenenergies arising from the three originally degenerate states?

(Note: You may need the results

$$\int_{-\pi/2}^{\pi/2}\theta^2\cos^2\theta\,d\theta = \frac{\pi^3}{24}-\frac{\pi}{4} \quad\text{and}\quad \int_{-\pi/2}^{\pi/2}\theta^2\sin^2 2\theta\,d\theta = \frac{\pi^3}{24}-\frac{\pi}{16} \quad)$$

See also Problem 10.5.9, which can be attempted once the hydrogen atom wavefunctions are understood.

6.5 Tight binding model

6.5.1 Consider three wells of equal thicknesses with equal barriers on either side of the middle well. Take the same tight-binding approach as used for two quantum wells, but now considering a 3 x 3 matrix. What are the approximate eigenenergies and wavefunctions of this coupled system? How many zeros are there in each of these wavefunctions (not counting the zeros at the extreme left and right of the system)?

6.5.2 Suppose we have a coupled potential well consisting of two weakly coupled identical potential wells with a barrier between them. We presume that we have solved this problem approximately using a tight-binding approach for the lowest two coupled states, giving approximate solutions

$$\psi_-(z) = \frac{1}{\sqrt{2}}\left(\psi_{left}(z) + \psi_{right}(z)\right) \text{ and } \psi_+(z) = \frac{1}{\sqrt{2}}\left(\psi_{left}(z) - \psi_{right}(z)\right)$$

with associated energies

$$E = E_1 \pm \left|\Delta E\right|$$

where E_1 is the energy of the lowest solution in either of the potential wells considered separately, $\psi_{left}(z)$ is the corresponding wavefunction of the first state in the left well considered separately, $\psi_{right}(z)$ is the corresponding wavefunction of the first state in the right well considered separately, and ΔE is a number that has been calculated based on the coupling.

Suppose now that the coupled system is initially prepared, at time $t = 0$, in the state such that the particle is in the left well, with initial wavefunction $\psi_{left}(z)$.

(i) Calculate expressions for the wavefunction and the probability density as a function of time after $t = 0$.
(ii) Describe in words the time-dependence of this probability density.
(Note: This problem requires an understanding of Chapter 3)

6.6 Variational method

6.6.1* Based on your understanding of the variational method and the principles behind it, prove that the finite basis subset method will always give an answer for the energy of the lowest energy eigenstate that is equal to or above the exact value.

6.6.2 (This problem may be used as a substantial assignment.) Solve this problem by any approximation method or methods you consider appropriate. Consider an electron in an infinitely deep potential well of thickness $L_z = 30$ Å, into which a potential barrier is introduced in the middle as shown in the figure. This barrier has thickness $\Delta L = 0.5$Å and height $V_o = 1$ eV.
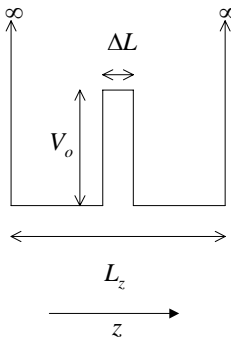
(i) Find the energies and plot the wavefunctions of the first two states (i.e., the ones with the lowest energies) in this potential. Though formal proof of accuracy is not required, you should have reasonable grounds for believing your energy calculation is accurate to ~5 percent or better for the first level.
(ii) Now we apply an electric field, F, to this structure along the z-direction. We consider the energy of the center of the well to be fixed as we apply field. We presume that for small fields, the energy E_1 of the first level changes quadratically with electric field; that is,

$$\Delta E_1 = -\frac{1}{2}\alpha F^2$$

(The quantity α is often called the *polarizability*.) Find a reasonable approximate numerical result for α, expressed in units appropriate for energies in eV and fields in V/Å.

Chapter 7

Time-dependent perturbation theory

7.1 Time-dependent perturbations

7.1.1* Consider a one-dimensional semiconductor potential well of width L_z with potential barriers on either side approximated as being infinitely high. An electron in this potential well is presumed to behave with an effective mass m_{eff}. Initially, there is an electron in the lowest state of this potential well.

We want to use this semiconductor structure as a detector for a very short electric field pulse. If the electron is found in the second energy state after the pulse, the electron is presumed to be collected as photocurrent by some mechanism and the pulse is therefore detected.

To model this device, we presume that the electric field pulse $F(t)$ can be approximated as a half-cycle pulse of length Δt; that is, a pulse of the form

$$F(t) = F_o \sin\left(\frac{\pi t}{\Delta t}\right)$$

for times t from 0 to Δt and zero for all other times.

(i)   Find an approximate expression, valid for sufficiently small field amplitude F_o, for the probability of finding the electron in its second state after the pulse.

(ii) For a pulse of length $\Delta t = 100$ fs and a GaAs semiconductor structure with $m_{eff} = 0.07 m_o$ and width $L_z = 10$ nm, for what minimum electric field magnitude F_o does this detector have at least a 1 percent chance of detecting the pulse?

(iii) For a full-cycle pulse (i.e., one of the form $F(t) = F_o \sin(2\pi t / \Delta t)$ for times t from 0 to Δt and zero for all other times), what is the probability of detecting the pulse with this detector? Justify your answer.

7.1.2 An electron is initially in the lowest state of an infinitely deep one-dimensional potential well of thickness L_z. An electric field pulse, with its field direction polarized perpendicular to the well, and of the form

$$F(t) = 0, \ t < 0; \quad F(t) = F_o \exp(-t/\tau), \ t \geq 0$$

is applied to the well. This pulse will create some probability for times $t \gg \tau$ of finding the electron in the second state and we presume that electrons excited into the second state are subsequently swept out to give a photocurrent on some timescale long compared to τ.

(i)   Find an expression, valid for sufficiently small values of F_o, for the probability of generating an electron of photocurrent from such a pulse.

(ii) Suppose now that we consider a pulse of a given fixed energy E_{pulse}, which we may take to be of the form $E_{pulse} = A F_o^2 \tau$, where A is some constant. For what value of characteristic pulse length

τ does this detector have the maximum sensitivity (i.e., maximum chance of generating an electron of photocurrent)?

(iii) Treating an electron in a GaAs quantum well as being modeled by such an infinitely deep well, with an electron effective mass of $m_{eff} = 0.07 m_o$, for a well of thickness 10 nm, calculate the probability of generating an electron of photocurrent for a field value of $F_o = 10^3$ V/cm and a characteristic time $\tau = 100$ fs.

(iv) If we were now to make 10^{11} such single electron systems (or, equivalently, to put 10^{11} electrons in one actual GaAs quantum well, a number quite feasible for ~ 1 cm^{-2} area), what now would be the average number of electrons of photocurrent generated per pulse?

(v) For the same pulse energy, what would be the optimum pulse length to maximize the photocurrent for the GaAs case of parts (iii) and (iv), and how much larger would the photocurrent be?

7.2 Simple oscillating perturbations

7.2.1* An electron is in the *second* state of a one-dimensional, infinitely deep potential well, with potential $V(z) = 0$ for $0 < z < L_z$ and infinite otherwise. An oscillating electric field of the form

$$F(t) = F_o \left[\exp(-i\omega t) + \exp(i\omega t) \right] = 2F_o \cos(\omega t)$$

is applied along the z direction for a large but finite time, leading to a perturbing Hamiltonian during that time of the form

$$\hat{H}_p(t) = eF(t)z = \hat{H}_{po} \left[\exp(-i\omega t) + \exp(i\omega t) \right]$$

(i) Consider the first four states of this well and presume that we are able to tune the frequency ω arbitrarily accurately to any frequency we wish. For each conceivable transition to another one of those states, say whether that transition is possible or essentially impossible, given appropriate choice of frequency.

(ii) What qualitative difference, if any, would it make if the well was of finite depth (though still considering only the first four states, all of which we presume to be bound in this finite well)?

7.2.2 I wish to make a quantum mechanical device that will sense static electric field F based on the shift of an optical transition energy. I want to make an estimate of the sensitivity of this device by considering optical transitions in an idealized infinitely deep one-dimensional potential well of thickness L_z, with an electron initially in the first state of that well, and considering the transition between the first and second states of the well. The electric field to be sensed is presumed to be in the direction perpendicular to the walls of the potential well, which we call the z direction.

(i) In what direction should the optical electric field be polarized for this device? Justify your answer.

(ii) Give an approximate expression for the shift of the transition energy with field, numerically evaluating any summations. (You may make reasonable simplifying calculational assumptions, such as retaining only the most important terms in a sum if they are clearly dominant.)

(iii) So that this estimate would correspond approximately to the situation we might encounter in atoms, we make the potential well 3 Å thick. Presuming that the minimum change of optical transition energy that can be measured is 0.1 percent, calculate the corresponding minimum static electric field that can be sensed.

(iv) Still using the electron transition energy in a well of this thickness and the same measurable change in optical transition energy, suggest a method that would increase the sensitivity of this device for measuring changes in electric field.

7.2.3 (Note: This problem can be used as a substantial assignment. It is an exercise in both time-independent calculation techniques and in consequences of Fermi's Golden Rule.) We wish to make a detector for radiation in the terahertz frequency regime. The concept for this detector is first that we make a coupled potential well structure using GaAs wells each of 5 nm thickness, surrounded by $Al_{0.3}Ga_{0.7}As$ layers on either side and with a barrier of the same $Al_{0.3}Ga_{0.7}As$ material between the wells, of a thickness w to be determined.
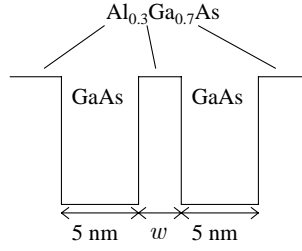
Initially, there will be electrons in the lowest level of this structure and, if we can raise the electrons by optical absorption from the first level into the second level, we presume that the carriers in the second level are then swept out as photocurrent by a mechanism not shown. The terahertz electric field is presumed to be polarized in the horizontal direction in the diagram. We presume that this detector is held at very low temperature so that, to a sufficient degree of approximation, all the electrons are initially in this lowest state. (The electrons are free to move in the other two directions, but this does not substantially change the result of this problem. The nature of optical absorption within the conduction band of semiconductors is such that, even if the electron does have momentum [and, hence, kinetic energy] in the other two directions, that momentum [and, hence, kinetic energy] is conserved in an optical transition, so the transition energy is unaffected by that initial momentum in this particular so-called *intersubband* transition.)

Assume that the electron can be treated like an ordinary electron, but with an effective mass, a mass that is different in different material layers (see Problem 2.9.4 for appropriate boundary conditions and a solution of the finite well problem in this case). Note the following parameters: separation between $Al_{0.3}Ga_{0.7}As$ and GaAs so-called "zone center" conduction band edges (i.e., the potential barrier height in this problem) = 0.235 eV; electron effective masses: 0.067 m_o in GaAs, 0.092 m_o in $Al_{0.3}Ga_{0.7}As$.

(i)   Deduce what thickness w of barrier should be chosen if this detector is to work for approximately 0.5 THz (500 GHz) frequency. (Hint: You may assume that the coupling is relatively weak and that a tight binding approach would be a good choice. Note: You may have to discard a solution here that goes beyond the validity of the approximate solution method you use.)

(ii) We wish to tune this detector by applying a static electric field in the horizontal direction.
     (a) Graph how the detected frequency changes with electric field up to a detected frequency of approximately 1 THz.
     (b) Graph how the sensitivity of the detector (i.e., the relative size of the photocurrent) changes as a function of static electric field.
     (c) Over what frequency range does this detector have a sensitivity that changes by less than 3 dB (i.e., a factor of two) as it is tuned?

7.3 Refractive index

7.4 Nonlinear optical coefficients

7.4.1 Consider a quantum mechanical system that has effectively only two levels of interest, levels 1 and 2, separated by some energy E_{21}. We presume that each of the levels has a spatial wavefunction with a definite parity. The system is subject to an oscillating electric field of the form

$$E(t) = E_o \left[\exp(-i\omega t) + \exp(i\omega t) \right] = 2E_o \cos(\omega t)$$

leading to a perturbing Hamiltonian, in the electric dipole approximation, of

$$\hat{H}_p(t) = eE(t)z = eE_o z \left[\exp(-i\omega t) + \exp(i\omega t) \right]$$

We presume that $\hbar\omega \neq E_{21}$ (so we avoid steady absorption from the radiation field and may consider the steady-state case as in the consideration of linear susceptibility or refractive index), and we take the system to be completely in the lower state in the absence of any perturbation.

(i) Show that the second-order perturbation of the upper state (state 2) is zero (or, at least, constant in time and, hence, not of interest here) (i.e., $a_2^{(2)} = 0$ or, at least, is constant)

(ii) What can you say about the parities of the two states if there is to be any response at all to the perturbing electric field?

7.4.2 (Note: This problem can be used as a substantial assignment.) Consider a quantum mechanical system in which a single electron has only three levels of interest, levels 1, 2, and 3, with energies E_1, E_2, and E_3 and spatial wavefunctions $|\psi_1\rangle$, $|\psi_2\rangle$, and $|\psi_3\rangle$, respectively. The system is initially in its lowest level (level 1). (We could imagine this system is, for example, a molecule of some kind.). The system is illuminated by a light beam of angular frequency ω, polarized in the z direction, which we can write as

$$\mathsf{E}(t) = \mathsf{E}_o\left[\exp(-i\omega t) + \exp(i\omega t)\right] = 2\mathsf{E}_o\cos(\omega t)$$

and which perturbs the molecule through the electric dipole interaction.

(i) Derive an expression for the contributions to the expectation value of the dipole moment, μ_{dip}, that are second-order in this perturbation. At least for this derivation, you may presume that all the matrix elements between the spatial parts of the wavefunctions

$$z_{ij} = \langle \psi_i | z | \psi_j \rangle$$

are finite. (Note: A term of the form $\langle \phi_i^{(1)} | z | \phi_j^{(1)} \rangle$ would give a second-order contribution, as would a term $\langle \phi_i^{(0)} | z | \phi_j^{(2)} \rangle$, whereas a term $\langle \phi_i^{(1)} | z | \phi_j^{(2)} \rangle$ would be a third-order contribution.) (This derivation may take quite a lot of algebra, though it is straightforward and does lead to a relatively simple expression in the end.)

(ii) You should find in your result to part (i) a term or set of terms corresponding to second harmonic generation; that is, a term or terms $\propto \cos(2\omega t)$. You should also have another term or set of terms that behaves differently in time. This second effect is sometimes known as *optical rectification*. What is the physical meaning of this second term; that is, if we shine such a light beam at this "molecule," what is the physical consequence that results from this term?

(iii) What will be the consequence for these second-order effects if the states all have definite parity?

(iv) Calculate the amplitudes of the second-harmonic and optical-rectification electric fields generated under the following set of conditions: Take $z_{ij} = 1$ Å for all of the z_{ij}, except we choose $z_{11} = 0$ (i.e., no static dipole in the lowest state). $E_2 - E_1 = 1$ eV, $E_3 - E_1 = 1.9$ eV, $\hbar\omega = 0.8$ eV, presume that there are 10^{19} cm^{-3} of these "molecules" per unit volume and consider an optical intensity I of the field $\mathsf{E}(t)$ of 10^{10} W/m^2. (Such an intensity corresponds to that of a 1 pJ, 1 ps long light pulse focused to a 10 x 10 micron spot, a situation easily achieved in the laboratory.) (Note that the relation between optical intensity (i.e., power per unit area) I and the amplitude E_o is

$$I = \frac{2\mathsf{E}_o^2}{Z_o}$$

where $Z_o \cong 377\Omega$. Note also that the polarization P is the same as the dipole moment per unit volume and the magnitude of a polarization can always be viewed in terms of an equivalent pair of equal and opposite surface charge densities $\pm\sigma$, unit distance apart, of magnitude $\sigma = \mathsf{P}$. The electric field from such charge densities, assuming no background dielectric constant [i.e., $\varepsilon_r = 1$] is of magnitude $\mathsf{E}_{dip} = \sigma/\varepsilon_o$, and so the electric field from a dipole moment per unit volume of magnitude P is $\mathsf{E}_{dip} = \mathsf{P}/\varepsilon_o$. This field, incidentally, is negative in direction if the dipole moment is positive in direction [positive dipole moment corresponds to positive charge on the right, negative on the left, which corresponds to a field pointing away from the positive charge].)

(v) Repeat the calculations of part (iv) but for $\hbar\omega = 0.98$ eV. (Note: You should only now need to calculate a few terms because these will dominate over all of the others.)

7.4.3 (Note: This problem can be used as a substantial assignment.) Consider a quantum mechanical system in which a single electron has only four states of interest, states 1, 2, 3, and 4, with energies E_1, E_2, E_3, and E_4 (all distinct) and spatial wavefunctions $|\psi_1\rangle$, $|\psi_2\rangle$, $|\psi_3\rangle$, and $|\psi_4\rangle$, respectively, all with definite parities. The system is initially in its lowest level (level 1). (We could imagine this system is, e.g., a molecule of some kind.) The system is illuminated by a light beam of angular frequency ω, polarized in the z direction, which we can write as

$$E(t) = E_o \left[\exp(-i\omega t) + \exp(i\omega t) \right] = 2E_o \cos(\omega t)$$

and which perturbs the molecule through the electric dipole interaction, with perturbing Hamiltonian

$$\hat{H}_p = \hat{H}_{po} \left[\exp(-i\omega t) + \exp(i\omega t) \right]$$

where

$$\hat{H}_{po} \equiv eE_o z$$

We presume that $\hbar\omega$ and its multiples (e.g., $2\hbar\omega$, $3\hbar\omega$) do not coincide with any of the energy differences between the states 1, 2, 3, and 4. Throughout this problem, use a notation where $\omega_n \equiv E_n / \hbar$ and $(E_p - E_q)/\hbar \equiv \omega_{pq}$ and $H_{pq} \equiv \langle \psi_p | \hat{H}_{po} | \psi_q \rangle$.

We are interested here in calculating the lowest order nonlinear refractive index contribution from such systems, a contribution that corresponds to a dipole μ_{dip} (strictly, its expectation value) that is third-order in the field E_o (i.e., third-order overall in the perturbation) and is at frequency ω.

As we do this, we will be considering terms up to the third order in the time-dependent perturbation expansion of the wavefunction

$$|\Psi\rangle \cong |\Psi^{(0)}\rangle + |\Psi^{(1)}\rangle + |\Psi^{(2)}\rangle + |\Psi^{(3)}\rangle$$

where $|\Psi^{(n)}\rangle \equiv \sum_{s=1}^{4} a_s^{(n)}(t) \exp(-i\omega_s t) |\psi_s\rangle$.

For simplicity in handling this problem, we choose $E_1 = 0$ (which we can do arbitrarily because this is simply an energy origin for the problem). Given this choice and our choice of state 1 as the starting state, we have $|\Psi^{(0)}\rangle = |\psi_1\rangle$; that is, $a_1^{(0)} = 1$, $a_2^{(0)} = a_3^{(0)} = a_4^{(0)} = 0$.

(i)   Show that the expression for the first-order expansion coefficients $a_j^{(1)}(t)$ is

$$a_j^{(1)}(t) = -\frac{H_{j1}}{\hbar} \left\{ \frac{\exp\left[i\left(\omega_{j1} - \omega\right)t \right]}{\omega_{j1} - \omega} + \frac{\exp\left[i\left(\omega_{j1} + \omega\right)t \right]}{\omega_{j1} + \omega} \right\} \quad .$$

(Note: In integrating over time to get the required result, you may neglect the formal constant of integration because we are only interested in the time varying parts here.)

(ii) Now show that the expression for the second-order expansion coefficients $a_m^{(2)}(t)$ is

$$a_m^{(2)}(t) = \frac{1}{\hbar^2} \sum_{j=1}^{4} H_{mj} H_{j1}$$

$$\times \left\{ \frac{\exp\left[i\left(\omega_{m1} - 2\omega\right)t \right]}{\left(\omega_{j1} - \omega\right)\left(\omega_{m1} - 2\omega\right)} + \frac{\exp\left(i\omega_{m1}t \right)}{\left(\omega_{j1} - \omega\right)\omega_{m1}} + \frac{\exp\left[i\omega_{m1}t \right]}{\left(\omega_{j1} + \omega\right)\omega_{m1}} + \frac{\exp\left[i\left(\omega_{m1} + 2\omega\right)t \right]}{\left(\omega_{j1} + \omega\right)\left(\omega_{m1} + 2\omega\right)} \right\}$$

noting that successive orders in the perturbation calculation of the state can be calculated from the previous one. (Note that $\omega_{mj} + \omega_{j1} = \omega_{m1}$, which may keep the algebra slightly simpler.) (For simplicity here and later, you may ignore the formal problem that $\omega_{11} = 0$.)

(iii) Now, similarly, show that the expression for the third-order expansion coefficients $a_q^{(3)}(t)$ is

$$a_q^{(3)} = \frac{-1}{\hbar^3} \sum_{m=1}^{4} \sum_{j=1}^{4} H_{qm} H_{mj} H_{j1}$$

$$\times \left\{ \frac{\exp\left[i\left(\omega_{q1} - 3\omega\right)t\right]}{\left(\omega_{j1} - \omega\right)\left(\omega_{m1} - 2\omega\right)\left(\omega_{q1} - 3\omega\right)} + \frac{\exp\left[i\left(\omega_{q1} - \omega\right)t\right]}{\left(\omega_{j1} - \omega\right)\left(\omega_{m1} - 2\omega\right)\left(\omega_{q1} - \omega\right)} \right.$$

$$+ \frac{\exp\left[i\left(\omega_{q1} - \omega\right)t\right]}{\left(\omega_{j1} - \omega\right)\omega_{m1}\left(\omega_{q1} - \omega\right)} + \frac{\exp\left[i\left(\omega_{q1} + \omega\right)t\right]}{\left(\omega_{j1} - \omega\right)\omega_{m1}\left(\omega_{q1} + \omega\right)} + \frac{\exp\left[i\left(\omega_{q1} - \omega\right)t\right]}{\left(\omega_{j1} + \omega\right)\omega_{m1}\left(\omega_{q1} - \omega\right)} + \frac{\exp\left[i\left(\omega_{q1} + \omega\right)t\right]}{\left(\omega_{j1} + \omega\right)\omega_{m1}\left(\omega_{q1} + \omega\right)}$$

$$\left. + \frac{\exp\left[i\left(\omega_{q1} + \omega\right)t\right]}{\left(\omega_{j1} + \omega\right)\left(\omega_{m1} + 2\omega\right)\left(\omega_{q1} + \omega\right)} + \frac{\exp\left[i\left(\omega_{q1} + 3\omega\right)t\right]}{\left(\omega_{j1} + \omega\right)\left(\omega_{m1} + 2\omega\right)\left(\omega_{q1} + 3\omega\right)} \right\}$$

(iv) Now derive an expression for the contributions to the expectation value of the dipole moment, $\mu_{dip} \equiv e\langle\Psi|z|\Psi\rangle$, that are third-order in this perturbation and that are oscillating at frequencies ω or $-\omega$. (Note: A term of the form $\langle\Psi^{(1)}|z|\Psi^{(1)}\rangle$ would give a second-order contribution, as would a term $\langle\Psi^{(0)}|z|\Psi^{(2)}\rangle$, whereas a term $\langle\Psi^{(1)}|z|\Psi^{(2)}\rangle$ or a term $\langle\Psi^{(0)}|z|\Psi^{(3)}\rangle$ would be a third-order contribution. Note also that $\langle\Psi^{(n)}|z|\Psi^{(r)}\rangle = \langle\Psi^{(r)}|z|\Psi^{(n)}\rangle^*$ and that $e\langle\psi_p|z|\psi_q\rangle = H_{pq}/E_o$. Note too that because by choice the states have definite parities, then $H_{pp} = 0$ for any p, which should help eliminate some terms in the sums here.)

(v) Now we restrict the problem to one where the parities of states 1 and 4 are the same and the parities of states 2 and 3 are the same as each other but opposite to those of states 1 and 4. For simplicity, we also choose all the nonzero perturbation matrix elements to be equal. Hence we have

$$H_{11} = H_{22} = H_{33} = H_{44} = H_{14} = H_{23} = 0 \; ; \; H_{12} = H_{13} = H_{24} = H_{34} = H_D \equiv e\mathsf{E}_o z_o$$

where H_D and z_o are constants characteristic of the specific system. We also presume that ω_{41} is very close (but not equal to) 2ω, though we also assume that ω_{21} and ω_{31} are not very close to ω (or $-\omega$). As a result, we may retain only the terms for which there is a term $\left(\omega_{41} - 2\omega\right)$ or its equivalent in the denominator. (Ignore again the formal problem that $\omega_{11} = 0$. In a full analysis, these terms cancel out, avoiding the apparent singularity here.)

(a) Write out the expression for μ_{dip} with these assumptions.

(b) Choose $\hbar\omega_{21} \equiv 3$ eV, $\hbar\omega_{31} \equiv 3.5$ eV, $\hbar\omega_{41} \equiv 5.05$ eV, $\hbar\omega \equiv 2.5$ eV, and $z_o = 1$ Å. Presume that there are 10^{22} cm^{-3} of such "molecules" per unit volume. Calculate the nonlinear refraction coefficient n_2, which is the change of refractive index per unit optical intensity.

(Note that (1) the polarization P is the same as the dipole moment per unit volume, (2) $\mathsf{P} = \varepsilon_o \chi \mathsf{E}$, where $\varepsilon_o \simeq 8.85 \times 10^{-12}$ F/m, and we assume for simplicity here that the only contribution to P is the nonlinear contribution we are calculating [there is also a linear contribution which we could also calculate, though we neglect it for simplicity here], (3) the relative dielectric constant $\varepsilon_r = 1 + \chi$, (4) the refractive index $n = \sqrt{\varepsilon_r}$, (5) the relation between optical intensity [i.e., power per unit area] I and the amplitude E_o is [strictly, in free space, but we use this relation here for simplicity] $I = 2\mathsf{E}_o^2/Z_o$ where $Z_o \cong 377\Omega$.)

(c) Suppose we imagine that this model approximately describes nonlinear refractive index in a hypothetical optical fiber intended for nonlinear optical switching applications. In such a fiber, the cross-sectional size of the optical mode is ~ 10 x 10 μm^2 and launched power into the fiber could be ~ 10 mW. Nonlinear refractive effects can have quite substantial consequences if they lead to changes in optical path length in the total length l of the fiber is of the order of half a wavelength. The change in index is ~ $n_2 I$, and the resulting change in optical path length is ~ $n_2 I l$. Considering a photon energy of 2.5 eV (as previously) with 10 mW power, what length l of fiber would lead to half a wavelength of optical path length change from this nonlinear effect?

(d) Repeat the calculation of part (b), changing $\hbar\omega_{31}$ to 2.0 eV. Explain your result.

Chapter 8

Quantum mechanics in crystalline materials

8.1 Crystals

8.2 One electron approximation

8.3 Bloch theorem

8.3.1 Consider a ring of six identical "atoms" or "unit cells" (e.g., like a benzene ring) with a repeat length (center to center distance between the atoms) of 0.5 nm. Explicitly, write out each of the different allowed Bloch forms (i.e., $\psi(v) = u(v)\exp(ikv)$) for the effective one-dimensional electron wavefunctions $\psi(v)$, where v is the distance coordinate as we move around the ring and $u(v)$ is a function that is periodic with period 0.5 nm. Be explicit about the numerical values and units of the allowed values of k.

8.4 Density of states in *k*-space

8.4.1 A two-dimensional crystal has a rectangular unit cell, with spacings between the centers of the atoms of 0.5 nm in one direction (e.g., the x direction) and 0.4 nm in the other direction (e.g., the y direction). Presuming that the crystal has 1,000 unit cells in each direction, sketch a representative portion of the reciprocal lattice of all the k-states in k-space on a scale drawing, showing the dimensions, units, and directions (i.e., k_x and k_y).

8.5 Band structure

8.5.1 Conventionally, we express Bloch functions within the first Brillouin zone, which for a simple one-dimensional crystal of repeat length a is the range $-\pi/a \le k \le \pi/a$. We could instead consider k values lying outside this range. Show, however, that any such Bloch function (i.e., a function of the form $\psi(x) = u(x)\exp(ikx)$, where $u(x)$ is a function periodic with repeat length a) for any k_{new} outside this first Brillouin zone can also be expressed as a Bloch function with a k value inside the first Brillouin zone. (Hint: Any k_{new} lying outside the first Brillouin zone can be written as $k_{new} = k + 2n\pi/a$ for some positive or negative integer n.)

8.6 Effective mass theory

8.6.1* Suppose we have a crystalline material that has an isotropic parabolic band with an energy minimum at some point $\mathbf{k}_{new} = \mathbf{k} - \mathbf{k}_o$ in the Brillouin zone; i.e., in general, *not* at $\mathbf{k} = 0$. Show that we can also construct an effective mass Schrödinger equation of the form

$$-\frac{\hbar^2}{2m_{eff}} \nabla^2 \Psi_{envnew}(\mathbf{r},t) + V(\mathbf{r}) \Psi_{envnew}(\mathbf{r},t) = i\hbar \frac{\partial}{\partial t} \Psi_{envnew}(\mathbf{r},t)$$

where the full wavefunction for the electron can be written as

$$\Psi(\mathbf{r},t) = u_0(\mathbf{r}) \exp(i\mathbf{k}_o \cdot \mathbf{r}) \Psi_{envnew}(\mathbf{r},t)$$

You may presume that the unit-cell function in the range of $\mathbf{k}$ of interest around $\mathbf{k}_o$ is approximately the same for all such $\mathbf{k}$, with a form $u_o(\mathbf{r})$. (Hint: Follow through the derivation of the effective mass envelope function equation, but centering the energy "parabola" around $\mathbf{k}_o$.)

8.6.2 Suppose that we have a material that has a different effective mass in each of the x, y, and z directions and, hence, has a dispersion relation (for a band minimum at $k = 0$)

$$E_{\mathbf{k}} = \frac{\hbar^2}{2} \left[\frac{k_x^2}{m_x} + \frac{k_y^2}{m_y} + \frac{k_z^2}{m_z} \right] + V$$

where m_x, m_y, and m_z are possibly different effective masses in the three different Cartesian directions and k_x, k_y, and k_z are the corresponding components of the $\mathbf{k}$ vector. Show that we can construct an effective mass Schrödinger equation for the envelope function, of the form

$$-\frac{\hbar^2}{2} \left[\frac{1}{m_x} \frac{\partial^2}{\partial x^2} + \frac{1}{m_y} \frac{\partial^2}{\partial y^2} + \frac{1}{m_z} \frac{\partial^2}{\partial z^2} \right] \Psi_{env}(\mathbf{r},t) + V(\mathbf{r}) \Psi_{env}(\mathbf{r},t) = i\hbar \frac{\partial}{\partial t} \Psi_{env}(\mathbf{r},t)$$

8.7 Density of states in energy

8.8 Densities of states in quantum wells

8.8.1 Derive an expression for the form of the density of states of a subband in a quantum "wire" with a rectangular cross-section – a cuboidal structure that is small in two directions but large (approximately infinite) in the third. Take the "walls" of the quantum wire to be infinitely "high" (i.e., this is an infinite quantum wire in the same sense as an infinite quantum well). (Note that the quantum wire problem, in this case, is "separable" into separate Schrödinger equations for each of the three directions.)

8.8.2* In the simplest form of a quantum well structure, a "quantum well" layer of one material (e.g., GaAs) is sandwiched between two "barrier" layers of a different material (e.g., AlGaAs alloy), resulting in a "rectangular" potential well (e.g., for electrons). The electrons are free to move in two (x and y) directions, but the wavefunction in the third direction (z) behaves like that of a particle in a box. Suppose now that instead of a simple uniform quantum well layer, the material is actually smoothly graded in the z direction so that the potential well seen by the electrons in this direction is parabolic, with the potential increasing quadratically as we move in the z direction from the center of the well. (Such structures can be made, for example, by progressively grading the aluminum concentration in an AlGaAs alloy.) For simplicity, we presume that the electron mass does not change as we change the material composition. Sketch the form of the electron density of states in this quantum well, including the first several subbands. (Note: You should not have to perform any actual calculations for this.)

8.9 k·p method

8.10   Use of Fermi's Golden Rule

8.10.1 (Notes: This is a substantial problem that could be used as an assignment. Section 8.9 should also have been studied before attempting this problem.) In this problem, we progressively consider direct optical transitions between the two bands in the simple two-band $\mathbf{k} \cdot \mathbf{p}$ model constructed previously, assuming that the lower band (band 1) is initially full of electrons and the upper band (band 2) is initially empty of electrons. For this problem, do not assume the small k approximation of Eq. (8.72). Work with the full roots of Eq. (8.72) for finding the eigenenergies and unit-cell functions.

(i)   Show that the wavefunction in the upper band may be written as

$$u_{2k}\left(\mathbf{r}\right) = \frac{1}{d_{+}} u_{10}\left(\mathbf{r}\right) + \frac{1 + \sqrt{1 + |b|^{2}}}{b d_{+}} u_{20}\left(\mathbf{r}\right)$$

where

$$d_{\pm} = \sqrt{1 + \frac{1}{|b|^{2}} \left(1 \pm \sqrt{1 + |b|^{2}}\right)^{2}}$$

where $b = 2\hbar k p_{12} / E_{g} m_{o}$ (so that $|b|^{2} = 2E_{p} \hbar^{2} k^{2} / E_{g}^{2} m_{o}$).

Hints:

(a) You may find it useful in the intermediate algebra to (1) work only in terms of p_{21} rather than E_{P} $(= 2|p_{21}|^{2} / m_{o})$, and (2) introduce the parameter b early in your manipulations.

(b) Note that if we find, for example, a_{2} in terms of a_{1}, then we actually can deduce both coefficients through the normalization of the overall unit-cell wavefunction (i.e., $|a_{1}|^{2} + |a_{2}|^{2} = 1$).

(ii)   Find a similar expression for $u_{1k}\left(\mathbf{r}\right)$.

(iii) Show for the interband momentum matrix element p_{21k} at Bloch wavevector k

$$p_{21k} = \int\limits_{unit\ cell} u_{2k}^{*}(\mathbf{r})\hat{\mathbf{p}}u_{1k}\left(\mathbf{r}\right)d^{3}\mathbf{r}$$

that

$$|p_{21k}|^{2} = \frac{m_{o}}{2} \frac{E_{p}}{1 + \dfrac{2E_{p}}{E_{g}^{2}} \dfrac{\hbar^{2}k^{2}}{m_{o}}}$$

Note that $p_{nn} = 0$ because we assume the unit-cell functions at $k = 0$ to have definite parity. (This part may take a fair amount of algebra, though it is straightforward algebra.)

(iv) Construct a mathematical expression for the absorption coefficient, $\alpha\left(\hbar\omega\right)$ for interband direct optical absorption in this model, expressed in terms of E_{p}, the band gap energy, E_{g}, the refractive index, n_{r}, the photon energy, $\hbar\omega$, and fundamental constants. (Note: Do *not* assume a simple parabolic density of states.)

(v) Assuming the refractive index is constant at $n_{r} \cong 3.5$, $E_{g} = 1\,\text{eV}$, and $E_{p} = 20\,\text{eV}$, graph the absorption coefficient, expressed in units of cm^{-1}, calculated using this model and compare it with the results for the simple parabolic band model with constant $|p_{21}|^{2}$. Graph your results up to a photon energy of 2 eV.

8.10.2 Here, we consider the equivalence of the electric dipole and "$\mathbf{A} \cdot \mathbf{p}$" versions of the Hamiltonian for certain optical absorption processes.

(i)   Prove for a single-electron Hamiltonian of the form

$$\hat{H}_{el} = \frac{-\hbar^{2}}{2m_{o}}\nabla^{2} + V\left(\mathbf{r}\right)$$

that

$$\left[\hat{H}_{el}, \mathbf{r}\right] = -i\frac{\hbar}{m_o}\hat{\mathbf{p}}$$

(ii) When $|\psi_1\rangle$ and $|\psi_2\rangle$ are eigenfunctions of $\hat{H}_{el}$, with corresponding eigenenergies E_1 and E_2, find an expression relating $\mathbf{p}_{21} = \langle\psi_2|\hat{\mathbf{p}}|\psi_1\rangle$ to $\mathbf{r}_{21} = \langle\psi_2|\mathbf{r}|\psi_1\rangle$.

(iii) Consider the two possible time-dependent perturbing Hamiltonians

$$\hat{H}_{pA} = -\frac{e}{m_o}\mathbf{A}\cdot\hat{\mathbf{p}}, \text{ with } \mathbf{A} = \mathbf{A}_o\cos\omega t$$

and

$$\hat{H}_{pE} = -e\mathbf{E}\cdot\mathbf{r}, \text{ with } \mathbf{E} = \mathbf{E}_o\cos\omega t$$

Show that, in Fermi's Golden Rule, these two Hamiltonians lead to the same transition rate for the same strength of electromagnetic field for transitions between eigenstates of $\hat{H}_{el}$. (You may use the relation $\mathbf{E} = -\partial\mathbf{A}/\partial t$.)

8.10.3 (Note: This problem can be used as a substantial assignment and should be attempted only after completing Problem 8.10.1.) Consider two-photon absorption in the simple two-band $\mathbf{k}\cdot\mathbf{p}$ theory semiconductor considered previously. Assume the lower band is initially full of electrons and the upper band is initially completely empty.

For the purposes of this exercise, you need only consider the process corresponding to two-photon absorption from the lower band (band 1) to the upper band (band 2) in which states in the upper band are available as the intermediate states. You also need only consider the first contribution to the process; that is, in the previous notation, you may presume

$$\left|a_j^{(2)}(t_o)\right|^2 =$$

$$\frac{t_o}{\hbar^4}\left[\sum_n\sum_q\frac{\langle\psi_m|\hat{H}_{po}|\psi_q\rangle\langle\psi_q|\hat{H}_{po}|\psi_j\rangle\langle\psi_j|\hat{H}_{po}|\psi_n\rangle\langle\psi_n|\hat{H}_{po}|\psi_m\rangle}{(\omega_{nm}-\omega)(\omega_{qm}-\omega)}t_o\left[\frac{\sin\left(\omega_{jm}-2\omega\right)t_o/2}{\left(\omega_{jm}-2\omega\right)t_o/2}\right]^2\right]$$

(Note that at least as part of a two-photon process, it is possible to consider the optical transition from a state within band 2 to an adjacent state in the same band. Though the optical wavevector is usually negligible numerically, its finite magnitude ensures that such a transition is between two different states, albeit ones of nearly identical wavevector $\mathbf{k}$.)

Specifically,

(i) Given these presumptions about the initial, intermediate, and final states; evaluate each of the matrix elements $H_{poij} = \langle\psi_i|\hat{H}_{po}|\psi_j\rangle$ in this expression in terms of the magnetic vector potential amplitude A_o of the oscillatory electromagnetic field, momentum matrix elements of the form $p_{nn'\mathbf{k}} = \int_{unit\ cell}u_{n\mathbf{k}}^*(\mathbf{r})pu_{n'\mathbf{k}}(\mathbf{r})d^3\mathbf{r}$, and fundamental constants; and deduce any restrictions these impose on the terms surviving in the summations. (Consider the optical wavevector $\mathbf{k}_{op}$ to be negligibly small.)

(ii) For a particular initial state with wavevector $\mathbf{k}_m$ in band 1, derive a mathematical expression for the two-photon transition rate $w_{\mathbf{k}m} = \left|a_j^{(2)}(t_o)\right|^2/t_o$ in terms of the optical intensity, I; the photon energy $\hbar\omega$; the energy separation, $E_J(\mathbf{k}_m)$, between the states in bands 1 and 2 at wavevector $\mathbf{k}_m$; the quantities $\left|p_{21\mathbf{k}m}\right|^2$ and $\left|p_{22\mathbf{k}m}\right|^2$; a function of the form $t_o[(\sin x)/x]^2$; the refractive index n_r; and fundamental constants.

(iii) Find an approximate expression for the matrix element $\left|p_{22\mathbf{k}m}\right|^2$, valid to lowest order in k_m, and expressed in terms of $\left|p_{21}\right|^2$, the band gap energy E_g, and fundamental constants. (This will be an expression proportional to k_m^2.)

(iv) Find an expression for the total two-photon transition rate from all possible initial states to all possible final states, valid to lowest order in k_m, and in terms of optical intensity, I, the photon energy, $\hbar\omega$, the quantity $E_p = 2\left|p_{21}\right|^2/m_o$, the refractive index n_r, and fundamental constants. (Note: Because we are only interested in the lowest order behavior with k_m, you may use the parabolic dispersion relations for the bands.)

(v) Consider a semiconductor with $n_r \cong 3.5$, $E_g = 1$ eV, and $E_p = 20$ eV. A short pulse laser has an average power of 1 mW and a photon energy of 0.6 eV. Its light is concentrated in pulses that

are 100 fs long with a repetition rate of 100 MHz. For simplicity of calculation, you may assume that the light intensity is constant throughout the pulse. This light shines on a 10 x 10 micron square area of the surface of the semiconductor, approximately uniformly (you may assume the surface is antireflection coated so there is no reflection from the surface). The semiconductor is 1 micron thick. The semiconductor is structured like a photodiode so that every electron-hole pair generated in the semiconductor gives rise to one electron of current. Approximately what will be the average current generated in this diode using the two-photon absorption model constructed here?

Chapter 9

Angular momentum

9.1 Angular momentum operators

9.1.1 Starting from the definition of the operators for the Cartesian components of the angular momentum, show that $\hat{\mathbf{L}} \times \hat{\mathbf{L}} = i\hbar\hat{\mathbf{L}}$. (Note that you should also explicitly derive any commutation relations that you need between the operators of the angular momentum components, starting from the known commutation properties of position and [linear] momentum operators.)

9.1.2 Starting from the definition in Cartesian coordinates and noting that

$$\frac{\partial}{\partial x} \equiv \frac{\partial r}{\partial x}\frac{\partial}{\partial r} + \frac{\partial \theta}{\partial x}\frac{\partial}{\partial \theta} + \frac{\partial \phi}{\partial x}\frac{\partial}{\partial \phi}$$

show that

$$L_x = i\hbar\left(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi} \right)$$

(Remember that $\dfrac{d\sin^{-1}x}{dx} = \dfrac{1}{\sqrt{1-x^2}}$ and $\dfrac{d\tan^{-1}x}{dx} = \dfrac{1}{1+x^2}$)

9.2 L squared operator

9.2.1* Show explicitly in Cartesian (x, y, z) coordinates that the ∇^2 and $\hat{L}_z$ operators commute; that is,

$$\left[\nabla^2, \hat{L}_z\right] = 0$$

9.2.2 Write out the associated Legendre functions for $l = 0$, 1, and 2 with $\cos\theta$ instead of x as the argument (possibly simplifying the results using $\cos^2\theta + \sin^2\theta = 1$) and, hence, state all the angles θ for which each of these associated Legendre functions has zeros.

9.3 Visualization of spherical harmonic functions

9.4 Comments on notation

9.5 Visualization of angular momentum

Chapter 10

The hydrogen atom

10.1 Multiple-particle wavefunctions

10.2 Hamiltonian for the hydrogen atom problem

10.3 Coordinates for the hydrogen atom problem

10.4 Solving for the internal states of the hydrogen atom

10.5 Solutions of the hydrogen atom problem

10.5.1* Consider an electron in a thin cylindrical shell potential. This potential is zero within the cylindrical shell and may be presumed infinite everywhere else. The shell has inner radius r_o and thickness L_r, where $r_o \gg L_r$. The cylindrical shell may be presumed to be infinite along its cylindrical (z) axis.

(i) Show that the energy eigenfunctions (i.e., solutions of the time-independent Schrödinger equation) are, approximately

$$\psi(r,\phi,z) \propto \sin\frac{n\pi(r-r_o)}{L_r}\exp(im\phi)\exp(ik_z z)$$

(ii) State what the restrictions are on the values of n, m, and k_z (e.g., are they real, integer, limited in their range?)

(iii) Give an approximate expression for the corresponding energy eigenvalues.

Note: In cylindrical polar coordinates

$$\nabla^2 = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial\phi^2} + \frac{\partial^2}{\partial z^2}$$

10.5.2* Consider the case of a spherical potential well – that is, a structure in which the potential energy is lower and constant for all radii $r < r_o$ and higher and constant for all $r > r_o$ – and a particle of mass m_o.

For the case of an infinite potential well (i.e., one in which the potential is infinite for all $r > r_o$), find the energy of the lowest state of a particle in the well relative to the bottom of the well. (You may presume the lowest state has the lowest possible angular momentum.) (Note: Remember that it can be shown that with a radial wavefunction $R(r) = \chi(r)/r$, $\chi(0) = 0$.)

(This problem is part of the analysis of spherical semiconductor quantum dots. Such structures can be made and are commonly used in color glass filters and as fluorescent markers for biological experiments. The color of the dots or of their fluorescence is partly determined and controlled by the size of the dot through these quantum size effects. Quantum dots are also interesting for optoelectronic devices.)

10.5.3 Consider the defining differential equation for the Hermite polynomials

$$\frac{d^2 H_n(x)}{dx^2} - 2x \frac{dH_n(x)}{dx} + 2nH_n(x) = 0$$

and solve it by the series solution method for functions $H_n(x)$ such that $H_n(x)\exp(-x^2/2)$ can be normalized

In your solution
  (i) find a recurrence relation between the coefficients of the power-series solutions (Note: This relation will be between c_q and c_{q+2}.)
  (ii) show that $H_n(x)\exp(-x^2/2)$ will not be normalizable unless the power series terminates (Note: You will have to consider two power series, one starting with c_0 and one starting with c_1, and show that neither will terminate unless n is an integer.)
  (iii) choosing $c_0 = 0$ or 1 and $c_1 = 0$ or 1, find the first five power-series solutions of the equation.

10.5.4 Consider a spherical quantum box or "dot" with an electron inside it. We presume the potential is infinite at the boundary of the dot and zero within, and that the "dot" has radius r_0.
  (i) Find an expression for the eigenenergies $E_{n\ell}$, where ℓ is the usual angular momentum quantum number and n is another integer quantum number (starting at $n = 1$), expressing your result in terms of the zeros $s_{n\ell}$ of the spherical Bessel function $j_\ell(x)$, where $s_{n\ell}$ is the nth zero for a given ℓ.
  (ii) Find the electron confinement energies for the nine conditions $n = 1, 2, 3$ with $\ell = 0, 1, 2$ for each n, for the case of a 10 nm diameter semiconductor dot with electron effective mass of $0.2 m_0$. (Note: You will have to find appropriate zeros of special functions from mathematical tables or otherwise.)

Notes:
  (a) The equation

$$\frac{d^2 y}{dx^2} + \left[a^2 + \left(\frac{1}{4} - p^2 \right) \frac{1}{x^2} \right] y = 0$$

has solutions

$$y = \sqrt{x} \left[A J_p(ax) + B Y_p(ax) \right]$$

where A and B are arbitrary constants, J_p is the Bessel function of order p, and Y_p is the Weber function of order p. Note that the Weber functions tend to infinity as $x \to 0$, though the Bessel functions remain finite as $x \to 0$.
  (b) The spherical Bessel functions are given by

$$j_\ell(x) = \sqrt{\frac{\pi}{2x}} J_{\ell+1/2}(x)$$

and these functions can also be expressed as

$$j_\ell(x) = x^\ell \left(-\frac{1}{x} \frac{d}{dx} \right)^\ell \frac{\sin x}{x}$$

10.5.5 Find an expression for the energy eigenstates of a cylindrical quantum wire of radius r_o for which we assume there is an infinitely high barrier at radius r_o. Specify all quantum numbers and state their allowed values.

(Note: In this case, it is left as an exercise for the reader to find the necessary special functions and their properties to solve this problem.)

10.5.6 Evaluate the matrix element $\langle U_{210} | z | U_{100} \rangle$, where by $|U_{nlm}\rangle$ we mean the hydrogen atom orbital where the quantum numbers n, l, and m take their usual meanings.

10.5.7 Suppose we are considering optical transitions between different states in the hydrogen atom. We presume that the hydrogen atom is initially in a given starting state and we want to know if, for a linearly polarized oscillating electromagnetic field (i.e., one for which the optical electric field can be taken to be along the z direction) of the appropriate frequency, it can make transitions to the given final state, at least for transition rates calculated using first-order time-dependent perturbation theory in the electric dipole approximation. State for each of the following combinations whether such optical transitions are possible. Explain your method and your results. (Note: This problem requires some understanding of transition matrix elements for optical transitions as discussed in Chapter 7.)

(a) Starting state $|1,0,0\rangle$, final state $|2,1,0\rangle$

(b) Starting state $|1,0,0\rangle$, final state $|2,1,1\rangle$

(c) Starting state $|1,0,0\rangle$, final state $|2,0,0\rangle$

(d) Starting state $|2,1,0\rangle$, final state $|1,0,0\rangle$

10.5.8 (This problem can be used as a substantial assignment.) Consider the problem of a "two-dimensional" hydrogen atom. Such a situation could arise for a hydrogen atom squeezed between two parallel plates, for example. (This problem is a good limiting model for excitons in semiconductor quantum wells.) We are not concerned with the motion in the z direction perpendicular to the plates and are hence left with a Schrödinger equation for the electron and proton

$$\left[-\frac{\hbar^2}{2m_e}\nabla^2_{xye} - \frac{\hbar^2}{2m_p}\nabla^2_{xyp} - \frac{e^2}{4\pi\varepsilon_o |\mathbf{r}_{xye} - \mathbf{r}_{xyp}|} \right] \psi\left(x_e, y_e, x_p, y_p\right) = E\psi\left(x_e, y_e, x_p, y_p\right)$$

where

$$\nabla^2_{xye} \equiv \frac{\partial^2}{\partial x_e^2} + \frac{\partial^2}{\partial y_e^2}$$

where x_e and y_e are the position coordinates of the electron and, similarly, for the proton.

Solve for the complete wavefunctions and eigenenergies for all states where the electron and proton are bound to one another (you need not normalize the wavefunctions).

Give an explicit expression for the coefficients of any polynomials you derive for solutions, in terms of the lowest order coefficient in the polynomial.

Explicitly state the allowed values of any quantum numbers and give the numerical answer for the lowest energy of the system in electron volts.

Hints:
(i)   This problem can be solved in a very similar fashion to the three-dimensional hydrogen atom. Use the same units as those used in that problem.
(ii) The Laplacian in two-dimensional polar coordinates is

$$\nabla^2 = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial\phi^2}$$

(iii) You should be able to get to an equation that looks something like

$$s\frac{d^2L}{ds^2} + (A - s)\frac{dL}{ds} + BL = 0$$

in solving for the radial motion, where A and B do not depend on s.

10.5.9 (This problem can be used as a substantial assignment.) Consider the effect of a small electric field on the $n = 2$ levels of the hydrogen atom. (Note: There are several such levels because of the different values of l and m possible for $n = 2$. This problem should, therefore, be approached using first-order degenerate perturbation theory. The algebra of the problem may be somewhat easier if the electric field is chosen in the z direction.)

Find how these $n = 2$ degenerate states are affected by the field. Give explicit numerical expressions for the shifts of those levels that are affected by the field *F*, and show how their wavefunctions are constructed as linear combinations of hydrogen wavefunctions of specific *n*, *l*, and *m* quantum numbers. Specify also the basis functions that can be used to describe any $n = 2$ state or states not affected by the field.

Give explicit numbers for the shifts of states for a field of 10^5 V/m. Specify energies in electron-Volts. (Note: Chapter 6 is a prerequisite for this problem.)

Chapter 11

Methods for one-dimensional problems

11.1 Tunneling probabilities

11.1.1 Consider a single barrier of thickness L, with height V much larger than the energy E of an electron wave incident on the left of the barrier. Presume that the barrier is thick enough that the amount of wave reflected back from the right-hand side of the barrier to the left is essentially negligible. Show that the fraction η of incident electrons transmitted by this barrier can be written approximately as

$$\eta \simeq \frac{16k^2\kappa^2}{\left(k^2 + \kappa^2\right)^2}\exp\left(-2\kappa L\right)$$

where $k = (2m_o E / \hbar^2)^{1/2}$ and $\kappa = [2m_o(V - E)/\hbar^2]^{1/2}$. (Note: Use the expression of the form $\eta = |F|^2 / |A|^2$, where F and A are the amplitudes of the transmitted and incident waves, respectively, to derive this; otherwise, the algebra becomes much more involved.)

11.2 Transfer matrix

11.2.1* Consider a double-barrier structure consisting of two barriers of height 1 eV and thickness 0.3 nm on either side of a 1 nm thick region of zero potential energy, with the regions on the left and the right of the entire structure assumed to have zero potential energy. Construct a transfer matrix model for that structure and calculate the tunneling probability of an electron through the structure as a function of electron energy from 0 to 1 eV, graphing the resulting transmission probability.

11.2.2 Perform a similar calculation to that of Problem 11.2.1 for the case of a semiconductor structure. The material on the left, on the right, and in the middle "well" is taken to be GaAs, and we are considering an electron in the conduction band of this and the other materials. The two barriers are now taken to be the specific AlGaAs material with aluminum fraction $x = 0.3$. The conduction band barrier height relative to the GaAs conduction band is given by the relation

$$V_{AlGaAs} \simeq 0.77x \text{ eV}$$

and the electron effective masses in the GaAs and AlGaAs layers are

$$m_f \simeq \left(0.067 + 0.083x\right)m_o$$

with $x = 0$ corresponding to the GaAs case. The middle GaAs "well" layer is 9 nm thick.

Specifically, find within 0.1 meV the energy of maximum transmission of the electron through the structure in the range 0 to 0.1 eV for the following AlGaAs barrier thicknesses on either side of the well

    (i) 4 nm

(ii) 6 nm

(iii) 8 nm

11.2.3 Consider a GaAs and AlGaAs structure, with a 9 nm thick GaAs layer, but with infinitely thick AlGaAs barriers on either side. Using the method of finding the energy that minimizes T_{11}, the top left element of the transfer matrix, find the bound state of this structure in the range 0 to 0.2 eV within 0.1 meV. (Note: Here, you will only have three layers in your structure altogether, with the "entering" and "exiting" materials being AlGaAs and only one GaAs intermediate layer, which makes the transfer matrix, in this case, only the product of three matrices altogether.)

11.2.4 Consider sets of one-dimensional potential wells that are 0.7 nm thick, with potential barriers separating the wells (i.e., on either side of the wells) that are 0.3 nm thick and 0.9 eV high, and consider the transmission resonances of an electron (in one dimension) in sets of these wells for energies up to 0.5 eV, presuming that the entering and exiting "materials" are the same as the potential well.

   (i)   Consider for reference one such well (i.e., a 0.7 nm well with two 0.3 nm barriers on either side) and find the resonance energy and sketch or graph the corresponding probability density inside the structure.

   (ii) Consider two such wells (i.e., two wells and three barriers):
      (a) graph the transmission probability as a function of energy with sufficient resolution to show all the resonances
      (b) state the number of resonances
      (c) find the lowest and highest resonance energies in the range
      (d) sketch or graph the probability amplitudes inside the structure corresponding to the lowest and highest energy resonances

   (iii) Repeat part (ii) for four such wells.

   (iv) Repeat part (ii) for eight such wells.

   (Note: This problem illustrates the emergence of band structure in periodic systems.)

11.3 Penetration factor for slowly varying barriers

11.4 Electron emission with a potential barrier

11.4.1 Consider a potential barrier of height 1 eV and thickness 1 nm. The same otherwise uniform material (taken here just to be vacuum) is on both sides of the barrier and no electric field is applied. There are electrons on the left of the barrier but none on the right. The electrons on the left are in a thermal distribution at room temperature (300K), with the Fermi energy of that distribution at -100 meV, below the lowest energy state of the electrons on the left, so we can approximately say the electrons are in a Maxwell–Boltzmann distribution. Using the approximate formula

$$\eta \simeq \frac{16 k_z^2 \kappa_z^2}{\left(k_z^2 + \kappa_z^2\right)^2} \exp\left(-2\kappa_z L\right)$$

where $k_z = (2m_o E_z / \hbar^2)^{1/2}$ and $\kappa_z = [2m_o(V - E_z)/\hbar^2]^{1/2}$, for the transmission probability of an electron of wavevector $+k_z$ (and kinetic energy E_z) in the z direction for tunneling from the left to the right of the barrier, calculate the total tunneling emission current density (in A/cm^2) from left to right of the barrier. (Note: You may well perform an appropriate numerical integral to get this result.)

11.4.2 (Note: This problem can be used as a substantial assignment.) Consider two GaAs layers separated by an Al$_{0.3}$Ga$_{0.7}$As barrier, 5 nm thick, which has a potential height for electrons of ~ 231 meV and an effective mass of ~0.0919 m_o. Presume that the electron effective mass in GaAs is 0.067 m_o. The temperature is 300K and the carrier density on the left of the barrier is such that the Fermi energy is at the bottom of the conduction band. (You may use the Maxwell–Boltzmann approximation to the thermal distribution of electrons.) There are presumed to be no carriers on the right-hand side of the

barrier, though the GaAs is assumed to be at the same uniform potential as the GaAs on the left-hand side of the barrier (i.e., assume the bottom of the GaAs conduction band is at the same constant energy on both sides).

(i)   Plot the transmission probability for an electron incident on the barrier from the left as a function of the energy of the electron, from 0 to 0.5 eV.

(ii)   Calculate the current density of electrons (in A/cm^2) moving from the left of the barrier to the right that we would expect on a simple classical calculation (i.e., the Richardson–Dushman equation).

(iii) Calculate the current density now using the quantum mechanical calculation with the transmission probability included.

(iv) Now replace the single barrier with a pair of $Al_{0.3}Ga_{0.7}As$ barriers each 3 nm thick around an empty GaAs "well" of thickness 4 nm. Plot the transmission probability for an electron incident on the barrier from the left as a function of the energy of the electron, from 0 to 0.5 eV.

(v)   With this new structure, calculate the current density now using the quantum mechanical calculation with the transmission probability included.

11.4.3 (Note: This problem can be used as a substantial assignment. It is similar to the previous problem, but here the electric field over the barrier is changed.) Consider the problem of emission of electrons from GaAs, through an AlGaAs barrier of thickness 10 nm and aluminum fraction of 30 percent, into another GaAs layer. The Fermi energy of the electrons in the conduction band of the emitting GaAs is presumed to be at the bottom of conduction band (which, incidentally, corresponds to an electron concentration of $\sim 3.2 \times 10^{17}$ cm^{-3}). Presume there is negligibly small carrier density in the GaAs layer on the other side of the barrier. The temperature is 300 K. You may assume the carrier distribution is approximately given by the Maxwell–Boltzmann distribution for all carriers that are important in the carrier emission. Answers for current densities need only be accurate to ~ 10 percent.

(i)   Calculate the thermionic emission current density across this barrier, in A/cm^{-2}, based on the classical Richardson–Dushman equation. (The presumption is that all carriers going to the "right" across the barrier are emitted.)

(ii)   Calculate the total emission current density at zero applied field across this barrier including the quantum mechanical transmission coefficient. Explain any difference in the value you get compared to the Richardson–Dushman result.

(iii) Calculate the total emission current density at a field of 20 V/micron. This field is presumed to be applied over the AlGaAs barrier only, in such a direction as to increase emission current substantially. The GaAs layers on either side of the barrier may be presumed to have zero field in them.

(iv) Graph the total emission current density over a field range from 0 to 40 V/micron over the AlGaAs barrier.

Note: Perform this calculation by constructing a transfer matrix model for the structure and dividing the barrier into a sufficient number of layers. The effect of electric field in the barrier is incorporated by progressively changing the potential in each successive layer of the barrier structure through the addition (or subtraction) of the potential due to the electric field in the barrier. You should not need a very large number of layers to get sufficiently accurate answers. You may need to take some care in numerical integrations over the Maxwell–Boltzmann exponential function because of its strongly decaying nature, though sophisticated numerical integration techniques should not be necessary.

Chapter 12

Spin

12.1 Angular momentum and magnetic moments

12.2 State vectors for spin angular momentum

12.3 Operators for spin angular momentum

See Problems 4.10.4 and 5.1.1.

12.4 The Bloch sphere

12.4.1* Show that for $|s\rangle = \cos(\theta/2)|\uparrow\rangle + \exp(i\phi)\sin(\theta/2)|\downarrow\rangle$

$$\langle s|\hat{\boldsymbol{\sigma}}|s\rangle = \mathbf{i}\sin\theta\cos\phi + \mathbf{j}\sin\theta\sin\phi + \mathbf{k}\cos\theta$$

12.4.2 Suppose an electron is in the spin state $|s\rangle = (1/\sqrt{2})[|\uparrow\rangle + i|\downarrow\rangle]$ and that the electron spin magnetic moment operator can be written as $\hat{\boldsymbol{\mu}}_e = g\mu_B\hat{\boldsymbol{\sigma}}$. What is the expectation value of the electron spin magnetic moment? (Note: The result is a vector).

12.4.3 Consider an arbitrary spin state $|s\rangle = \cos(\theta/2)|\uparrow\rangle + \exp(i\phi)\sin(\theta/2)|\downarrow\rangle$ and operate on it with the $\hat{\sigma}_z$ operator. Describe the result of this operation in terms of a rotation of the spin polarization vector on the Bloch sphere.

12.5 Direct product spaces and wavefunctions with spin

12.6 Pauli equation

12.7 Where does spin come from?

Chapter 13

Identical particles

13.1 Scattering of identical particles

13.1.1 Suppose that the initial state of the pair of identical particles (not restricted to being electrons) on the left in Fig. 13.1 is one of the states required for identical particles; that is,

$$\psi_{tpbefore}\left(\mathbf{r}_1,\mathbf{r}_2\right) = \psi_{abefore}\left(\mathbf{r}_1\right)\psi_{bbefore}\left(\mathbf{r}_2\right) \pm \psi_{abefore}\left(\mathbf{r}_2\right)\psi_{bbefore}\left(\mathbf{r}_1\right)$$

Suppose also that, mathematically, the effect of the scattering in Fig. 13.1 on a state $\psi_{abefore}\left(\mathbf{r}_1\right)\psi_{bbefore}\left(\mathbf{r}_2\right)$ is

$$\psi_{abefore}\left(\mathbf{r}_1\right)\psi_{bbefore}\left(\mathbf{r}_2\right) \rightarrow s_{straight}\psi_{aafter}\left(\mathbf{r}_1\right)\psi_{bafter}\left(\mathbf{r}_2\right) + s_{swap}\psi_{bafter}\left(\mathbf{r}_1\right)\psi_{aafter}\left(\mathbf{r}_2\right)$$

where $s_{straight}$ and s_{swap} are constant complex numbers. Show that the resulting state after the scattering is still of the right form required for identical particles.

13.2 Pauli exclusion principle

13.3 States, single-particle states, and modes

13.4 Exchange energy

13.4.1 Suppose that we have two ^{4}He nuclei, which are bosons, and also have electric charge because they have been stripped of their electrons. Suppose that they interact with one another through a potential energy that can be written in the form $V(\mathbf{r}_1,\mathbf{r}_2)$ (this potential could just be the Coulomb repulsion between these nuclei, for example, though the precise form does not matter for this problem). Suppose also that these particles are sufficiently weakly interacting that we can approximate their wavefunctions using products of the form $\psi_a\left(\mathbf{r}_1\right)\psi_b\left(\mathbf{r}_2\right)$, though we have to remember to symmetrize the overall wavefunction with respect to exchange. Write down an expression for the exchange energy of this pair of particles in terms of the Hamiltonian $\hat{H}$ for this pair of particles. (In other words, essentially go through the preceding argument for electrons, but presume bosons instead of fermions.)

13.4.2 *The classical beamsplitter.* An optical beamsplitter is a partially reflecting and partially transmitting mirror. One common form of a beamsplitter is in the form of a cube, with the reflecting surface being a diagonal one, as in the sketch.
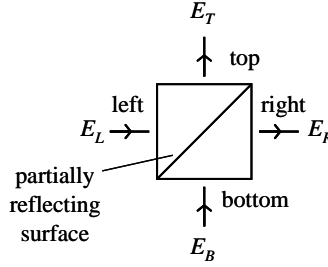
The beamsplitter is presumed loss-less, so an input beam on, say, the left face or the bottom face has its power split between the top and right output beams. E_L, E_B, E_T, and E_R are the electric field amplitudes of the various light beams as shown. For convenience, we take a complex representation for the fields, all of which we presume to be of the same frequency (i.e., $E_L = E_{Lo} \exp(-i\omega t)$ and similarly for the other beams) and of the same polarization (in the direction out of the page). The power in the left beam can, therefore, be taken to be $|E_L|^2$ (within a constant that will not matter for this problem) and similarly for the other beams. Because the beamsplitter is a linear optical component, we can write the relation between the input (left and bottom) beams and the output (right and top) beams using a matrix; that is, in general, we can write

$$\begin{bmatrix} E_T \\ E_R \end{bmatrix} = \hat{S} \begin{bmatrix} E_L \\ E_B \end{bmatrix} \quad \text{where} \quad \hat{S} = \begin{bmatrix} R_{LT} & T_{BT} \\ T_{LR} & R_{BR} \end{bmatrix}$$

where R_{LT}, R_{BR}, T_{BT}, and T_{LR} are constants for a given beamsplitter (with a self-evident notation in terms of reflection and transmission coefficients).

(i) Show for this lossless beamsplitter that

$$R_{LT} T_{BT}^* + R_{BR}^* T_{LR} = 0 \quad \text{and} \quad |R_{LT}|^2 + |T_{LR}|^2 = |R_{BR}|^2 + |T_{BT}|^2 = 1$$

(Hints: Conservation of power between the total input power ($|E_L|^2 + |E_B|^2$) and the total output power must hold for (a) arbitrary phase difference between E_L and E_B; and (b) arbitrary field magnitudes $|E_L|$ and $|E_B|$.)

(ii) Given the conditions proved in part (i), show that the matrix $\hat{S}$ is unitary.

13.4.3 *The boson beamsplitter.* Consider a 50:50 optical beamsplitter; that is, one that takes an input beam in the left or bottom input port and splits it equally in power between the top and right output ports. Following Problem 13.4.2, a suitable matrix that could describe such a beamsplitter would be

$$\hat{S} = \frac{1}{\sqrt{2}} \begin{bmatrix} i & 1 \\ 1 & i \end{bmatrix}$$

where we are considering two possible input beams, "left" and "bottom," and two possible output beams, "top" and "right," all of which are presumed to have exactly the same frequency and polarization (out of the page). When viewed quantum mechanically, these different beams each represent different modes (or single-particle states). In this way of viewing a beamsplitter, it couples the quantum mechanical amplitudes as follows:

$$\begin{bmatrix} \text{amplitude in top mode} \\ \text{amplitude in right mode} \end{bmatrix} = \hat{S} \begin{bmatrix} \text{amplitude in left mode} \\ \text{amplitude in bottom mode} \end{bmatrix}$$

Hence, the state $|1, L\rangle$ corresponding to a photon 1 in the left input mode is transformed according to the rule

$$|1, L\rangle \rightarrow \frac{1}{\sqrt{2}} \left(i|1, T\rangle + |1, R\rangle \right)$$

(" $\rightarrow$ " means "is transformed into") and, similarly, for photon 1 initially in the bottom input mode

$$|1, B\rangle \rightarrow \frac{1}{\sqrt{2}} \left(|1, T\rangle + i|1, R\rangle \right)$$

where L, R, T, and B refer to the left, right, top, and bottom modes, respectively.

Presume that the initial state of the system is one photon in the left input mode and one in the bottom input mode.

(i) Construct a state for these two photons in these two (input) modes that is correctly symmetrized with respect to exchange.

(ii) Using the transformation rules for the effect of the beamsplitter on any single photon state, deduce the output state after the beamsplitter, simplifying as much as possible.

(iii) Now suppose we perform a measurement on the output state and find one photon in the top mode. In what mode will we find the second photon?

(iv) In general, what can we say about the output modes in which we find the two photons?

(Note: This problem illustrates a particularly intriguing quantum mechanical behavior of a simple beamsplitter that is not predicted classically.)

13.4.4* *The fermion beamsplitter*. Imagine that a beamsplitter represented by the same matrix as in Problem 13.4.3 is operating as an electron (rather than photon) beamsplitter (for electrons of the same spin); deduce by a similar analysis to that of Problem 13.4.3:

(i) What will be the output quantum mechanical state of the two electrons if the input state is one electron in the left mode (or single-particle state) and one in the bottom mode (or single-particle state), simplifying as much as possible?

(ii) In general, what can we say about the output modes (single-particle states) in which we find the two electrons?

13.5 Extension to more than two identical particles

13.6 Multiple-particle basis functions

13.6.1 Suppose we have three particles, labeled 1, 2, and 3, and three single-particle states or modes, *a*, *b*, and *c*. We presume the particles are essentially not interacting, so the state of the three particles can be written in terms of products of the form $|1,a\rangle|2,b\rangle|3,c\rangle$, though we do presume that the states have to obey appropriate symmetries with respect to interchange of particles if the particles are identical. For the purposes of this problem, we are only interested in situations where each particle is in a different single-particle state or mode. For example, if the different states correspond to substantially different positions in space, we presume that we are considering states in which we would always find one and only one particle near each of these three positions if we performed a measurement.

Write out all the possible states of the three particles:
(i) if the particles are identical bosons
(ii) if the particles are identical fermions
(iii) if the particles are each different (e.g., one is an electron, one is a proton, and one is a neutron)

13.7 Thermal distribution functions

13.8 Important extreme examples of states of multiple identical particles

13.9 Quantum mechanical particles reconsidered

13.10 Distinguishable and indistinguishable particles

Chapter 14

The density matrix

14.1 Pure and mixed states

14.1.1 Suppose that we are measuring the value of the spin magnetic moment of electrons. We take the spin magnetic dipole moment operator to be $\hat{\boldsymbol{\mu}}_e = g\mu_B\hat{\boldsymbol{\sigma}}$. We compare the average value we measure in two different states, both of which are equal mixtures of x and y spin character for the electrons.

(i) Consider the pure spin state $\left|s_p\right\rangle = (1/\sqrt{3})(\left|s_x\right\rangle + \left|s_y\right\rangle)$. Here, $\left|s_x\right\rangle$ and $\left|s_y\right\rangle$ are, respectively, spin states oriented along the $+x$ and $+y$ directions. (Hint: See Eq. (12.27) and the associated discussion of the Bloch sphere to see how to write out these two states.)

    (a) Show that this pure state is normalized.
    (b) Find the expected value (which is a vector) of the spin magnetic dipole moment (i.e., the average result on measuring the magnetic dipole on multiple successive electrons all prepared in this state).
    (c) What is the magnitude of this average dipole moment (i.e., the length of the vector)?

(ii) Consider now the mixed spin state, with equal probabilities of the electrons being in the pure state $\left|s_x\right\rangle$ and the pure state $\left|s_y\right\rangle$.

    (a) What is the resulting average expected value (again a vector) of the spin magnetic dipole moment when measuring an ensemble of successive electrons prepared this way?
    (b) What is the magnitude of this ensemble average value?

(iii) What differences are there between the measured magnetic dipole moments in the two different cases of pure and mixed states?

14.2 Density operator

14.3 Density matrix and ensemble average values

14.3.1* Suppose we have a set of photons in a mixed state, with probabilities $P_1 = 0.2$ and $P_2 = 0.8$, respectively, of being in the two different pure states

$$\left|\psi_1\right\rangle = \left|\psi_H\right\rangle \ \text{ and } \ \left|\psi_2\right\rangle = \frac{3}{5}\left|\psi_H\right\rangle + \frac{4i}{5}\left|\psi_V\right\rangle$$

where $\left|\psi_H\right\rangle$ and $\left|\psi_V\right\rangle$ are the normalized and orthogonal basis states representing horizontal and vertical polarization, respectively. ($\left|\psi_1\right\rangle$, therefore, is a horizontally polarized state and $\left|\psi_2\right\rangle$ is an elliptically polarized state.) Write the density matrix for this state, in the $\left|\psi_H\right\rangle$ and $\left|\psi_V\right\rangle$ basis, with $\left\langle\psi_H\middle|\rho\middle|\psi_H\right\rangle$ as the top left element.

14.3.2 Consider the mixed spin state, with equal probabilities of the electrons being in the pure state $|s_x\rangle$ and the pure state $|s_y\rangle$. Here, $|s_x\rangle$ and $|s_y\rangle$ are, respectively, spin states oriented along the $+x$ and $+y$ directions. (See Problem 14.1.1)

(i) Evaluate the density operator ρ on the z spin basis (i.e., $|\uparrow\rangle$ and $|\downarrow\rangle$).

(ii) Now write this density operator as a density matrix, with the term in $|\uparrow\rangle\langle\uparrow|$ in the top left element.

(iii) Taking the spin magnetic dipole moment operator to be $\hat{\boldsymbol{\mu}}_e = g\mu_B\hat{\boldsymbol{\sigma}}$, evaluate $\hat{\boldsymbol{\mu}}_e$ as a matrix on the same z spin basis (i.e., $|\uparrow\rangle$ and $|\downarrow\rangle$), with the element $\langle\uparrow|\hat{\boldsymbol{\mu}}_e|\uparrow\rangle$ in the top left corner.

(iv) Using the expression of the form $\overline{\langle A\rangle} = Tr(\rho\hat{A})$, evaluate the ensemble average expectation value for the spin magnetic dipole moment in this mixed state. (Hint: The answer should be the same as that for Problem 14.1.1 (ii)(a).)

14.4 Time evolution of the density matrix

14.5 Interaction of light with a two-level "atomic" system

14.5.1 Suppose we have been driving an ensemble of two-level atoms with an energy separation between the two levels of $\hbar\omega_{21}$ and a (real) dipole matrix element μ_d between these two levels. The atoms have been illuminated with an electric field of the form $E_o\cos\omega t$ for a sufficiently long time that the system has reached a steady state. We work in the approximation where we have characteristic times T_1 and T_2 to describe the population recovery time and the dephasing time, respectively. For simplicity also, we presume we are at a low temperature so that the equilibrium condition (in the absence of optical electric field) is that all the atoms are in their lower state.

(i) Write down expressions for the values of the fractional difference $\rho_{11} - \rho_{22}$ between the lower and upper-state populations of the atoms and for the ensemble average $\langle\mu\rangle$ of the polarization of these atoms at time $t = 0$.

(ii) At time $t = 0$, we suddenly cut off this driving field (i.e., we suddenly set $E_o = 0$). Find expressions for the subsequent behavior of $\rho_{11} - \rho_{22}$ and $\langle\mu\rangle$. (Note: You may neglect the additional electric field that results from the polarization, for simplicity assuming that the total electric field is always zero for $t \geq 0$. You may use expressions based on the rotating wave approximation for this part.)

(iii) Presuming that $T_1 \gg T_2 \gg 1/\omega_{21}$ (e.g., $T_1 = 4T_2 = 20 \times 2\pi/\omega_{21}$) and, for simplicity, presuming we are operating far from resonance (i.e., $|\omega - \omega_{21}| \gg 1/T_2$), sketch the resulting behavior as a function of time of both the fraction of the population of atoms that are in their upper state and the ensemble average of the polarization (in arbitrary units for both these quantities), indicating all the characteristic times on your sketch. (Note: It is easier here *not* to use the slowly-varying or rotating-wave expressions for the off-diagonal elements.)

(iv) It might be that radiative recombination is the only process by which the atoms recover to their ground state (and, hence, that is the only process that contributes to T_1). You may find in part (ii) that the ensemble average of the overall magnitude of the polarization decays faster than the population recovers to its ground state. Explain why that rapid polarization decay can still be consistent with the longer overall (radiative) recovery of the population.

14.6 Density matrix and perturbation theory

Chapter 15

Harmonic oscillators and photons

15.1 Harmonic oscillator and raising and lowering operators

15.1.1. Prove the relation

$$\left[\hat{a},\hat{a}^{\dagger}\right]=\hat{a}\hat{a}^{\dagger}-\hat{a}^{\dagger}\hat{a}=1$$

for the harmonic oscillator raising and lowering operators, starting from their definitions

$$\hat{a}^{\dagger}\equiv\frac{1}{\sqrt{2}}\left(-\frac{d}{d\xi}+\xi\right) \text{ and } \hat{a}\equiv\frac{1}{\sqrt{2}}\left(\frac{d}{d\xi}+\xi\right)$$

15.1.2. Given that

$$\hat{a}^{\dagger}\hat{a}\left|\psi_{n}\right\rangle=n\left|\psi_{n}\right\rangle$$

and

$$\left[\hat{a},\hat{a}^{\dagger}\right]=\hat{a}\hat{a}^{\dagger}-\hat{a}^{\dagger}\hat{a}=1$$

show that

$$\hat{a}^{\dagger}\hat{a}\left(\hat{a}^{\dagger}\left|\psi_{n}\right\rangle\right)=(n+1)\left(\hat{a}^{\dagger}\left|\psi_{n}\right\rangle\right)$$

15.2 Hamilton's equations and generalized position and momentum

15.3 Quantization of electromagnetic fields

15.4 Nature of the quantum mechanical states of an electromagnetic mode

15.5 Field operators

15.5.1* Find the commutator $[\hat{\xi}_{\lambda},\hat{\pi}_{\lambda}]$ starting from the operator definitions

$$\hat{\xi}_{\lambda}\equiv\frac{1}{\sqrt{2}}\left(\hat{a}_{\lambda}+\hat{a}_{\lambda}^{\dagger}\right) \text{ and } \hat{\pi}_{\lambda}=\frac{i}{\sqrt{2}}\left(\hat{a}_{\lambda}^{\dagger}-\hat{a}_{\lambda}\right)$$

15.6 Quantum mechanical states of an electromagnetic field mode

15.6.1 Show that the coherent state in Eq. (15.94) is an eigenstate of the annihilation operator $\hat{a}_\lambda$, with eigenvalue $\sqrt{\bar{n}} \exp(-i\omega_\lambda t)$.

15.6.2* Using the results of Problem 15.6.1, find an expression for the expectation value of the "position" ξ_λ for the coherent state in Eq. (15.94) in terms of $\bar{n}$, ω_λ, and time t.

15.6.3 Consider the uncertainty relation for position and momentum in the coherent state of Eq. (15.94).

(i) Deduce the uncertainty relation for the operators $\hat{\xi}_\lambda$ and $\hat{\pi}_\lambda$.

(ii) By evaluating $\left\langle \hat{\xi}_\lambda^2 \right\rangle - \bar{\xi}_\lambda^2$ for the coherent state, show that the standard deviation of the width of the resulting probability distribution for the "position" ξ is $1/\sqrt{2}$, independent of time.

(iii) Repeat the calculation in (ii) for "momentum," with operator $\hat{\pi}_\lambda$, instead of "position."

(iv) Deduce that the coherent state is a "minimum uncertainty" state; that is, it has the minimum possible product of the standard deviations of "position" and "momentum."

(Hints: Use the results of Probs. 15.6.1 and 15.6.2, and the general relations for uncertainty principles in Chapter 5.)

15.7 Generalization to sets of modes

15.7.1 Consider a set of modes of the electromagnetic field in which the electric field is polarized along the *x* direction and the magnetic field is polarized in the *y* direction. Restricting consideration only to those modes, find the simplest expression you can for the commutation relation $\left[\hat{E}_x, \hat{B}_y \right]$ for this multimode field.

15.8 Vibrational modes

Chapter 16

Fermion operators

16.1 Postulation of fermion annihilation and creation operators

16.1.1* Consider a system that has two possible single-fermion states, 1 and 2, and can have anywhere from zero to two particles in it. There are, therefore, four possible states of this system: $|0_1, 0_2\rangle$ (the state with no particles in either single-fermion state, a state we could also write as the empty state $|0\rangle$), $|1_1, 0_2\rangle$, $|0_1, 1_2\rangle$, and $|1_1, 1_2\rangle$. (We also choose the standard ordering of the states to be in the order 1, 2.) Any state of the system could be described as a linear combination of these four basis states; that is,

$$|\Psi\rangle = c_1 |0_1, 0_2\rangle + c_2 |1_1, 0_2\rangle + c_3 |0_1, 1_2\rangle + c_4 |1_1, 1_2\rangle$$

which we could also choose to write as a vector

$$|\Psi\rangle = \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{bmatrix}$$

(i)   Construct 4 x 4 matrices for each of the operators $\hat{b}_1^\dagger$, $\hat{b}_1$, $\hat{b}_2^\dagger$, and $\hat{b}_2$.

(ii) Explicitly verify by matrix multiplication the anticommutation relations

$$\hat{b}_1^\dagger \hat{b}_1 + \hat{b}_1 \hat{b}_1^\dagger = 1$$
$$\hat{b}_2^\dagger \hat{b}_2 + \hat{b}_2 \hat{b}_2^\dagger = 1$$
$$\hat{b}_1^\dagger \hat{b}_2^\dagger + \hat{b}_2^\dagger \hat{b}_1^\dagger = 0$$
$$\hat{b}_1^\dagger \hat{b}_1^\dagger + \hat{b}_1^\dagger \hat{b}_1^\dagger = 0$$

16.1.2 Prove the relation

$$\hat{b}_j \hat{b}_k + \hat{b}_k \hat{b}_j = 0$$

by considering the swapping of rows in determinants (i.e., follow similar arguments to the analogous relation for creation operators in the previous section), considering all relevant initial states and choices of j and k.

16.2 Wavefunction operator

16.2.1 Consider the two-particle wavefunction operator

$$\hat{\psi}(\mathbf{r}_1,\mathbf{r}_2) = \frac{1}{\sqrt{2}}\sum_{j,n}\hat{b}_n\hat{b}_j\phi_j(\mathbf{r}_1)\phi_n(\mathbf{r}_2)$$

and a state $\left|\ldots,1_k,\ldots,1_m,\ldots\right\rangle \equiv \hat{b}_k^\dagger\hat{b}_m^\dagger\left|0\right\rangle$ that has one fermion in single-particle state k and an identical fermion in single-particle state m. Show that

$$\hat{\psi}(\mathbf{r}_1,\mathbf{r}_2)\left|\ldots,1_k,\ldots,1_m,\ldots\right\rangle = \frac{1}{\sqrt{2}}\left[\phi_k(\mathbf{r}_1)\phi_m(\mathbf{r}_2) - \phi_k(\mathbf{r}_2)\phi_m(\mathbf{r}_1)\right]\left|0\right\rangle$$

(i.e., this operator correctly constructs the combination of wavefunction products that is antisymmetric with respect to exchange of identical particles).

16.3 Fermion Hamiltonians

16.3.1 For identical fermions, prove

$$\left\langle 0\left|\hat{b}_m\hat{b}_k\hat{b}_a^\dagger\hat{b}_b^\dagger\hat{b}_d\hat{b}_c\hat{b}_k^\dagger\hat{b}_m^\dagger\right|0\right\rangle = \delta_{ak}\delta_{bm}\delta_{ck}\delta_{dm} + \delta_{am}\delta_{bk}\delta_{cm}\delta_{dk} - \delta_{am}\delta_{bk}\delta_{ck}\delta_{dm} - \delta_{ak}\delta_{bm}\delta_{cm}\delta_{dk}$$

16.3.2 Consider electrons and protons and construct the Hamiltonian in the **r** form for one electron and one proton assuming Coulomb interaction only.

(i) Transform this Hamiltonian into an occupation number form with creation and annihilation operators for both electrons and protons. (Hint: Use separate wavefunction operators for the electron wavefunction and for the proton wavefunction, noting any commutation relation between the operators corresponding to different kinds of particles.)

(ii) By presuming that the system is in a state $\left|\psi\right\rangle$ in which the electron is in some electron basis state k and the proton is in some proton basis state m, formally evaluate the expectation value of the energy of this system of one electron and one proton using this occupation number form of the Hamiltonian. Make use of the commutation and/or anticommutation relations appropriate for the operators (you need not actually evaluate any integrals), showing that, in this case, there is no exchange-energy term in the resulting energy expectation value.

16.3.3* (i) Using a complete orthonormal spatial basis set $\phi_n(\mathbf{r})$, write a general expression in terms of creation and annihilation operators for the position operator $\hat{\mathbf{r}}$ of a fermion.

(ii) Suppose now the fermion is explicitly in a one-dimensional potential well with infinitely high potential barrier on each side. Write an explicit expression for the position operator using the energy eigenfunctions $\phi_n(z)$ of this one-dimensional potential well problem as a basis. You may need the result

$$\int_0^\pi (x-\pi/2)\sin(nx)\sin(mx)\,dx = \frac{-4nm}{(n-m)^2(n+m)^2},\ \text{ for } n+m \text{ odd}$$

$$= 0,\ \text{ for } n+m \text{ even}$$

Chapter 17

Interaction of different kinds of particles

17.1 States and commutation relations for different kinds of particles

17.2 Operators for systems with different kinds of particles

17.2.1 Suppose that we are going to describe a number of particles in each case using the basis set of plane waves of different directions and/or different wavevector magnitudes, indexed by the wavevector $\mathbf{k}$. Suppose we have one or more electrons (all of the same spin), with the annihilation operator $\hat{b}_{\mathbf{k}}$ corresponding to the annihilation of an electron in basis plane-wave state of wavevector $\mathbf{k}$. Similarly, consider one or more protons (all with the same spin) with annihilation operators $\hat{d}_{\mathbf{k}}$, and one or more photons (all with the same polarization in any given plane-wave state) with annihilation operators $\hat{a}_{\mathbf{k}}$. For each of the following sets of operators, describe the process being represented by the operators and if that process necessarily cannot ever actually happen because of basic rules such as Pauli exclusion, say so. (E.g., the operators $\hat{b}_{\mathbf{k}1}^{\dagger}\hat{b}_{\mathbf{k}2}\hat{a}_{\mathbf{k}3}$ correspond to the process of absorption of a photon from the plane-wave state with wavevector $\mathbf{k}_3$ and changing an electron from the plane wave state with wavevector $\mathbf{k}_2$ to that with wavevector $\mathbf{k}_1$.)

(i) $\hat{d}_{\mathbf{k}1}^{\dagger}\hat{d}_{\mathbf{k}2}\hat{a}_{\mathbf{k}3}$

(ii) $\hat{b}_{\mathbf{k}1}^{\dagger}\hat{b}_{\mathbf{k}2}\left(\hat{a}_{\mathbf{k}3}\right)^{2}$

(iii) $\hat{d}_{\mathbf{k}1}^{\dagger}\hat{d}_{\mathbf{k}2}^{\dagger}\hat{d}_{\mathbf{k}3}\hat{d}_{\mathbf{k}4}$

(iv) $\left(\hat{b}_{\mathbf{k}1}^{\dagger}\right)^{2}\hat{b}_{\mathbf{k}3}\hat{b}_{\mathbf{k}4}$

(v) $\hat{b}_{\mathbf{k}1}^{\dagger}\hat{d}_{\mathbf{k}1}^{\dagger}\hat{b}_{\mathbf{k}3}\hat{d}_{\mathbf{k}4}$

(vi) $\hat{b}_{\mathbf{k}1}^{\dagger}\hat{a}_{\mathbf{k}2}^{\dagger}\hat{b}_{\mathbf{k}3}\hat{a}_{\mathbf{k}4}$

17.3 Perturbation theory with annihilation and creation operators

17.3.1* Suppose we have electrons (which are fermions with annihilation operator $\hat{b}$) and ^{4}He nuclei (which are bosons [here with an annihilation operator $\hat{c}$] because they consist of an even number of

fermions and which are also charged because they are ionized). The Coulomb interaction between these two particles can be described by a (perturbing) Hamiltonian of the form

$$\hat{H}_{Cen} = \sum_{j,k,\lambda,\mu} H_{Cjk\lambda\mu} \hat{b}_j^\dagger \hat{c}_\lambda^\dagger \hat{b}_k \hat{c}_\mu$$

Evaluate using the creation and annihilation operator formalism the matrix element $\left\langle N_{fq}; N_{bq} \middle| \hat{H}_{Cen} \middle| N_{fm}; N_{bm} \right\rangle$ for an initial state (i.e., $\left| N_{fm}; N_{bm} \right\rangle$) corresponding to one electron in single-particle state u with no other electron states occupied and one ^{4}He nucleus in mode α with no other ^{4}He states occupied, and a final state $\left| N_{fq}; N_{bq} \right\rangle$ corresponding to one electron in state v with no other electron states occupied and one ^{4}He nucleus in state β with no other ^{4}He states occupied. (Note: The answer to this is rather simple and even obvious, but this problem gives an elementary exercise in using the commutation properties of the various operators.)

17.4 Stimulated emission, spontaneous emission, and optical absorption

17.4.1 Consider an electron that may be in one of two states, state 1 with electron energy E_1 or state 2 with electron energy E_2, where $E_2 > E_1$. This electron is assumed to interact with the electromagnetic field through the electric-dipole interaction

$$\hat{H}_{ed} = \sum_{j,k,\lambda} H_{ed\lambda jk} \hat{b}_j^\dagger \hat{b}_k \left(\hat{a}_\lambda - \hat{a}_\lambda^\dagger \right)$$

where λ indexes the photon modes and j and k refer to electron states. The initial state of this system is presumed to be that the electron is in state 2, there are $n_{\lambda 1}$ photons in mode λ_1, and no photons in other modes.

(i) Show that the stimulated emission transition rate into the state q_{stim} with $n_{\lambda 1} + 1$ photons in mode λ_1 is

$$w_{qstim} = \frac{2\pi}{\hbar} (n_{\lambda 1} + 1) \left| H_{ed\lambda_1 21} \right|^2 \delta\left(E_2 - E_1 - h\omega_{\lambda 1} \right)$$

(ii) Show that the spontaneous emission transition rate into a state q_{spon} with $n_{\lambda 1}$ photons still in mode λ_1 and one photon in another mode λ is

$$w_{qspon} = \frac{2\pi}{\hbar} \left| H_{ed\lambda 21} \right|^2 \delta\left(E_2 - E_1 - h\omega_\lambda \right)$$

(iii) Suppose now that the initial state is still with $n_{\lambda 1} + 1$ photons in the mode λ_1, but that the electron is in state 1. Show that the absorption transition rate into the state with electron in state 2 and $n_{\lambda 1}$ photons in mode λ_1 is identical to the rate w_{qstim} calculated above for the stimulated emission.

17.4.2 (This problem can be used as a substantial assignment.) Consider a mass m on a spring. The mass is constrained in such a way that it can only move along one axis (e.g., the z axis) and, because of the linear restoring force of the spring, the mass has a natural oscillation (angular) frequency of Ω, behaving like a simple harmonic oscillator. The mass has a charge q and, consequently, it can interact with electromagnetic radiation.

(i) Write an expression for the quantum mechanical Hamiltonian for this simple harmonic oscillator (neglecting any interaction with the electromagnetic field) in terms of raising and lowering (annihilation and creation) operators. (Note: To avoid confusion with annihilation and creation operators for photons, you may want to use a different letter for these, for example, $\hat{d}^\dagger$ and $\hat{d}$.)

(ii) Give an expression for the position operator for the mass in terms of raising and lowering (annihilation and creation) operators of the harmonic oscillator formed by the mass and its spring. (Note: Do not write the position operator in terms of fermion annihilation and creation operators for the mass. That makes this problem much harder and, anyway, we have not even specified here whether this mass is a fermion or a boson.)

(iii) The electromagnetic field and the charged mass are presumed to interact through the electric dipole interaction. Give an expression for the Hamiltonian for this interaction with the

electromagnetic field in terms of raising and lowering and/or annihilation and creation operators, considering all possible modes of the electromagnetic field. (You should make the approximation that the field amplitude of the mode is taken to be approximately constant over the size of the oscillator and can be replaced by its value at some specific point in space in the region of the oscillator.)

(iv) Presume that the harmonic oscillator is initially in its lowest state. Considering for the moment only electromagnetic modes with electric field polarized in the *z* direction, describe the form of the optical absorption spectrum as a function of frequency. You may do this by considering the interaction with an electromagnetic mode initially containing one photon.

(v) Now consider a situation where the harmonic oscillator is in its first excited state and consider the interactions with all possible electromagnetic modes, all presumed initially empty of photons. Derive an expression for the spontaneous emission lifetime of this first excited state of the harmonic oscillator (i.e., how long will it take on average to emit a photon and decay to its lowest state).

(vi) Suppose that $m = 10^{-26}$ kg (roughly, the mass of a small atom), $q = +e$ (corresponding to an ion with a positive charge), and $\Omega = 2\pi \times 10^{14}$ s^{-1} (a typical frequency for some kinds of vibration modes in solids). In this case, what is the spontaneous emission lifetime?

(vii) Describe qualitatively in words the angular dependence of the emission rate of photons from such a system if the harmonic oscillator is initially in its first excited state.

Chapter 18

Quantum information

18.1 Quantum mechanical measurements and wavefunction collapse

18.2 Quantum cryptography

18.3 Entanglement

18.3.1 State whether each of the following states is entangled (i.e., can it be factored into a product of states of the individual particles, in which case it is not entangled):

(i) $\dfrac{1}{\sqrt{2}}\left(|H\rangle_1|V\rangle_2 - |H\rangle_1|H\rangle_2\right)$

(ii) $\dfrac{1}{\sqrt{2}}\left(|H\rangle_1|V\rangle_2 - |V\rangle_1|H\rangle_2\right)$

(iii) $\dfrac{3}{5}|H\rangle_1|V\rangle_2 + \dfrac{4i}{5}|V\rangle_1|V\rangle_2$

(iv) $\dfrac{1}{2}\left(|H\rangle_1|H\rangle_2 + |H\rangle_1|V\rangle_2 + |V\rangle_1|H\rangle_2 + |V\rangle_1|V\rangle_2\right)$

18.3.2 Show that the Bell states $|\Phi^-\rangle_{12}$ and $|\Psi^+\rangle_{12}$ are orthogonal.

18.3.3* Show that the set of four Bell states is complete as a basis for two-particle states where each particle has two available basis states (i.e., show that the general state of Eq. (18.16) can be written in terms of the Bell states and write that state out in terms of Bell states and the coefficients c_{HH}, c_{HV}, c_{VH}, and c_{VV}.) (Hint: Note that, e.g., $|H\rangle_1|H\rangle_2$ can be written as a sum of two different Bell states.)

18.3.4 (i) Consider the Bell state $|\Phi^-\rangle_{12} = (1/\sqrt{2})(|H\rangle_1|H\rangle_2 - |V\rangle_1|V\rangle_2)$ of two photons and suppose now that we wish to express it not on a basis of horizontal ($|H\rangle$) and vertical ($|V\rangle$) polarized states, but instead on a basis rotated by 45°; that is, a new basis

$$|+45\rangle = \left(1/\sqrt{2}\right)(|H\rangle + |V\rangle) \qquad |-45\rangle = \left(1/\sqrt{2}\right)(|H\rangle - |V\rangle)$$

Show that expressed on this particular basis, the resulting state is still a Bell state.

(ii) Repeat part (i) but with the Bell state $|\Phi^+\rangle_{12} = (1/\sqrt{2})(|H\rangle_1|H\rangle_2 + |V\rangle_1|V\rangle_2)$. What difference do you note between the two results?

See also Problems 13.4.2–13.4.4.

18.4 Quantum computing

18.5 Quantum teleportation

Chapter 19

Interpretation of quantum mechanics

19.1 Hidden variables and Bell's inequalities

19.1.1 (i) Consider the Bell state $|\Phi^+\rangle_{12} = (1/\sqrt{2})(|H\rangle_1|H\rangle_2 + |V\rangle_1|V\rangle_2)$ of two photons. Express it now not on a basis of horizontal ($|H\rangle$) and vertical ($|V\rangle$) polarized states but instead on a basis $|\theta\rangle$ and $|\theta + \pi/2\rangle$ rotated by an angle θ in a positive (i.e., anticlockwise) direction relative to the horizontal axis. (Hint: On such a basis, $|V\rangle = \sin\theta|\theta\rangle + \cos\theta|\theta + \pi/2\rangle$ and a similar expression exists for $|H\rangle$.)

(ii) Hence, show that the two photons in such a state will always come out of the same arm of each polarizer when two aligned polarizers are used to examine the pair of photons.

19.2 Solutions to the measurement problem

19.2.1 Derive the relations

$$\text{(i)} \quad \frac{\partial S}{\partial t} + \frac{(\nabla S)^2}{2m} + V + Q = 0 \quad \text{and (ii)} \quad \frac{\partial R^2}{\partial t} + \nabla \cdot \left(R^2 \frac{\nabla S}{m} \right) = 0$$

from Schrödinger's time-dependent equation, where

$$Q = -\frac{\hbar^2}{2m} \frac{\nabla^2 R}{R}$$

and the wavefunction is written in the form

$$\psi(\mathbf{r},t) = R(\mathbf{r},t)\exp\big(iS(\mathbf{r},t)\big).$$

(Note: The second relation (ii) corresponds to conservation of particles or probability density because $(\nabla S)/m$ can be interpreted as velocity; hence, $R^2(\nabla S)/m$ represents the flow of probability density.)

19.3 Epilogue

Problem Solutions

Chapter 2 problem solutions

2.3.1

(i) From Eq. (2.17) in the book and the following text, we have the expression $d_s=\lambda z_o/s$ for the separation of the fringes. Here z_o = 10cm and s = 5nm. We can calculate λ using the de Broglie formula $\lambda = h/p$. Remembering also that $E = p^2/2m$ for a free particle, we have

$$p = \sqrt{2mE} = \sqrt{2 \cdot (9.11 \times 10^{-31} \text{kg}) \cdot (1\text{eV}) \cdot (1.6 \times 10^{-19} \text{J/eV})} = 5.4 \text{x} 10^{-25} \text{ kg/s}$$

$$d_s = \lambda z_o / s = h z_o / sp = [(6.626 \times 10^{-34} \text{J} \cdot \text{s}) \times (1 \times 10^{-1} \text{m})]/[(5 \times 10^{-9} \text{m}) \times (5.4 \times 10^{-25})] = 25\text{mm}$$

(ii) The mass of the proton is 1836 times larger than the mass of the electron. Since p is proportional to the square root of m and d is inversely proportional to p, then the answer should be $25\text{mm}/\sqrt{1836} = 583 \mu\text{m}$.

2.3.2

(i) The slit is of width d and the screen is z_o away. Each point in the slit is the source of a spherically expanding wave. The wavefunction at a point (x, z_o) on the screen is the sum of the waves from all the points in the slit. Since it is a continuous set of points, our summation limits to an integral.
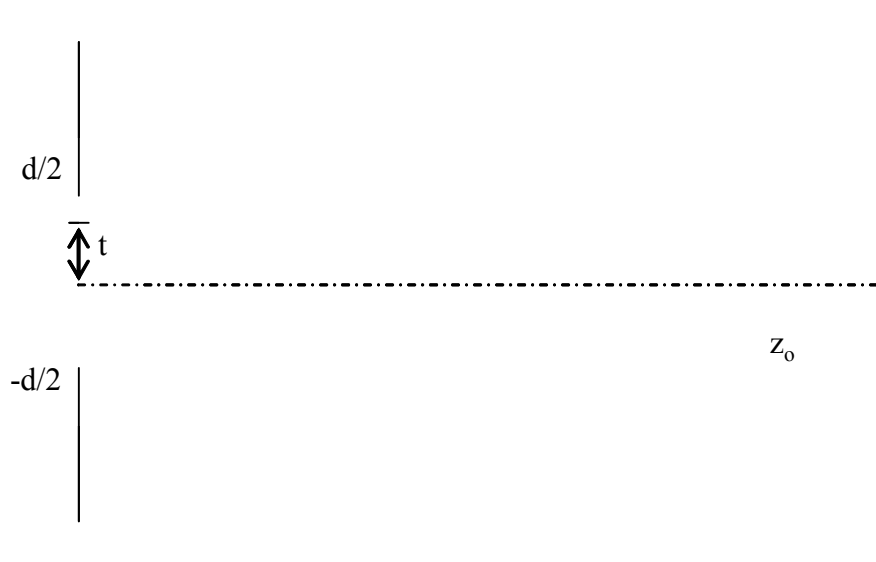
Taking the center of the slit as the origin, consider a small section of the slit at a distance t from the center having a width dt. To find the wave function at x on the screen, due to all the point sources within this section, we must propagate the expanding waves through the distance between $(0, t)$ and (x, z_o). This distance r is

$$r = \left(z_o^2 + (x-t)^2\right)^{(1/2)}$$

The wave function at (x, z_o) due to the section dt is

$$d\psi(x, z_o) = \frac{1}{r}\exp(ikr)dt$$

The paraxial approximation that $x \ll z_o$ implies that $r \sim z_o.$ For the $1/r$ term, we can safely assume $1/r \sim 1/z_o$, and neglect that as a constant factor; i.e.,

$$d\psi(x, z_o) = \frac{1}{z_o}\exp(ikr)dt \propto \exp(ikr)dt$$

However, an exponential is very sensitive to small changes in its argument so we cannot assume $r \sim z_o$ in the phase term. The paraxial approximation $x \ll z_o$ allows us to expand the square root in a Taylor series keeping only first order terms in $(x - t)^2$. Also using $t < x \ll z_o$

$$r = \left(z_o^2 + (x-t)^2\right)^{(1/2)} \approx z_o\left[1 + \frac{1}{2}\left(\frac{x^2 + t^2 - 2xt}{z_o^2}\right)\right]$$

$$\approx z_o\left[1 + \frac{1}{2}\left(\frac{x^2 - 2xt}{z_o^2}\right)\right] = \left[z_o + \frac{x^2}{2z_o} - \frac{xt}{z_o}\right]$$

Hence,

$$d\psi(x,z_o) \propto \exp(ikr)dt = \exp\left[ik\left(z_o + \frac{x^2}{2z_o}\right)\right]\exp\left(-ik\frac{xt}{z_o}\right)dt$$

Integrating this over t we get the contribution from the entire slit

$$\psi(x,z_o) = \exp(ik\phi)\int_{-d/2}^{d/2} \exp\left(-ik\frac{xt}{z_o}\right)dt$$

where

$$\phi = \left(z_o + \frac{x^2}{2z_o}\right)$$

$$\psi(x,z_o) = \exp(ik\phi)\frac{2z_o}{kx}\sin\left(\frac{kxd}{2z_o}\right) = d\exp(i\phi)\frac{\sin\left(\dfrac{kxd}{2z_o}\right)}{\left(\dfrac{kxd}{2z_o}\right)}$$

We have a function of the form $(\sin x)/x$, also known as the sinc function. Below is a plot of $\psi(x,z_o)$.

distance on screen (microns)
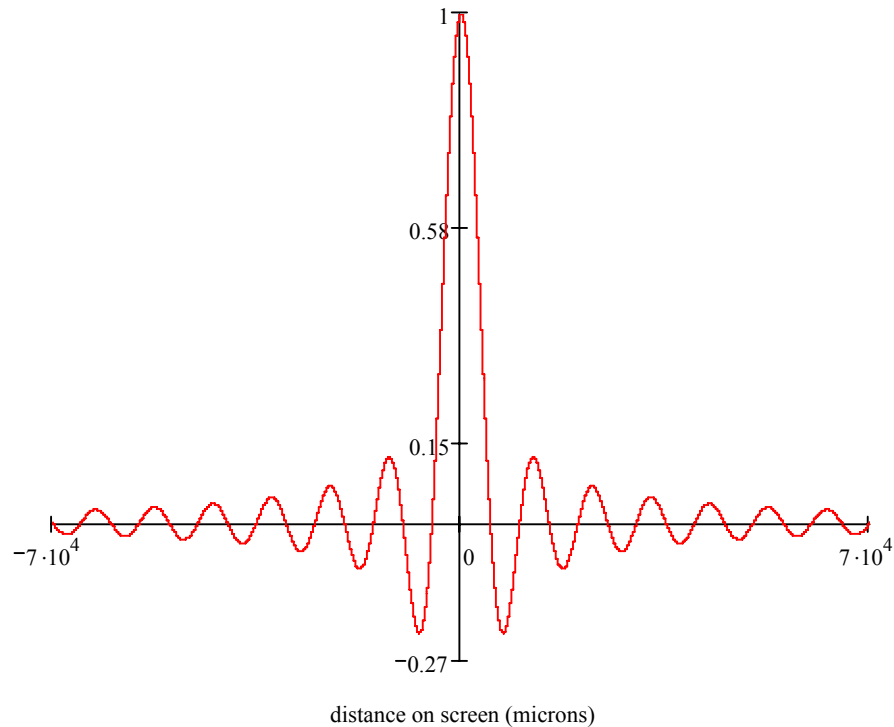
The function crosses zero each time the argument of the sine is a non-zero multiple of π, so the widths of each of the side fringes is $\dfrac{\lambda z_o}{d}$. More importantly, the width of the bright central lobe is $2\dfrac{\lambda z_o}{d}$, which says the electrons diffract more as

(a) the slit gets narrower for given λ

(b) the wavelength gets larger for a given slit width

The z_o term just says the farther the screen, the larger the spot.

(ii) The intensity of light at a point on the phosphorescent screen is proportional to the probability density of the electron at that point

$$I(x,z_o) = |\psi(x,z_o)|^2 = \text{sinc}^2\left(\frac{kxd}{2z_o}\right)$$

d/2

-d/2

w

z_o
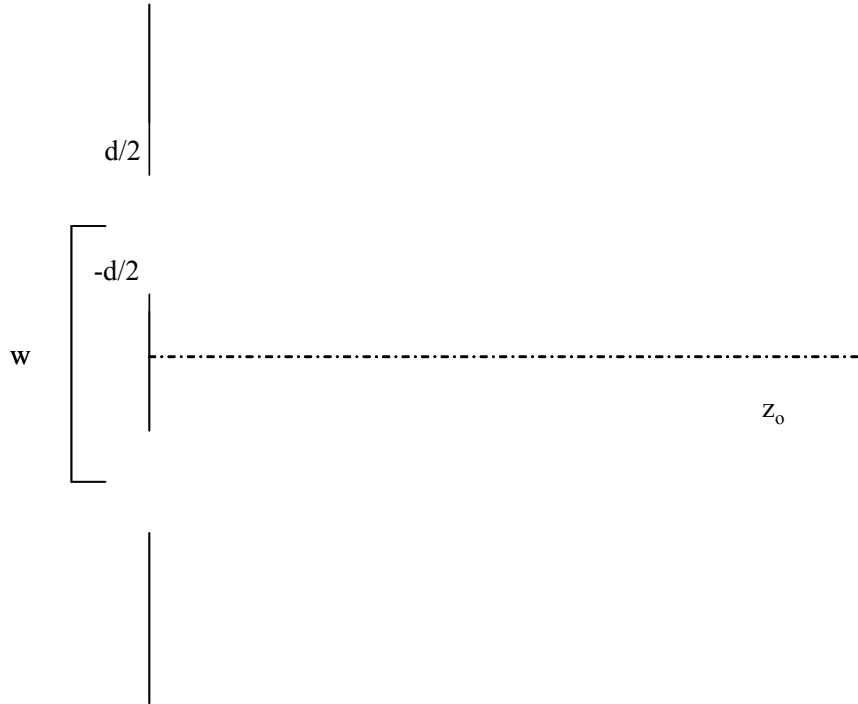
(iii) Two finite slits

For two slits we can essentially use the technique in part (i). We integrate over each slit separately and add the results. Let the slit separation (center to center) be w and the variable of integration t measured from the center of each slit. The limits of integration are $t = -d/2$ to $t = d/2$.

For the top slit this results in

$$r = \left(z_o^2 + (x - \frac{w}{2} - t)^2\right)^{(1/2)} \approx z_o\left[1 + \frac{1}{2}\left(\frac{(x-\frac{w}{2})^2 + t^2 - 2(x-\frac{w}{2})t}{z_o^2}\right)\right]$$

$$\approx z_o\left[1 + \frac{1}{2}\left(\frac{(x-w/2)^2 - 2(x-w/2)t}{z_o^2}\right)\right] = \left[z_o + \frac{(x-w/2)^2}{2z_o} - \frac{(x-w/2)t}{z_o}\right]$$

Note that this is the same form as we had for the single slit just with x shifted to $x - w/2$. For the bottom slit the shift is $x \to x + w/2$ i.e.,

$$d\psi(x,z_o) = \exp\left(ik\left(z_o + \frac{(x-w/2)^2}{2z_o}\right)\right)\exp\left(-ik\frac{(x-w/2)t}{z_o}\right)dt \qquad \text{from the top slit}$$

$$d\psi(x,z_o) = \exp\left[ik\left(z_o + \frac{(x+w/2)^2}{2z_o}\right)\right]\exp\left(-ik\frac{(x+w/2)t}{z_o}\right)dt \quad \text{from the bottom slit}$$

Integrating each and adding gives

$$d\exp\left[ik\left(z_o + \frac{(x-w/2)^2}{2z_o}\right)\right]\frac{\sin\left(\frac{k(x-w/2)d}{2z_o}\right)}{\left(\frac{k(x-w/2)d}{2z_o}\right)} + d\exp\left[ik\left(z_o + \frac{(x+w/2)^2}{2z_o}\right)\right]\frac{\sin\left(\frac{k(x+w/2)d}{2z_o}\right)}{\left(\frac{k(x+w/2)d}{2z_o}\right)}$$

Ignoring constant phase factors and constants we have

$$\exp\left[ik\frac{(x-w/2)^2}{2z_o}\right]\frac{\sin\left(\frac{k(x-w/2)d}{2z_o}\right)}{\left(\frac{k(x-w/2)d}{2z_o}\right)} + \exp\left[ik\frac{(x+w/2)^2}{2z_o}\right]\frac{\sin\left(\frac{k(x+w/2)d}{2z_o}\right)}{\left(\frac{k(x+w/2)d}{2z_o}\right)}$$

Plotting the modulus squared of this we get
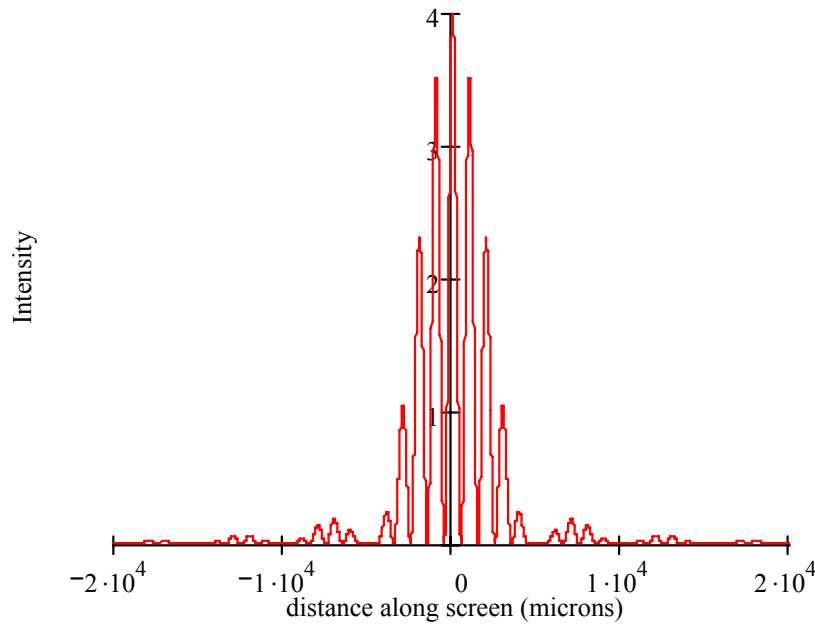
Note: Given the numbers in the problem w^2/z_0^2 was very small so neglecting this will still give essentially the correct plot. However, in general it may not be the case that the slit spacing is negligible.

2.4.1

We will use the following test for linearity for a non-zero solution $\psi(x)$.

   If $\psi(x)$ is a solution then $a\psi(x)$ is also a solution where a is an arbitrary constant.

If we substitute $a\psi(x)$ into each of the equations we get the following.

i) $az\dfrac{d\psi}{dz} + ag(z)\psi(z) = 0$

We see that the a's will cancel, meaning that therefore $a\psi(x)$ is also a solution, so this equation is **LINEAR.**

ii) $a^2\psi(z)\dfrac{d\psi(z)}{dz} + a\psi(z) = 0$

The constant a cannot be canceled in this equation, so it is **NOT LINEAR. (**In other words, given that $\psi(x)$ is a solution of $\psi(z)\dfrac{d\psi(z)}{dz} + \psi(z) = 0$, the only value of a for which $a\psi(x)$ is also a solution is $a = 1$.)

iii) $a\dfrac{d^2\psi(z)}{dz^2} + ab\dfrac{d\psi(z)}{dz} = ac\psi(z)$

We see that the a's will cancel, so this is **LINEAR.**

iv) $a\dfrac{d^3\psi(z)}{dz^3} = 1$

The constant a cannot be canceled in this equation, so it is **NOT LINEAR.**

v) $a\dfrac{d^2\psi(z)}{dz^2} + a(1 + a^2|\psi(z)^2|)\dfrac{d\psi(z)}{dz} = ag\psi(z)$

The constant a cannot be canceled in this equation, so it is **NOT LINEAR.**

2.6.1

The normalized wavefunctions for the various different levels in the potential well are

$$\psi_n(z) = \sqrt{\frac{2}{L_z}} \sin\left(\frac{n\pi z}{L_z}\right)$$

The lowest energy state is $n = 1$, and we are given $L_z = 1$ nm.

The probability of finding the electron between 0.1 and 0.2 nm from one side of the well is, using nanometer units for distance,

$$P = \int_{0.1}^{0.2} \left|\psi_1(z)\right|^2 dz = \int_{0.1}^{0.2} 2\sin^2(\pi z)dz$$

$$= \int_{0.1}^{0.2} \left[1 - \cos(2\pi z)\right] dz$$

$$= 0.1 - \int_{0.1}^{0.2} \cos(2\pi z)dz$$

$$= 0.1 - \frac{1}{2\pi}\left[\sin(2\pi \times 0.2) - \sin(2\pi \times 0.1)\right]$$

$$= 0.042$$

(Note: For computation purposes, remember that the argument of the sine is in radians and not degrees. For example, when we say $\sin(\pi) = 0$, it is implicit here that we mean π radians.)

2.6.2

(i) Odd, since

$$f(x) = \sin(x)$$
$$f(-x) = \sin(-x) = -\sin(x) = -f(x)$$

(ii) Neither even nor odd, since

$$f(x) = \exp(ix) = \cos(x) + i\sin(x)$$
$$f(-x) = \exp(-ix) = \cos(x) - i\sin(x)$$

(iii) Even, since

$$f(x) = (x-a)(x+a) = x^2 - a^2$$
$$f(-x) = x^2 - a^2 = f(x)$$

(iv) Even, since

$$f(x) = \exp(ix) + \exp(-ix) = 2\cos(x)$$
$$f(-x) = 2\cos(-x) = 2\cos(x) = f(x)$$

(v) Odd, since

$$f(x) = x(x^2 - 1)$$
$$f(-x) = -x(x^2 - 1) = -f(x)$$

2.6.3

(i) $\sin\left(7\pi z / L_z\right)$

Yes (this is the solution for $n = 7$ for such a simple well)

(ii) $\cos\left(2\pi z / L_z\right)$

No (this does not fit the boundary conditions at the walls of the well, not being zero amplitude at the walls)

(iii) $0.5\sin\left(3\pi z / L_z\right) + 0.2\sin\left(\pi z / L_z\right)$

No (this is a superposition of two eigenfunctions, but that is not a solution of the time-independent Schrödinger equation)

(iv) $\exp(-0.4i)\sin\left(2\pi z / L_z\right)$

Yes (This is the solution for $n = 2$, with a complex factor that makes no difference in the time-independent Schrödinger equation.)

2.6.4

We have an infinite potential well of width L_z in each of the three dimensions.

(i) Given the note at the end of the problem, we can write the solution as a product of three solutions

$$\psi_{n_x n_y n_z}(x,y,z) = \sqrt{\frac{2}{L_z}}\sin\left(\frac{n_x \pi x}{L_z}\right) \times \sqrt{\frac{2}{L_z}}\sin\left(\frac{n_y \pi y}{L_z}\right) \times \sqrt{\frac{2}{L_z}}\sin\left(\frac{n_z \pi z}{L_z}\right)$$

With the allowed energies of the three dimensional system being

$$E_n = E_{n_x} + E_{n_y} + E_{n_z} = E_1^\infty(n_x^2 + n_y^2 + n_z^2)$$

where

$$E_1^\infty = \frac{\hbar^2}{2m}\left(\frac{\pi}{L_z}\right)^2$$

is the lowest allowed energy of a particle in a one-dimensional infinite potential well.

(ii) The lowest allowed state corresponds to $(n_x, n_y, n_z) = (1,1,1)$ and has an energy $E_1 = 3E_1^\infty$. In this state the wave function in each of the three directions looks like
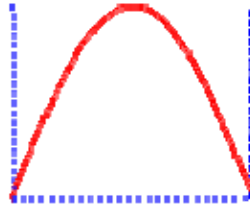
The next three states all have the same energy $E_{2,3,4} = 6E_1^\infty$ and correspond to $(n_x, n_y, n_z) = (2,1,1)$, $(n_x, n_y, n_z) = (1,2,1)$, $(n_x, n_y, n_z) = (1,1,2)$. In these three cases, the wave function along two of the dimensions looks as above, but along the third dimension it is the next higher state of the infinite well
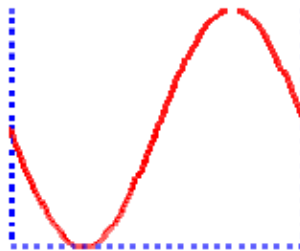
(iii) These last three states have equal energy and hence are degenerate (i.e., they have a degeneracy of 3) because the width of the well is the same in all three dimensions.

2.7.1

To check orthogonality on [-1,1] we take the inner product of the two functions. If they are orthogonal on the interval, then the inner product (orthogonality integral) is zero, i.e.,

$$\int_{-1}^{1} f(x)g^*(x)dx = 0$$

Since the interval is symmetric about $x = 0$, we can use the parity of the integrand to determine by inspection whether the integral is zero or not. But we should be careful with periodic functions, as in (v).

(i) orthogonal

$$\int_{-1}^{1} x^3 = 0 \qquad\qquad\qquad \text{(since } x^3 \text{ is odd)}$$

(ii) not orthogonal

$$\int_{-1}^{1} x^4 \neq 0 \qquad\qquad\qquad \text{(since } x^4 \text{ is even)}$$

(iii) not orthogonal

$$\int_{-1}^{1} x \sin x \, dx \neq 0 \qquad\qquad\qquad \text{(since } x \sin x \text{ is even)}$$

(iv) not orthogonal

$$\int_{-1}^{1} x \exp\left(\frac{-i\pi x}{2}\right)dx = \int_{-1}^{1}\left(x\cos\frac{\pi x}{2} - ix\sin\frac{\pi x}{2}\right)dx$$

note that $\cos(\pi x/2)$ and $\sin(\pi x/2)$ are periodic with period 4, so the interval is less than a period.

$$0 - i\int_{-1}^{1}\left(x\sin\frac{\pi x}{2}\right)dx \neq 0$$

(since $x\cos\dfrac{\pi x}{2}$ is odd and $x\sin\dfrac{\pi x}{2}$ is even)

(v) orthogonal

$$\int_{-1}^{1} \exp(-4\pi i x)dx = \int_{-1}^{1} [\cos(4\pi x) - i\sin(4\pi x)]dx = 0$$

because the period of both $\cos(4\pi x)$ and $\sin(4\pi x)$ is 2, so the interval is an integral number of periods (in this case one full period). The integral of a sinusoid over one period is zero.

2.7.2

(i) $$f_0(x)=1, \quad f_1(x)=x, \quad f_2(x)=x^2 \quad ...f_n(x)=x^n$$

For a counter example to show these functions are not all orthogonal, we can choose the x and x^3 functions, leading to an orthogonality integral

$$\int_{-1}^{1} x \times x^3 dx = \int_{-1}^{1} x^4 dx \neq 0 \qquad \text{(since } x^4 \text{ is even)}$$

(ii) Let the unnormalized functions be labeled as $h_i(x)$. So we have, for our first member of this set of functions

$$h_0(x) = f_0(x) = 1$$

To normalize a function we divide it by the appropriate normalization factor, which is the square root of the integral of its modulus squared over the interval of interest. For this function, the integral of its modulus squared over the interval of interest is

$$\int_{-1}^{1} |f_0(x)|^2 \, dx = \int_{-1}^{1} 1 dx = 2$$

Thus the normalized version is $g_0(x) = \dfrac{1}{\sqrt{2}}$

We can check that $g_0(x)$ is normalized; i.e.,

$$\int_{-1}^{1} |g_0(x)|^2 = 1 \qquad (1)$$

Now we try to construct a function that is orthogonal to $g_0(x)$ by constructing a combination of $g_0(x)$ and $f_1(x)$ that is orthogonal to $g_0(x)$. One appropriate way of writing such a combination is $h_1(x) = f_1(x) + a_{10}g_0(x)$. We want this to be orthogonal to $g_0(x)$, so we require

$$\int_{-1}^{1} \left(f_1(x) + a_{10}g_0(x) \right) g_0(x) dx = 0$$

so, using Eq. (1) $$\int_{-1}^{1} f_1(x) g_0(x) dx = -a_{10}$$

Hence $-a_{10} = \int_{-1}^{1} \dfrac{x}{\sqrt{2}} dx = 0$. Thus, in this particular case, $h_1(x) = f_1(x) = x$.

Normalizing $$\int_{-1}^{1} |h_1(x)|^2 dx = \int_{-1}^{1} x^2 dx = 2/3$$

Hence $$g_1(x) = \sqrt{\frac{3}{2}} x$$

So now we have constructed a function $g_1(x)$ that is normalized and orthogonal to $g_0(x)$.

c) Similarly, we now try to construct a function $h_2(x)$ that is orthogonal to $g_0(x)$ and $g_1(x)$ by adding amounts of these two functions and some of the next linearly independent function in our set, i.e.,

$$h_2(x) = f_2(x) + a_{20}g_0(x) + a_{21}(x)g_1(x)$$

Orthogonalizing to g_0 and g_1 gives

$$a_{21} = -\int_{-1}^{1} x^2 \sqrt{\frac{3}{2}} x \, dx = 0 \quad \text{and} \quad a_{20} = \int_{-1}^{1} x^2 \sqrt{\frac{1}{2}} dx = -\sqrt{\frac{2}{3}}$$

So
$$h_2(x) = x^2 - \frac{1}{3}$$

Normalizing, we have
$$\int_{-1}^{1} |h_2(x)|^2 \, dx = \int_{-1}^{1} (x^4 + \frac{1}{9} - \frac{2}{3}x^2) dx = \frac{8}{45}$$

and hence
$$g_2(x) = \frac{1}{3}\sqrt{\frac{45}{8}}(3x^2 - 1) = \frac{1}{2}\sqrt{\frac{5}{2}}(3x^2 - 1)$$

d) We write

$$h_i(x) = f_i(x) + a_{i0}g_0(x) + a_{i1}g_1(x) + \ldots + a_{i,i-1}g_{i-1}(x)$$

Orthogonalizing to $g_j(x)$, we have

$$\int_{-1}^{1} h_i(x)g_j(x)dx = 0 \implies \int_{-1}^{1} f_i(x)g_j(x)dx + a_{ij} \int_{-1}^{1} g_j(x)g_j(x)dx = 0$$

$$\implies a_{ij} = -\int_{-1}^{1} f_i(x)g_j(x)dx$$

e) For the function $g_3(x)$, we start with $h_3(x) = f_3(x) + a_{30}g_0(x) + a_{31}g_1(x) + a_{32}g_2(x)$

Orthogonalizing to $g_0(x)$, $g_1(x)$, and $g_2(x)$ leads to

$$a_{30} = -\int_{-1}^{1} x^3 \sqrt{\frac{1}{2}}dx = 0 \qquad a_{31} = \int_{-1}^{1} x^3 \sqrt{\frac{3}{2}}x dx = -\frac{2}{5}\sqrt{\frac{3}{2}} \qquad a_{32} = \int_{-1}^{1} x^3 \frac{1}{2}\sqrt{\frac{5}{2}}(3x^2 - 1)dx = 0$$

So
$$h_3(x) = x^3 - \frac{2}{5}(\frac{3}{2})x = 5x^3 - 3x$$

Normalizing, we have
$$\int_{-1}^{1} |h_3(x)|^2 \, dx = \int_{-1}^{1} (25x^6 + 9x^2 - 30x^4)dx = \frac{8}{7}$$

Hence
$$g_3(x) = \frac{1}{2}\sqrt{\frac{7}{2}}(5x^3 - 3x)$$

So finally we have

$$g_0(x) = \sqrt{\frac{1}{2}} \qquad g_1(x) = \sqrt{\frac{3}{2}}x \qquad g_2(x) = \frac{1}{2}\sqrt{\frac{5}{2}}(3x^2 - 1) \qquad g_3(x) = \frac{1}{2}\sqrt{\frac{7}{2}}(5x^3 - 3x)$$

f) The above is not the only set of orthogonal normalized functions for this interval in powers of x. If we start with a different function in the series we will in general get a new set. For instance, we could make the following choice for our first function

$$h_0 = f_3(x) = x$$

Normalizing this choice gives $\qquad g_0(x) = \sqrt{\frac{3}{2}}x$

Then for our second function, we would have

$$h_1(x) = f_2(x) + a_{10}g_0(x)$$

Orthogonalizing to $g_0(x)$ leads to $\qquad a_{10} = -\int_{-1}^{1} x^2 \sqrt{\frac{3}{2}}x\,dx = 0$

Hence $\qquad h_1(x) = x^2$

Normalizing this function gives $\qquad g_1(x) = \sqrt{\frac{5}{2}}x^2$

and so on. Note that these functions g are a different and orthonormal set; for example, we have no function that is simply proportional to x^2 in the set of functions in part (e) above.

2.8.1

The wave incident from the left on the infinite barrier will be reflected completely because of the boundary condition that the wavefunction must be zero at the edge of, and everywhere inside of, the infinite barrier. So if the barrier is located at $x = 0$

$$\psi(x) = 0 \qquad\qquad (x > 0)$$

Now, for an electron of energy E, which here is 1 eV, we know that it will have a wavevector

$$k = \sqrt{\frac{2m_o E}{\hbar^2}} = 5.12 \times 10^9 \text{ m}^{-1}$$

The general solution for a wave on the left of the barrier is a sum of a forward and a backward wave each with this magnitude of wavevector, with amplitudes A and B, respectively; that is

$$\psi(x) = A\exp(ikx) + B\exp(-ikx) \quad (x < 0)$$

Knowing from our boundary condition that the wave must be zero at the boundary at $x = 0$,

$$A + B = 0 \;\Rightarrow\; A = -B$$
$$\Rightarrow\; \psi(x) = A(\exp(ikx) - \exp(-ikx)) = 2iA\sin(ikx) \quad (x < 0)$$

Thus, the wave function on the left hand side of the infinite barrier is a standing wave.

The probability density for finding the electron at any given position is

$$|\psi(x)|^2 = 0 \qquad\qquad (x > 0)$$
$$|\psi(x)|^2 = 4|A|^2 \sin^2(kx) \qquad (x < 0)$$

which has a period π / k.

The period of the standing wave shown in the graph is therefore ~ 6.1 Angstroms.
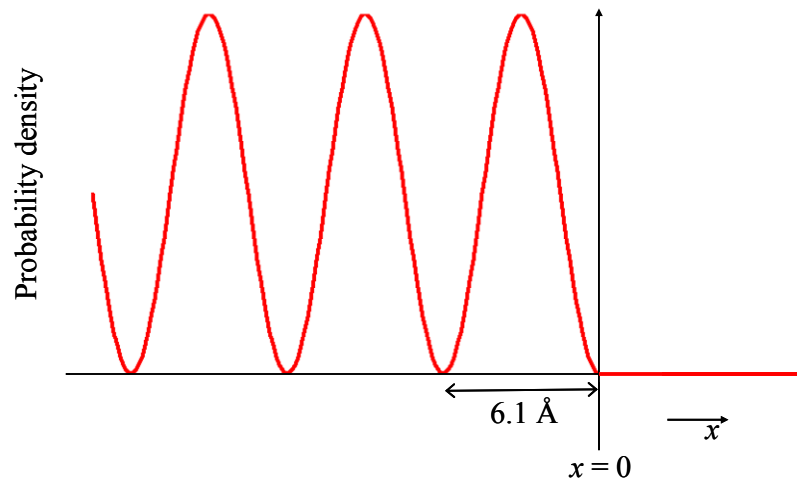
(The amplitude of the standing wave is $4|A|^2$, but A here has to remain as an arbitrary number. We cannot actually normalize such an infinite plane wave, though this problem can be resolved for any actual situation, for example by considering a wavepacket or pulse rather than just an idealized plane wave.)

2.8.2

The wavefunction in the barrier will be a dying exponential. Therefore, $\psi = A\exp(-\kappa x)$. We just need to calculate the probability in the two regions requested.

$$\kappa = \frac{\sqrt{2m(V-E)}}{\hbar} = 3.62 \times 10^9 \, m^{-1}$$

$$x_0 = 1 \times 10^{-10} \, m$$

$$P_1 = \int_0^{x_0} |A|^2 \exp(-2\kappa x) \; dx = |A|^2 \left(\frac{1}{-2\kappa}\right) \left[\exp(-2\kappa x)\right]_0^{x_0} = \frac{|A|^2}{-2\kappa}\left[\exp(-2\kappa x_0)-1\right]$$

$$P_2 = \int_{x_0}^{\infty} |A|^2 \exp(-2\kappa x) \; dx = |A|^2 \left(\frac{1}{-2\kappa}\right) \left[\exp(-2\kappa x)\right]_{x_0}^{\infty} = \frac{|A|^2}{-2\kappa}\left[-\exp(-2\kappa x_0)\right]$$

$$\exp(-2\kappa x_0) = 0.485$$

$$\Rightarrow P_1 = \frac{|A|^2}{2\kappa}[0.515]$$

$$\Rightarrow P_2 = \frac{|A|^2}{2\kappa}[0.485]$$

The electron is more likely to be *within the first Angstrom of the barrier*.

2.8.3

For $E = 1.5$ eV and $V_o = 1$ eV, the incoming particle/wave from the left will be partly reflected and partly transmitted at the barrier. We write the general form of the wavefunctions on both sides of the barrier

$$\psi_{left}(z) = C\exp(ik_L z) + D\exp(-ik_L z) \qquad \text{i.e., the sum of the incident and reflected waves}$$

$$\psi_{right}(z) = F\exp(ik_R z) \qquad \text{i.e., the transmitted wave}$$

(Note that we do not have a backward propagating wave on the right hand side because there is no reflection beyond the barrier.)

Here $\qquad k_L = \sqrt{\dfrac{2mE}{\hbar^2}} = 6.27 \times 10^9$ m^{-1} and $k_R = \sqrt{\dfrac{2m(E - V_o)}{\hbar^2}} = 3.62 \times 10^9$ m^{-1}

Now applying boundary conditions

(a) the continuity of the wavefunction at $z=0$ (barrier edge): $(C + D) = F$

(b) continuity of the derivative of the wavefunction at $z=0$: $(C - D)k_L = k_R F$

Adding and subtracting, we get $\quad D = \dfrac{k_L - k_R}{k_L + k_R}C$ and $F = \dfrac{2k_L C}{(k_L + k_R)}$

The absolute phase of any one of these wave components is arbitrary because it does not affect any measurable result, including the probability density (we are always free to choose such an overall phase factor). If we choose that phase such that C is real, then our algebra becomes particularly simple and, from the above equations, D and F are also real. The probability density on each side will thus be

$$\left|\psi_{left}(z)\right|^2 = \left|C\right|^2 + \left|D\right|^2 + 2CD\cos(2k_L z) \qquad \left|\psi_{right}(z)\right|^2 = \left|F\right|^2$$

Taking $C=1$ and plotting the wave on both sides we see a standing wave on the left, which does not quite go down to zero because of the finite transmission over the barrier.
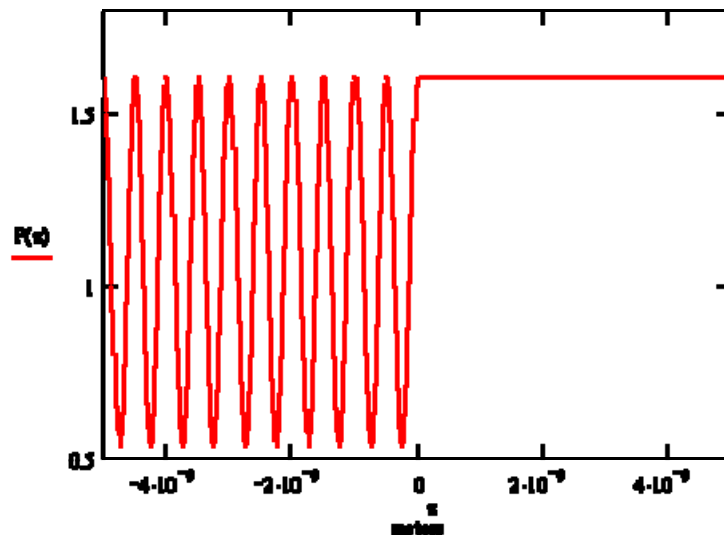
2.8.4

In a region where the potential is constant at some value V, the general solution of the Schrödinger wave equation is, for an electron wave of energy E,

$$\psi(z) = A \exp(ikz) + B \exp(-ikz)$$

where
$$k = \sqrt{\frac{2m_0(E-V)}{\hbar^2}}$$

In the incident region on the left in this problem, the wave will have this form with, in general, both A and B non-zero because we expect reflection from the potential discontinuity at $z = 0$. So, explicitly, we will have for $z < 0$

$$\psi_L(z) = A \exp(ik_L z) + B \exp(-ik_L z)$$

where
$$k_L = \sqrt{\frac{2m_0}{\hbar^2}(E - V_L)}$$

where V_L is the potential on the left. In the region to the right of $z = 0$, we will only have a forward propagating wave, so there we will have

$$\psi_R(z) = C \exp(ik_R z)$$

where
$$k_R = \sqrt{\frac{2m_0}{\hbar 2}(E - V_R)}$$

where V_R is the potential on the right. The boundary conditions to join these waves are

$$\text{continuity of the wavefunction, so } A + B = C \tag{1}$$

$$\text{continuity of the derivative, so } ik_L(A - B) = ik_R C \tag{2}$$

i.e.,
$$A - B = \frac{k_R}{k_L}C$$

Adding (1) and (2) gives

$$2A = \left(1 + \frac{k_R}{k_L}\right)C$$

or
$$A = \left[\frac{k_L + k_R}{2k_L}\right]C$$

and so

$$B = C - A = C\left[1 - \frac{(k_L + k_R)}{2k_L}\right] = \frac{2k_L - k_L - k_R}{2k_L} = \left[\frac{k_L - k_R}{2k_L}\right]C$$

For this problem, there are two k values of interest. One is the value in the barrier, k_b,

$$k_b = \sqrt{\frac{2m_0}{\hbar^2}(E - V_0)}$$

and the other is the value in the zero potential region

$$k_0 = \sqrt{\frac{2m_0}{\hbar^2}E}$$

Hence we have the following answers.

(i) (a) For $z < 0$

$$\psi_L(z) = C\left[\left(\frac{k_0 + k_b}{2k_0}\right)\exp(ik_0 z) + \left(\frac{k_0 - k_b}{2k_0}\right)\exp(-ik_0 z)\right]$$

For $z > 0$

$$\psi_R(z) = C\exp(ik_b z)$$

The probability density is, for $z < 0$, proportional to

$$|\psi_L(z)|^2 = |C|^2\left[\left(\frac{k_0 + k_b}{2k_0}\right)^2 + \left(\frac{k_0 - k_b}{2k_0}\right)^2 + \left(\frac{k_0 + k_b}{2k_0}\right)\left(\frac{k_0 - k_b}{2k_0}\right)\times\right.$$

$$\left.\left\{\exp(2ik_0 z) + \exp(-z_i k_0 z)\right\}\right]$$

$$= |C|^2\left[\left(\frac{k_0 + k_b}{2k_0}\right)^2 + \left(\frac{k_0 - k_b}{2k_0}\right)^2 + 2\left(\frac{k_0 + k_b}{2k_0}\right)\left(\frac{k_0 - k_b}{2k_0}\right)\cos(2k_0 z)\right]$$

which has a standing wave pattern to it, with the standing wave not going to zero at the minima. The period of the standing wave is

$$\lambda_{SL} = \frac{2\pi}{2k_0} = \frac{\pi}{k_0}$$

We also need to consider the phase of the probability amplitude so we can sketch it properly. For this case, since $k_0 > k_b$, the factor in front of the cosine is positive, so at $z = 0$, we are at a maximum in the standing wave pattern at $z = 0$. Note that, since the wavefunction is continuous across the boundary, so also is the probability density. For $z > 0$, the probability density is simply uniform, with

$$|\psi_R(z)|^2 = |C|^2$$

(b) Hence the probability density has the form
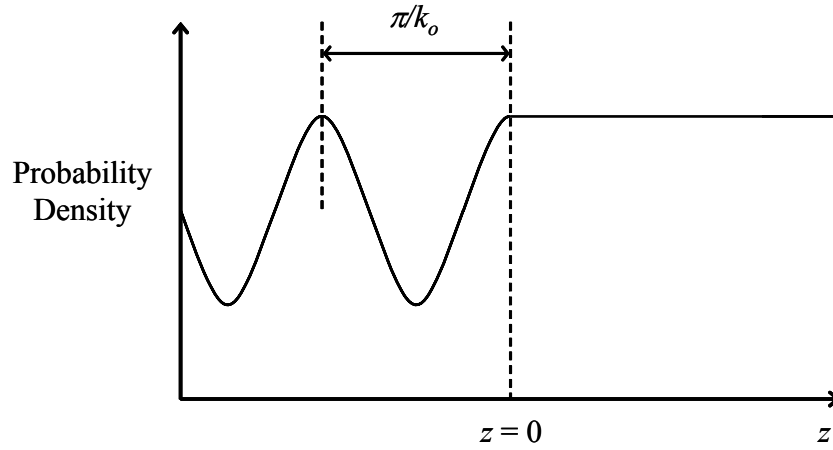
(ii) (a) For $z < 0$

$$\psi_L(z) = C\left[\left(\frac{k_b + k_0}{2k_b}\right)\exp(ik_b z) + \left(\frac{k_b - k_0}{2k_b}\right)\exp(-ik_b z)\right]$$

For $z > 0$
$$\psi_R(z) = C\exp(ik_0 z)$$

The probability density is, for $z < 0$, proportional to

$$|\psi_L(z)| = |C|^2\left[\left(\frac{k_b + k_0}{2k_b}\right)^2 + \left(\frac{k_b - k_0}{2k_b}\right)^2 + 2\left(\frac{k_b + k_0}{2k_b}\right)\left(\frac{k_b - k_0}{2k_b}\right)(\cos 2k_b z)\right]$$

(b) Now we also have a standing wave pattern on the left, with period

$$\lambda_{SL} = \pi / k_b$$

The standing wave pattern is now at a minimum at $z = 0$ because $k_b - k_0 < 0$, so we have
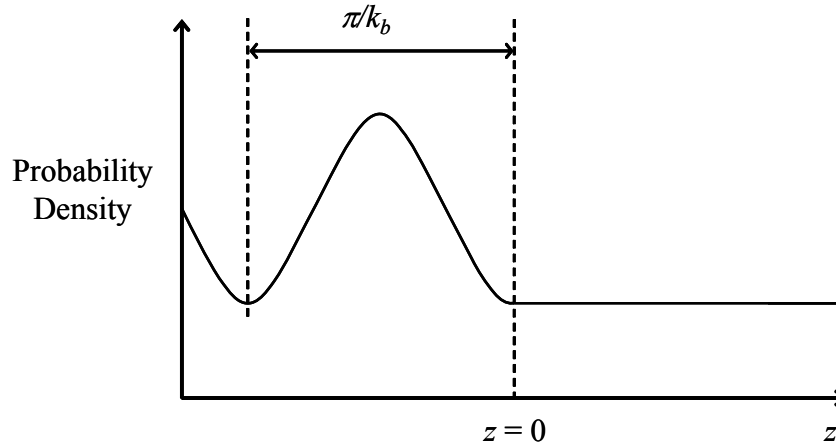
Note that the period of the standing wave is now much larger than in the first case.

2.8.5

On the "left" of the barrier, we have a wave of the form

$$\phi_{left}(z) = A\exp(i\,k_L z) + B\exp(-i\,k_L z)$$

where

$$k_L = \sqrt{\frac{2m_0 E}{\hbar^2}}$$

On the "right" of the barrier, we have a wave of the form

$$\phi_{right}(z) = C\exp(ik_R z)$$

where

$$k_R = \sqrt{\frac{2m_0(E-V_0)}{\hbar^2}}$$

(Note there is no left-going wave in the barrier region by the set-up of the problem.)

Equating the wavefunction at the barrier gives

$$A + B = C$$

Equating the derivatives at the barrier gives

$$ik_L(A - B) = ik_R C$$

i.e.,

$$A - B = \frac{k_R}{k_L}C = \sqrt{\frac{E-V_0}{E}}C = aC$$

Hence

$$2A = (1+a)C$$
$$2B = (1-a)C$$

Hence

$$\frac{B}{A} = \left(\frac{1-a}{1+a}\right)$$

and

$$\frac{|B|^2}{|A|^2} = \left(\frac{1-a}{1+a}\right)^2$$

But, $\dfrac{|B|^2}{|A|^2}$ is simply the probability of reflection. Hence

$$R = \left(\frac{1-a}{1+a}\right)^2 \qquad Q.E.D.$$

2.8.6
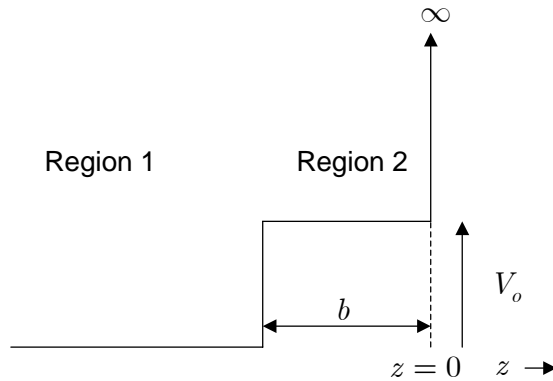
We write the wavefunction in each of the three regions

$$\text{Region1} \quad \psi_1(z) = A\exp(ik_1z) + B\exp(-ik_1z) \quad \text{where} \quad k_1 = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\text{Region2} \quad \psi_2(z) = M\exp(ik_2z) + N\exp(-ik_2z) \quad \text{where} \quad k_2 = \sqrt{\frac{2m(E-V_o)}{\hbar^2}}$$

$$\text{Region3} \quad \psi_3(z) = 0$$

We also have the following boundary conditions:

Continuity of the wavefunction at $z = 0$

$$0 = M + N \quad \Rightarrow \quad M = -N \tag{1}$$

Continuity of the wavefunction at $z = -b$

$$A\exp(-ik_1b) + B\exp(ik_1b) = M[\exp(-ik_2b) - \exp(ik_2b)] \tag{2}$$

Continuity of the wavefunction derivative at $z = -b$

$$k_1[A\exp(-ik_1b) - B\exp(ik_1b)] = Mk_2[\exp(-ik_2b) + \exp(ik_2b)]$$

(i) Rewriting $\psi_2(z)$ using the result from Eq. (1)

$$\psi_2(z) = M[\exp(ik_2z) - \exp(-ik_2z)] \ = 2iM\sin(k_2z) = C\sin(fz)$$

where $C = 2iM$ is a complex constant and f is $k_2 = \sqrt{\frac{2m(E-V_o)}{\hbar^2}}$.

(ii) Since there is 100% reflection from the infinite barrier, the reflected wave has amplitude 1. Thus $|A| = |B| = 1$

(iii) From the boundary conditions, we have

$$A\exp(-ik_1b) + B\exp(ik_1b) = -C\sin(k_2b)$$

and $\qquad\qquad A\exp(-ik_1b) - B\exp(ik_1b) = C(k_2/k_1i)\cos(k_2b)$

Adding these to eliminate B gives us

$$2A\exp(-ik_1b) = C[(k_2/k_1i)\cos(k_2b) - \sin(k_2b)]$$

So
$$C = 2iA \exp(-ik_1b) / [(k_2/k_1)\cos(k_2b) - i\sin(k_2b)]$$

In terms of E, V_o, and b, therefore, we have

$$C = \frac{2iA\exp(-ib\sqrt{\frac{2mE}{\hbar^2}})}{[(\sqrt{\frac{E-V_o}{E}})\cos(\sqrt{\frac{2m(E-V_o)}{\hbar^2}}b) - i\sin(\sqrt{\frac{2m(E-V_o)}{\hbar^2}}b)]}$$

(iv). We have

$$|C|^2 = \frac{4|A|^2}{[(k_2/k_1)^2 \cos^2(k_2b) + \sin^2(k_2b)]}$$

or, in terms of E, V_o, and b

$$|C|^2 = \frac{4|A|^2}{[(1-\frac{V_o}{E})\cos^2(\sqrt{\frac{2m(E-V_o)}{\hbar^2}}b) + \sin^2(\sqrt{\frac{2m(E-V_o)}{\hbar^2}}b)]}$$

i.e.,
$$|C|^2 = \frac{4|A|^2}{[1-\frac{V_o}{E}\cos^2(\sqrt{\frac{2m(E-V_o)}{\hbar^2}}b)]}$$

Sketching this as a function of energy from 1.1eV to 3 eV, choosing $A = 1$ for simplicity
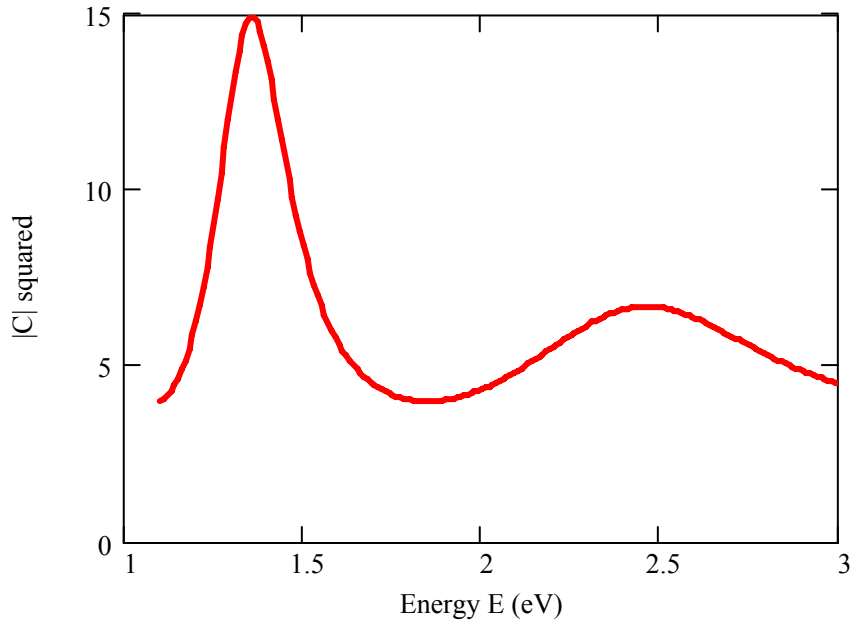
(v) All that is required here is a sketch. 1.356 eV is approximately the position of the resonance inside region 2, so we expect a large single peak inside that region, and a standing wave to the left, of lower amplitude. Since we know C in terms of A from part (iii), we can deduce B in terms of A from

the boundary conditions we can formally calculate the wave everywhere if we wish, as in the following graph.
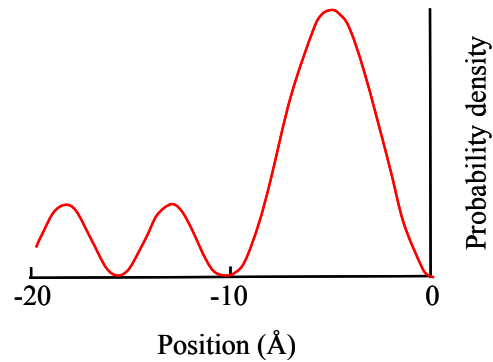
(vi) The curve in part (iv) shows that there is a "Fabry-Perot" resonance in the structure at roughly 1.35eV and another one near 2.5eV. (A Fabry-Perot resonator in optics is a simple resonator made from two parallel mirrors.) At higher energies $|C|^2 \to 4$ matching the amplitude of the standing wave on the left of the structure. Since the energy is related to the wave number inside the structure we only expect resonances at energies that give wave numbers that correspond to constructive interference of the incoming wave with the wave within the structure.

2.8.7

(i) The solution in the left half of the well is of the form

$$\sin(k_L z) \text{ with } k_L = \sqrt{\frac{2m_o E_S}{\hbar^2}}$$

Note that this has a zero at the left wall as required.

The solution in the right half of the well is of the form

$$\sin(k_R(L_z - z)) \text{ (or } \sin(k_R(z - L_z))) \text{ with } k_R = \sqrt{\frac{2m_o(E_S - V_S)}{\hbar^2}}$$

Note that this has a zero at the right wall, as required.

Note that both of these solutions correspond to sine waves, not decaying exponentials, because V_S is substantially less than $(\hbar^2/2m_o)(\pi/L_z)^2$, which is the energy of the first state in a well without a step. Adding a step like this will only increase the eigenenergy, and so we can be quite sure that $E_S > V_S$.
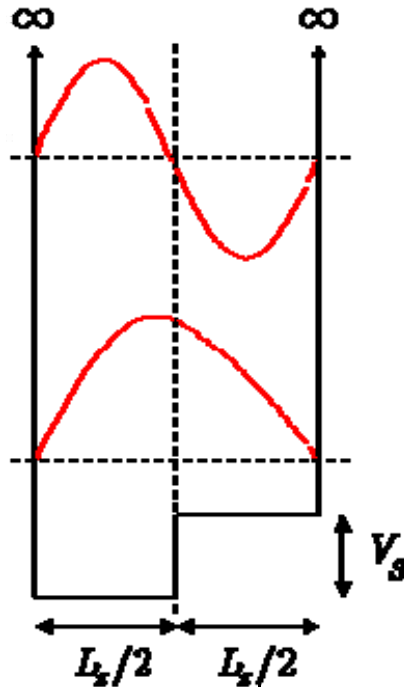
(ii) The lowest eigenstate we expect to have no zeros within the well. It will be sinusoidal in both halves, but will be more rapidly changing in the left half. This means that more than one quarter cycle will be in the left half, and less than one quarter cycle will be in the right half, hence the function as drawn in the figure. Note that the result should also have constant derivative as we pass from the left half to the right half because of the derivative boundary condition at the interface.

The second eigenstate we expect to have one zero within the well, and because $k_L > k_R$, we expect the zero to occur in the left half of the well. Again, the derivative should be constant across the interface, as in the figure. (One might make an intelligent (and correct) guess that the maximum amplitude is also larger in the right half, though this would be a very subtle point to realize here.)

(iii) Neither of these functions have definite parity.

(iv)
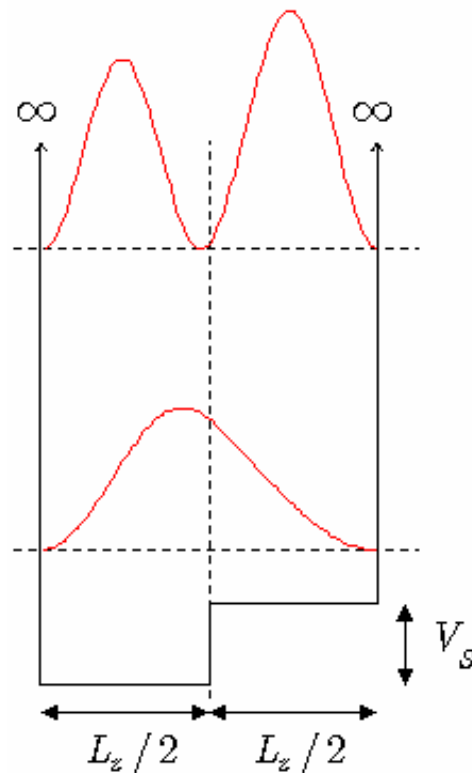
(Again, noticing that the amplitude of the probability density is higher on the right hand side for the second state would a rather subtle point to realize here.)

(v) For the lowest state, obviously there will be more integrated squared amplitude on the left side, and so the electron is more likely to be found there.

For the second state, there is a zero in the left half which is not present in the right half, and this reduces the relative average value of the probability density on the left side. As a result, the electron is actually more likely to be found on the right half of the well in this second state, which is quite a counter-intuitive conclusion. (It is also true that the amplitude on the right half will actually rise to a larger peak value as shown in the figure. It might be unreasonable to expect the reader to notice this particular point here, though it would be a satisfactory reason for coming to the correct conclusion.)

(The particular curves on the graphs here are actual solutions of such a stepped well problem for an electron, with $L_z = 1$ nm and $V_S = 0.35$ eV. The energy of the first state of a simple well of the same total thickness is $E_1 = 0.376$ eV. The energies of the first two solutions are 0.531 eV and 1.695 eV (the graphs are not to scale for the energies). The relative probabilities of finding the electron on the left and the right are, for the first state, 61.3% on the left, 38.7% on the right, and for the second state, 41.7% on the left, and 58.3% on the right.)

2.9.1

(i) The sketch shows a standing wave pattern to the left of the barrier that does not go all the way down to zero (there is finite transmission through the barrier, so the reflected wave is weaker than the incident wave). Inside the barrier, there is a combination of exponential decay (to the right) from the wave entering from the left and also some contribution of exponential "growth" to the right (i.e., exponential decay to the left) from the wave reflected from the right hand side of the barrier, though the exponential decay term is much stronger. To the right of the barrier, there is a constant, positive probability density corresponding to the fact that there is a right-propagating plane wave, but no left-propagating plane wave, so there is no interference. (Remember that the modulus squared of a single complex plane wave is a constant.)

(ii) One correct answer: By introducing a new barrier (identical to the old) to the left of the old barrier by a distance corresponding to roughly an integral number of half-wavelengths, one can create a resonant cavity, a Fabry-Perot-like structure, enhancing the transmission probability. (Perhaps surprisingly, for two identical barriers, one can actually get 100% transmission at the resonance of such a structure.)

2.9.2
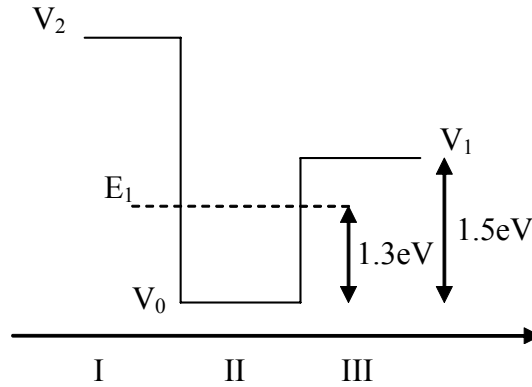
In general, the wavefunction solution in the well is of the form

$$\psi_w(z) = A\sin k_1 z + B\cos k_1 z$$

and in the barrier, because we can neglect the growing exponential solution as unphysical for an infinitely thick barrier,

$$\psi_b(z) = F\exp(-\kappa_2 z)$$

where

$$\begin{cases} k_1 = \dfrac{\sqrt{2m(E_1 - V_0)}}{\hbar} \\[2mm] \kappa_2 = \dfrac{\sqrt{2m(V_1 - E_1)}}{\hbar} \end{cases}$$

with

$$k_1 = \frac{\sqrt{2*9.11*10^{-31}*1.3*1.6*10^{-19}}}{1.055*10^{-34}} = 5.84*10^9 \text{ m}^{-1}$$

$$\kappa_2 = \frac{\sqrt{2*9.11*10^{-31}*0.2*1.6*10^{-19}}}{1.055*10^{-34}} = 2.29*10^9 \text{ m}^{-1}$$

Now these solutions have three constants altogether, and we need to reduce this to only one normalizing constant. We need to look at the boundary conditions. For simplicity, we will choose the origin at the position of the boundary between the well and the barrier on the "right", so we have the following.

Continuity of the wavefunction

$$B = F$$

Continuity of the derivative of the wavefunction

$$A = \frac{-\kappa_2}{k_1}F$$

So the general form, within the one normalizing constant F, is

a) within the well

$$\psi_w(z) = F\left(\cos k_1 z - \frac{\kappa_1}{k_2}\sin k_1 z\right)$$

b) in the barrier on the right hand side

$$\psi_b(z) = F\exp(-\kappa_2 z)$$

2.9.3

(i)

$V_0 = 1\text{eV}$

$z = 0 \qquad z = L$
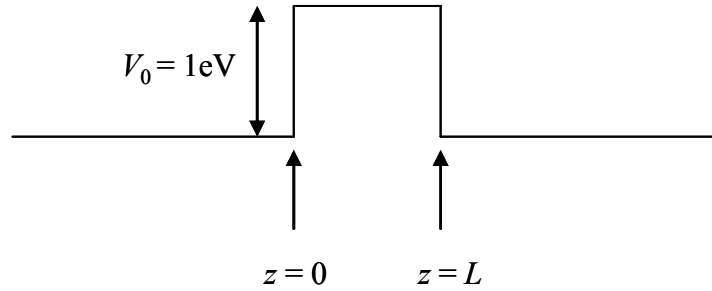
This problem is very similar to the ones solved in the book for the infinite barrier and the finite quantum well. The basic philosophy in attacking this problem is the following: One must satisfy the wave equation in all regions of interest while also satisfying the boundary conditions at the interfaces.

Note that we have a choice of coordinates here. For simplicity, we choose the zero of z to be at the left edge of the finite barrier. The other edge then lies at $z = L = 10$ Å. We choose the zero of energy to be the value of the potential at the left or the right. Therefore, the barrier has height $+1\text{eV}$.

Note that there are three distinct regions in which we must solve the wave equation (left, inside the barrier, and right), which we denote 1, 2, and 3, respectively, and, thus, there are two interfaces. In any given region, the potential is constant, so the solutions to the wave equation will be exponentials. If the energy is above the potential in a given region, then the solutions will be oscillating complex exponentials, like exp(ikz) or exp($-ikz$). If the energy is below the potential in a given region, then the solutions will be growing or decaying real exponentials, like exp(kz) or exp($-kz$). However, we can consider all cases at once by treating all the wavefunctions as complex exponentials, because if $E < V$, the value we will get for k will be purely imaginary and so exp(ikz) will become exp($i\,(ik)z$)=exp($-kz$). This will become clearer by example as we proceed.

First of all, what are the values of k in each region? Let us denote them as k_1, k_2, and k_3.

$$E - V = \hbar^2 k^2 / 2m$$

So,

$$k = \sqrt{2m(E - V)} / \hbar$$

Therefore, since $V = 0$ in regions 1 and 3, $k_1 = k_3 = \sqrt{2mE} / \hbar$. In region 2, $k_2 = \sqrt{2m(E - V_0)} / \hbar$. Note that these are all known quantities (since we will be using E as a parameter in our graph). Also, when $E < V_0$, k_2 will be purely imaginary, and thus, we must remember that our exponentials are real growing or decaying exponentials. Now we must write down the most general solution to the wave equation in all three regions.

$$\psi_1 = A \exp(ik_1 z) + B \exp(-ik_1 z)$$

$$\psi_2 = C \exp(ik_2 z) + D \exp(-ik_2 z)$$

$$\psi_3 = F \exp(ik_1 z)$$

Note that for this problem we presume that there is a wave incident from the left but there is no wave coming in from the right from infinity. This sets the coefficient of exp($-ik_1z$) in region 3 equal to zero, so no such term appears for the wave in region 3.

The next step is to impose the boundary conditions. There is an interface at $z = 0$ and another at $z = L$. At each interface, we require that *both* the wavefunction ψ and its derivative $\partial \psi / \partial z$ be continuous. This gives us four equations.

ψ continuous at $z = 0$

$$\psi_1 = \psi_2 \Rightarrow A \exp(ik_1 z) + B \exp(-ik_1 z) = C \exp(ik_2 z) + D \exp(-ik_2 z)$$

so
$$A + B = C + D \tag{1}$$

$\partial \psi / \partial z$ continuous at $z = 0$

$$\frac{\partial \psi_1}{\partial z} = \frac{\partial \psi_2}{\partial z} \Rightarrow ik_1 A \exp(ik_1 z) + (-ik_1) B \exp(-ik_1 z) = ik_2 C \exp(ik_2 z) + (-ik_2) D \exp(-ik_2 z)$$

so
$$ik_1(A - B) = ik_2(C - D) \tag{2}$$

ψ continuous at $z = L$

$$\psi_2 = \psi_3 \Rightarrow C \exp(ik_2 z) + D \exp(-ik_2 z) = F \exp(ik_1 z)$$

so
$$C \exp(ik_2 L) + D \exp(-ik_2 L) = F \exp(ik_1 L) \tag{3}$$

$\partial \psi / \partial z$ continuous at $z = 0$

$$\frac{\partial \psi_2}{\partial z} = \frac{\partial \psi_3}{\partial z} \Rightarrow ik_2 C \exp(ik_2 z) + (-ik_2) D \exp(-ik_2 z) = (ik_1) F \exp(ik_1 z)$$

so
$$ik_2 \left[C \exp(ik_2 L) - D \exp(-ik_2 L) \right] = ik_1 F \exp(ik_1 L) \tag{4}$$

Remember that in the end, all we care about is the relative values of the coefficients A and F. Combining these equations, we can solve for the value of A in terms of F.

(a) $ik_2 \times$ [Eq. (3) + Eq. (4)]

$$2ik_2 C \exp(ik_2 L) = i(k_1 + k_2) F \exp(ik_1 L)$$

$$\Rightarrow C = \frac{k_1 + k_2}{2k_2} F \exp(i(k_1 - k_2)L)$$

(b) $ik_2 \times$ [Eq. (3) − Eq. (4)]

$$2ik_2 D \exp(-ik_2 L) = i(k_1 - k_2) F \exp(ik_1 L)$$

$$\Rightarrow D = -\frac{k_1 - k_2}{2k_2} F \exp(i(k_1 + k_2)L)$$

(c) $ik_1 \times$ [Eq. (1) + Eq. (2)]

$$2ik_1 A = iC(k_1 + k_2) + iD(k_1 - k_2)$$

$$\Rightarrow A = \frac{1}{2}\left[C \frac{k_1 + k_2}{k_1} + D \frac{k_1 - k_2}{k_1} \right]$$

(d) $ik_1 \times$ [Eq. (1) - Eq. (2)]

$$2ik_1 B = iC(k_1 - k_2) + iD(k_1 + k_2)$$

$$\Rightarrow B = \frac{1}{2}\left[C\frac{k_1 - k_2}{k_1} + D\frac{k_1 + k_2}{k_1}\right]$$

Ultimately, we want the value of the transmission $\dfrac{|\psi_{out}|^2}{|\psi_{inc}|^2} = \dfrac{|F|^2}{|A|^2}$, so we need to get A in terms of F.
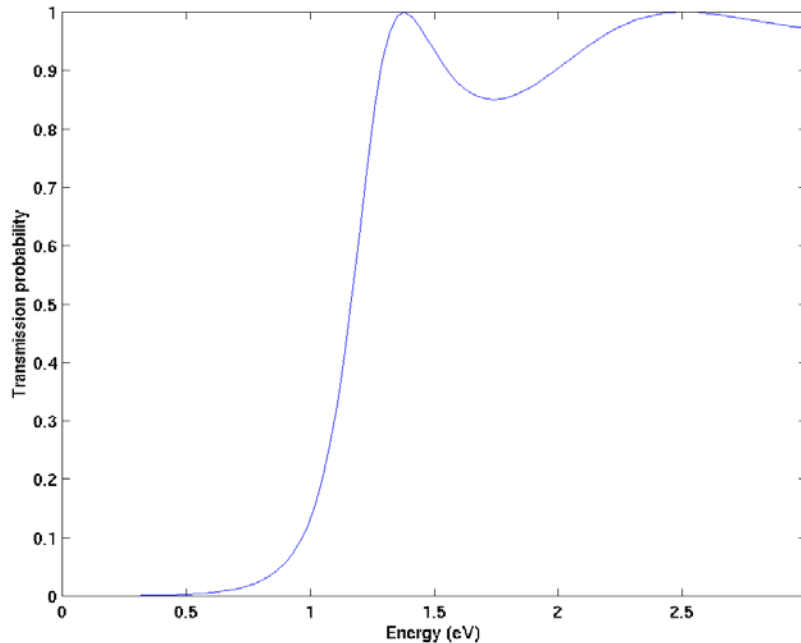
So, using the above results

$$A = \frac{1}{2}\left[\frac{k_1 + k_2}{k_1}C + \frac{k_1 - k_2}{k_1}D\right]$$

$$= \frac{1}{2}\left[\left(\frac{k_1 + k_2}{2k_2}F\exp\left(i(k_1 - k_2)L\right)\right)\frac{k_1 + k_2}{k_1} + \left(-\frac{k_1 - k_2}{2k_2}F\exp\left(i(k_1 + k_2)L\right)\right)\frac{k_1 - k_2}{k_1}\right]$$

$$= \frac{1}{4k_1 k_2}F\left[(k_1 + k_2)^2\exp\left(i(k_1 - k_2)L\right) - (k_1 - k_2)^2\exp\left(i(k_1 + k_2)L\right)\right]$$

Graphing the transmission from this point is simple. (E.g., in MATLAB.)

Note that there are maxima above the barrier height of 1 eV. (We will discuss this in part (iii))The first maximum appears at $E = 1.3763$ eV, and the second around $E = 2.060$eV.

(ii) To plot the probability density, we now just need to calculate the values of the coefficients A, B, C, and D for the value of energy $E = 1.3763$ eV. This is easily done on the computer as well. (See MATLAB code at the end of the solutions for this, in detail.)

Note that, as is common in quantum mechanics, the wavefunctions must be added first before taking the modulus squared. We may not simply add $|A|^2 + |B|^2$ to get the probability density. For example,

$$\psi_1 = A\exp(ik_1 z) + B\exp(-ik_1 z) \Rightarrow |\psi_1|^2 = |A\exp(ik_1 z) + B\exp(-ik_1 z)|^2$$

$$\neq |A\exp(ik_1 z)|^2 + |B\exp(-ik_1 z)|^2 = |A|^2 + |B|^2$$

The following graph plots the probability density (in arbitrary units) as a function of position at this resonant energy $E = 1.3763$ eV.
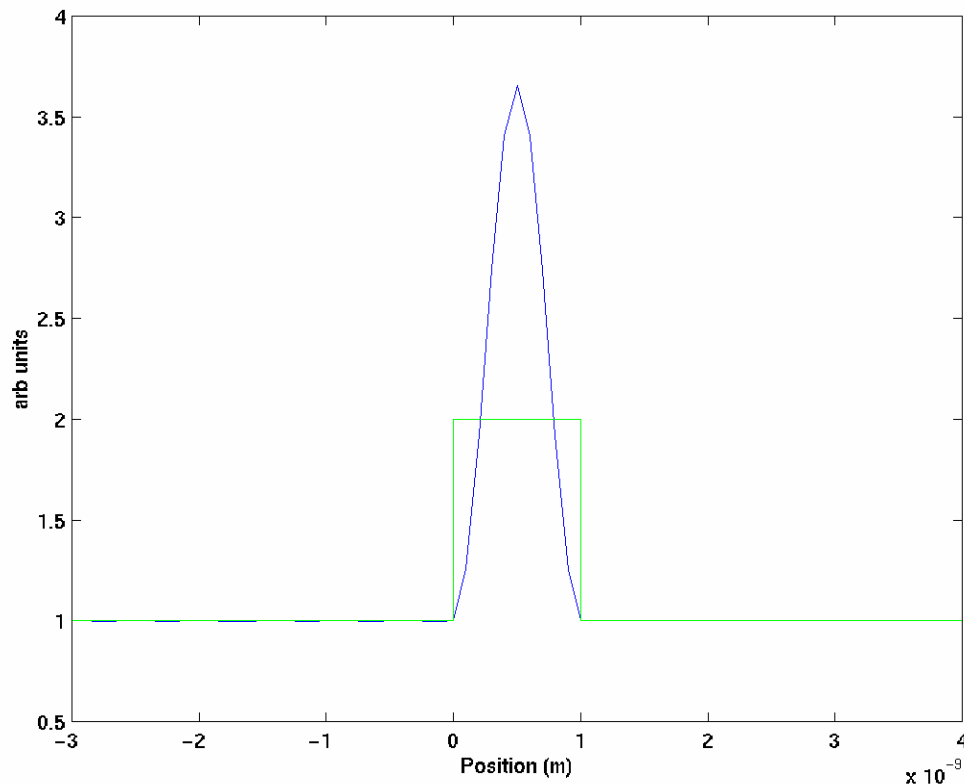
 (iii) A physical explanation for the form of the transmission is that the electron wave encountering a potential barrier is totally akin to an optical wave encountering a change in the index of refraction. (The analogy is quite strict – for any given energy of quantum mechanical wave, the mathematics is identical in that the wave equation derived from Maxwell's equations for light waves in a solid of variable index of refraction is the same as the time-independent Schrödinger equation; the main difference is the relation between energy and frequency, which is substantially different in quantum mechanics compared to electromagnetism. For any particular electromagnetic frequency and quantum mechanical energy, the two wave equations are essentially identical, however.)

For energies above the barrier height, the electron wave is reflected partially from both sides of the barrier. At certain energies, therefore, we see Fabry-Perot-like resonances, where the electron wave builds up significantly inside the barrier. The picture above is very much an indication of that phenomenon. (A Fabry-Perot resonator in optics is a resonator formed from two parallel reflecting surfaces.)

```
APPENDIX : MATLAB code
% Physical Constants
m = 9.11e-31;              % mass of electron
e = 1.6e-19;               % electronic charge (converts eV to J)
hbar = 1.055e-34; % Planck's constant over 2*pi

% Problem-specific constants:
V=1;                       % height of the barrier
L = 1e-9;          % width of the barrier
E = [0.01:0.004:3];        % energy scale

% Calculate the values of k in each region, for every value of E (as a vector):
```

```
k1 = sqrt(2*m*E*e)/hbar;
k2 = sqrt(2*m*(E-V)*e)/hbar;

% Calculate the coefficients of the wavefunction parts (as derived in soln set):
C =  exp(i.*(k1-k2).*L).*( (k1+k2)./(2*k2) );
D = -exp(i.*(k1+k2).*L).*( (k1-k2)./(2*k2) );
A = 0.5*(C.*(k1+k2)./k1 + D.*(k1-k2)./k1);
B = 0.5*(C.*(k1-k2)./k1 + D.*(k1+k2)./k1);

% Calculate transmission probability assuming outgoing wave (F=1) is normalized to 1:
trans = 1./(A.*conj(A));

% Plot
figure(1);
plot(E,trans);
xlabel('Energy (eV)');
ylabel('Transmission probability');
% if the first max is Efirstmax, then this will plot the probability density
% for that energy.  The basic idea is just to calculate the coefficients
% of the wavefunctions and then take the complex square of the wavefunction.

% Recalculate several things above, except this time only for the max energy:
Efirstmax = 1.3763;
k1m = sqrt(2*m*Efirstmax*e)/hbar;
k2m = sqrt(2*m*(Efirstmax-V)*e)/hbar;

% Define the z-axis:
z_step = 1e-10;
z_left = [-3e-9:z_step:0];
z_center = [0:z_step:1e-9];
z_right = [1e-9:z_step:4e-9];
z = cat(2, z_left, z_center, z_right);

% Recalculate the coefficients:
Cm =  exp(i*(k1m-k2m)*L)*( (k1m+k2m)/(2*k2m) );
Dm = -exp(i*(k1m+k2m)*L)*( (k1m-k2m)/(2*k2m) );
Am = 0.5*(Cm*(k1m+k2m)/k1m + Dm*(k1m-k2m)/k1m);
Bm = 0.5*(Cm*(k1m-k2m)/k1m + Dm*(k1m+k2m)/k1m);

% Calculate the wavefunction in pieces:
psi_left = Am.*exp(i.*k1m.*z_left) + Bm.*exp(-i.*k1m.*z_left);
psi_center = Cm.*exp(i.*k2m.*z_center) + Dm.*exp(-i.*k2m.*z_center);
psi_right = exp(i.*k1m.*z_right);

% Calculate the probability function as the square of the wavefunction in each region:
psi_left_sq = psi_left.*conj(psi_left);
psi_center_sq = psi_center.*conj(psi_center);
psi_right_sq = psi_right.*conj(psi_right);

% Concatenate them all together so that they graph nicely:
psi_sq = cat(2, psi_left_sq, psi_center_sq, psi_right_sq);

figure(2);
hold off
plot(z,psi_sq);
xlabel('Position (m)');
ylabel('arb units');

% Put a graph representing the potential barrier on there at the same time for comparison:
V_z = cat(2, zeros(1,length(z_left)), ones(1, length(z_center)), zeros(1, length(z_right)));
V_z = V_z + 1;
hold on;
plot(z,V_z,'g-');
```

2.9.4

(i) This derivation is very similar to the one in the book, except with added factors of $\dfrac{m_w^*}{m_b^*}$ at various points. Therefore, using the same notation as in the book

$$\psi(z < -L/2) = G\exp(+\kappa z)$$
$$\psi(-L/2 < z < L/2) = A\sin kz + B\cos kz$$
$$\psi(z > L/2) = F\exp(-\kappa z)$$

$$X = \exp(-\kappa L/2)$$
$$C = \cos(kL/2)$$
$$S = \sin(kL/2)$$

Continuity of ψ at $z = -L/2$ and $z = L/2$ yields equations

$$GX = -AS + BC$$
$$FX = AS + BC$$

Continuity of $\dfrac{1}{m^*}\dfrac{\partial \psi}{\partial z}$ at $z = -L/2$ and $z = L/2$ yields equations

$$\frac{1}{m_b^*}\kappa GX = \frac{1}{m_w^*}k(AC - B(-S))$$

$$\Rightarrow \frac{m_w^*}{m_b^*}\frac{\kappa}{k}GX = AC + BS$$

$$\frac{1}{m_b^*}(-\kappa)FX = \frac{1}{m_w^*}k(AC - BS)$$

$$\Rightarrow \frac{m_w^*}{m_b^*}\frac{\kappa}{k}FX = -AC + BS$$

These four equations can be added and subtracted, as in the book, to yield the equations

$$2BC = (F + G)X$$
$$2AS = (F - G)X$$
$$2BS = \frac{m_w^*}{m_b^*}\frac{\kappa}{k}(F + G)X$$
$$2AC = \frac{m_w^*}{m_b^*}\frac{\kappa}{k}(-F + G)X$$

If $F \neq -G$, then we can divide the third equation by the first equation and get the tangent relation

$$\frac{S}{C} = \tan(kL/2) = \frac{m_w^*}{m_b^*}\frac{\kappa}{k}$$

If $F \neq G$, then we can divide the fourth equation by the third equation and get the cotangent relation

$$\cot(kL/2) = -\frac{m_w^*}{m_b^*}\frac{\kappa}{k}$$

As in the book, if we define ε and v_0 as dimensionless energies, we get the desired relations, remembering that m^* is different for k and κ

$$\tan(\frac{\pi}{2}\sqrt{\varepsilon}) = \sqrt{\frac{m_w^*}{m_b^*}}\sqrt{\frac{v_0 - \varepsilon}{\varepsilon}}$$

$$\cot(\frac{\pi}{2}\sqrt{\varepsilon}) = -\sqrt{\frac{m_w^*}{m_b^*}}\sqrt{\frac{v_0 - \varepsilon}{\varepsilon}}$$

(ii) Since 1.55μm corresponds to 1.24/1.55 = 0.800eV = 800meV, and InGaAs has a bandgap ~750meV, it is necessary to make the zero-point energy be ~50meV.

$$V_0 = 260meV = 4.16\times10^{-20}J$$
$$E = 50meV = 8.0\times10^{-21}J$$
$$m_b^* = 0.080m_0 = 7.288\times10^{-32}kg$$
$$m_w^* = 0.041m_0 = 3.735\times10^{-32}kg$$

$$\kappa = \frac{\sqrt{2m_b^*(V_0 - E)}}{\hbar} = 6.633\times10^8\,m^{-1}$$

$$k = \frac{\sqrt{2m_w^*E}}{\hbar} = 2.317\times10^8\,m^{-1}$$

It is the tangent relation that yields the lowest energy solution. Therefore, we solve

$$\tan(kL/2) = \frac{m_w^*}{m_b^*}\frac{\kappa}{k}$$

$$L = \frac{2}{k}\arctan\left(\frac{m_w^*}{m_b^*}\frac{\kappa}{k}\right) = 8.4nm$$

2.10.1

The effect of putting an infinitely high barrier at the middle and for all points to the left of center is to impose the boundary condition that the wavefunction must be zero at the center (and for all points to the left of the center). The energy eigenfunctions of this half oscillator are therefore all of the odd-parity energy eigenfunctions of the full oscillator; that is, all the ones that have a zero in the middle. We can see by inspection that those will all be solutions, because we already know that they satisfy the Schrödinger equation for all points z to the right of the center at these energies and they also satisfy our new boundary condition at the middle.

These are also all the solutions to this problem. The even parity solutions to the full harmonic oscillator problem were all the solutions that are symmetric and solve Schrödinger's equation for the harmonic oscillator potential, but none of those are solutions to this problem, and the odd parity solutions to the full harmonic oscillator problem were all the solutions that are antisymmetric (and that have a zero in the middle) that solve Schrödinger's equation for the harmonic oscillator potential.

The allowed energies in this half harmonic oscillator problem are therefore, in units of $\hbar\omega$ and expressed relative to the bottom of the potential, 3/2, 7/2, 11/2, and so on, all spaced by $2\hbar\omega$.

Finally, we consider the issue of normalization of the wavefunctions. In order that the total probability add up to one, the wavefunctions must be renormalized. Since we are cutting off half of the probability by cutting the wavefunctions in half, we must double the contribution from the wave we are keeping. Therefore, each eigenfunction must be multiplied by $\sqrt{2}$, such that its modulus squared is doubled.

2.11.1

For this problem, we use the expression for the eigenenergies in a linear varying potential

$$E_i = -\left(\frac{\hbar^2}{2m}\right)^{1/3} (e\mathsf{E})^{2/3} \zeta_i$$

or, in electron-volts, dividing by the electronic charge, e,

$$E_i = -\left(\frac{\hbar^2}{2me}\right)^{1/3} \mathsf{E}^{2/3}\zeta_i ,$$

and the first three zeros of the Ai Airy function, which are known to be $\zeta_1 \simeq -2.338$, $\zeta_2 \simeq -4.088$, and $\zeta_3 \simeq -5.521$.

Calculating, we have

$$\left(\frac{\hbar^2}{2me}\right)^{1/3} \simeq 3.366 \times 10^{-7}$$

and for a field of 1 V/Å (10^{10} V/m), we have

$$\mathsf{E}^{2/3} \simeq 4.642 \times 10^6$$

so

$$E_i (\text{in eV}) \simeq -1.562 \times \zeta_i$$

i.e.,

$$E_1 \simeq 3.65 \text{ eV}, \ E_2 \simeq 6.39 \text{ eV}, \text{ and } E_3 \simeq 8.62 \text{ eV}$$

2.11.2

In this case, we now have

$$E_i = -\left(\frac{\hbar^2}{2m_{\text{eff}}e}\right)^{1/3} \mathsf{E}^{2/3}\zeta_i \text{ with } \left(\frac{\hbar^2}{2m_{\text{eff}}e}\right)^{1/3} = 8.167\times10^{-7} \text{ in MKS units}$$

For 1 V/µm (10^6 V/m), we have $\mathsf{E}^{2/3} = 10^4$, so

$$E_i(\text{eV}) \simeq -8.167\times10^{-3} \times \zeta_i$$

So

$$E_1 \simeq 19.1\,\text{meV},\, E_2 \simeq 33.4\,\text{meV},\, E_3 \simeq 45.1\,\text{meV}$$

For 10 V/µm (10^7 V/m), we have $\mathsf{E}^{2/3} = 4.642\times10^4$, so

$$E_i(\text{eV}) \simeq -3.791\times10^{-2} \times \zeta_i$$

So

$$E_1 \simeq 88.6\,\text{meV},\, E_2 \simeq 155\,\text{meV},\, E_3 \simeq 209\,\text{meV}$$

The classical turning point occurs at

$$z_i = E_i / e\mathsf{E}$$

for an eigenenergy E_i, or, for energies in electron-volts

$$z_i = E_i(\text{eV}) / \mathsf{E}$$

Hence for 1 V/µm (10^6 V/m), the classical turning points are, respectively

$$z_1 \simeq 19.1\,\text{nm},\, z_2 \simeq 33.4\,\text{nm},\, z_3 \simeq 45.1\,\text{nm}$$

and for 10 V/µm (10^7 V/m), the classical turning points are, respectively

$$z_1 \simeq 8.86\,\text{nm},\, z_2 \simeq 15.5\,\text{nm},\, z_3 \simeq 20.9\,\text{nm}$$

2.11.3

(i) For zero field, the energies of the first three levels are given by the particle-in-a-box (infinitely deep quantum well) solutions as

$$E_n = \frac{\hbar^2}{2m_{eff}} \left(\frac{n\pi}{L_z} \right)^2$$

where the effective mass $m_{eff} = 0.07 m_o$. The resulting energies for the infinitely deep potential well without field are

$$E_1 \simeq 53.8 \text{ meV}, \; E_2 \simeq 215.1 \text{ meV}, \; E_3 \simeq 483.9 \text{ meV}$$

The associated eigenfunctions are

$$\psi_n(z) = \sqrt{\frac{2}{L_z}} \sin\left(\frac{n\pi z}{L_z} \right)$$

where here $L_z = 10^{-8}$ m. If we want to normalize to get the probability per Ångstrom, we should express the distances in Ångstroms, in which case, we use $L_z = 100$ (Å) in this expression. The resulting probability densities are in Fig. 1 below.
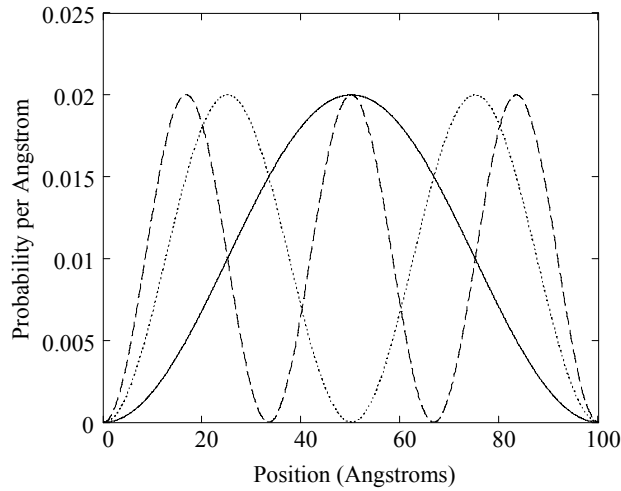
Fig. 1. Probability densities at zero field. Solid line – level 1. Dotted line – level 2. Dashed line – level 3.

(ii) For a field of 20 V/μm, we follow the method in the text. For these numbers, the potential drop across the well, expressed in units of E_1^∞ (the energy of the first state in the well at zero field), is $v_L = 3.7197$. To find the solutions, we need to find the zeros of the determinant function

$$D(\varepsilon) = Ai\big(\zeta_0(\varepsilon)\big) Bi\big(\zeta_L(\varepsilon)\big) - Ai\big(\zeta_L(\varepsilon)\big) Bi\big(\zeta_0(\varepsilon)\big)$$

The resulting values of ε will be the energy eigenvalues in units of E_1^∞ (expressed relative to the bottom corner of the potential). For the particular value of $v_L = 3.7197$, this determinant function is graphed in Fig. 2.

Using a root finder, we can find the precise numerical positions where this function crosses the axis, which are $\varepsilon_1 \simeq 2.7139$, $\varepsilon_2 \simeq 5.9008$, $\varepsilon_1 \simeq 10.8864$. Changing back to electron-volts (by multiplying by E_1^∞), we have, relative to the bottom corner of the well, energies of 145.9 meV, 317.3 meV, and

585.3 meV. The center of the well is at a potential of 100 meV relative to the bottom corner (there is 200 meV potential drop across the well in this field), and so the final energies relative to the center of the well are
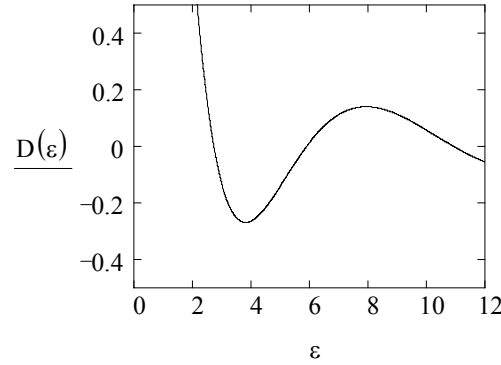

$\underline{D(\varepsilon)}$

Fig. 2. Graph of the determinant function, showing zero crossings near 3, 6, and 11.

$$E_1 = 45.9 \text{ meV, } 217.3 \text{ meV, } 485.3 \text{ meV}$$

Now we use these values and the relation

$$\frac{b_i}{a_i} = -\frac{Ai\left(\zeta_0\left(\varepsilon_i\right)\right)}{Bi\left(\zeta_0\left(\varepsilon_i\right)\right)}$$

to find the relative amplitude of the *Bi* and *Ai* functions in the wavefunction solution

$$\psi_i(z) = a_i Ai\left(\left(\frac{\pi}{v_L}\right)^{2/3}\left(v_L\frac{z}{L_z} - \varepsilon\right)\right) + b_i Bi\left(\left(\frac{\pi}{v_L}\right)^{2/3}\left(v_L\frac{z}{L_z} - \varepsilon\right)\right)$$

The resulting values for b_i / a_i are -0.1359, 0.651, and 1.5071 for levels 1, 2, and 3, respectively. To normalize this wavefunction, in practice, we will simply choose $a_i = 1$ in the unnormalized wavefunction, then perform a numerical normalization integral to find the appropriate normalization constant to put in front of the entire wavefunction. The resulting probability densities are graphed in Fig. 3.
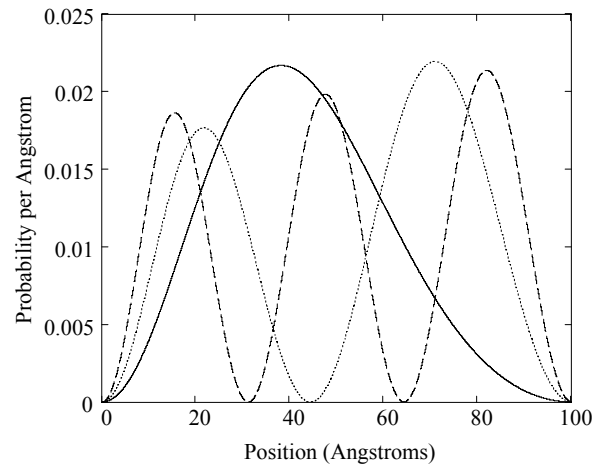
Fig. 3. Probability densities at 20 V/μm. Solid line – level 1. Dotted line – level 2. Dashed line – level 3.

Chapter 3 problem solutions

3.1.1

We start with Schrödinger's time-dependent equation, in one dimension

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

Then we substitute $\Psi = \exp\left[i(kz - \omega t)\right]$ with $V(z,t) = V_o$ to obtain

$$\frac{\hbar^2 k^2}{2m}\Psi + V_o\Psi = \hbar\omega\Psi$$

Hence to have a solution for each point on the wave we require

$$\frac{\hbar^2 k^2}{2m} + V_o = \hbar\omega$$

i.e.,

$$k^2 = \frac{2m}{\hbar^2}(\hbar\omega - V_o)$$

i.e.,

$$k = \sqrt{\frac{2m}{\hbar^2}(\hbar\omega - V_o)}$$

For real k

$$\hbar\omega \geq V_o$$

3.1.2

The time dependent Schrödinger equation with zero potential is

$$\left(-\frac{\hbar^2}{2m_o}\nabla^2\right)\Psi(r,t) = i\hbar\frac{\partial\Psi(r,t)}{\partial t}$$

(i) $\sin(kz-\omega t)$ is not a solution. Substituting it in, we would require

$$\frac{\hbar^2 k^2}{2m_o}\sin(kz\text{-}\omega t) = -i\hbar\omega\cos(kz-\omega t)$$

One reason why this is impossible for arbitrary z and t is that the left hand side is real while the right hand side is imaginary. (The problem with this wavefunction is that the wavefunction must be complex to satisfy Schrödinger's time dependent equation because of the i on the right hand side.)

(ii) $\exp(ikz)$ is not a solution. Substituting it in, we would require

$$\frac{\hbar^2 k^2}{2m_o}\exp(ikz) = 0$$

which is impossible for arbitrary z for a non-zero value of k. (The problem with this wavefunction is that it had no time dependence.)

(iii) $\exp\left[-i(\omega t+kz)\right]$ is a solution. Substituting it in, we have

$$\frac{\hbar^2 k^2}{2m_o}\exp[-i(\omega t+kz)] = i\hbar(-i\omega)\exp[-i(\omega t+kz)] = \hbar\omega\exp[-i(\omega t+kz)]$$

which is possible for real positive values of k and ω provided $\frac{\hbar^2 k^2}{2m_o} = \hbar\omega$.

(iv) $\exp\left[i(\omega t-kz)\right]$ is not a solution. Substituting it in, we would require

$$\frac{\hbar^2 k^2}{2m_o}\exp[i(\omega t-kz)] = -\hbar\omega\exp[-i(\omega t+kz)]$$

which is impossible for positive, real values of k and ω. (The problem with this wavefunction is that the time dependence has to be exp(-$i\omega t$), not exp($i\omega t$) for a solution of the time dependent Schrödinger equation with positive ω.)

3.1.3

(i) $\exp\left(-i\dfrac{\hbar\pi^2}{2m_o L_z^2}t\right)\sin\left(\dfrac{\pi z}{L_z}\right)$

Yes (the spatial part is the $n=1$ solution, and the temporal exponential is the correct one for this spatial solution)

(ii) $\exp\left(i\dfrac{4\hbar\pi^2}{2m_o L_z^2}t\right)\sin\left(\dfrac{2\pi z}{L_z}\right)$

No (the temporal exponent has the wrong sign)

(iii) $\exp\left(-i\left(\dfrac{\hbar\pi^2}{2m_o L_z^2}t+\dfrac{\pi}{2}\right)\right)\cos\left(\dfrac{\pi z}{L_z}+\dfrac{\pi}{2}\right)$

Yes (the $\pi/2$ in the cosine argument turns the cosine into a sine, making the spatial part the solution for $n=1$, and the additional constant $\pi/2$ in the temporal argument merely corresponds to multiplying the whole solution by a complex constant)

(iv) $2\exp\left(-i\dfrac{\hbar\pi^2}{2m_o L_z^2}t\right)\sin\left(\dfrac{\pi z}{L_z}\right)-i\exp\left(-i\dfrac{9\hbar\pi^2}{2m_o L_z^2}t\right)\sin\left(\dfrac{3\pi z}{L_z}\right)$

Yes (this is a superposition of two solutions, one for $n=1$ and the other for $n=3$, each with the correct temporal factor, and such superpositions are solutions of the time-dependent Schrödinger equation)

3.3.1

We know already that the energy eigenstates (as solutions of the time-independent Schrödinger equation) are

$$\psi_n(z) = \sqrt{\frac{2}{L_z}} \sin\left(\frac{n\pi z}{L_z}\right) \text{ with eigenenergies } E_n = \frac{\hbar^2 (n\pi)^2}{2m(L_z)^2}, \text{ where } n = 1, 2, \ldots.$$

and the time-dependent version of such an eigen solution will be $\Psi(z,t) = \psi_n(z) \exp\left(\frac{-iE_n t}{\hbar}\right)$.

(i). The time-independent Schrödinger equation is $-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(z)}{\partial z^2} = E\psi(z)$

(a) Yes, this is a solution, for $n = 3$

(b) No, this is not a solution; n has to be a non-zero integer

(c) No, this is not a solution; indeed, no linear superposition of eigenfunctions corresponding to different energy eigenvalues is a solution of the time-independent Schrödinger equation (as can be checked by substituting into the time-independent Schrödinger equation)

(d) No, this is not a solution, for the same reason as in (i) (c)

(ii) The time-dependent Schrödinger equation is $-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(z,t)}{\partial z^2} = -i\hbar \frac{\partial \Psi(z,t)}{\partial t}$

(a) No, this is not a solution, because there is no time dependence in the wavefunction

(b) No, this is not a solution. This function might appear to be a solution of the time-dependent Schrödinger equation within the well, but is not a solution of the whole problem because this wavefunction cannot meet the boundary condition on the spatial solution that it must be zero at the walls. (This would also have been a sufficient reason to reject this as a solution in (i)(b) above.)

(c) No, this is not a solution; there is no time dependence in the wavefunction

(d) Yes, this is a solution; it is a superposition of two eigenstates with $n = 1$ and $n = 4$

3.6.1

We know that a particle in a linear superposition of two eigenstates will have a probability density that oscillates at the difference or beat frequency.

For an infinite well, we have

$$\omega_3 - \omega_1 = \frac{E_3^\infty - E_1^\infty}{\hbar} = (3^2 - 1^2)\frac{\hbar}{2m_o}\left(\frac{\pi}{L_z}\right)^2 = 8\frac{\hbar}{2m_o}\left(\frac{\pi}{4\text{x}10^{-10}}\right)^2 m^{-1}$$

$$= 2.8\text{x}10^{16} rad/\sec = 4.55\text{x}10^{15} Hz$$

3.6.2

(i) We know that the frequency f of the oscillator in its classical limit (e.g., in a coherent state) is also the frequency that goes into the expression for the energy separation between two adjacent levels in the harmonic oscillator. So we can conclude that the energy separation between adjacent levels in this quantum mechanical harmonic oscillator is given by $E = hf$.

(ii) The energy separation will decrease because the potential is now shallower or less sloped, and hence wider for a given energy. This is consistent with the behavior of an infinitely deep potential well where the eigen energies E are proportional to $1/L^2$, that is, a wider well corresponds to more closely spaced energy levels.

3.6.3

The state is of the form

$$\Psi(z,t) = A\exp(-i\omega_1 t)\sin\left(\frac{\pi z}{L_z}\right) + B\exp(-i\omega_2 t)\sin\left(\frac{2\pi z}{L_z}\right) + C\exp(-i\omega_3 t)\sin\left(\frac{3\pi z}{L_z}\right)$$

where in this case A, B, and C are all of equal magnitude (though that actually makes no difference to the resulting solution), and where we use the notation

$$\omega_n = \frac{E_n}{\hbar} = \frac{\hbar}{2m_o}\left(\frac{n\pi}{L_z}\right)^2$$

and, explicitly, $\omega_2 = 4\omega_1$, $\omega_3 = 9\omega_1$. The charge density is proportional to

$$\begin{aligned}|\Psi(z,t)|^2 = {}& |A|^2 + |B|^2 + |C|^2 \\ & + AB^* S_{12}(z)\exp\left(-i(\omega_1 - \omega_2)t\right) + c.c. \\ & + AC^* S_{13}(z)\exp\left(-i(\omega_1 - \omega_3)t\right) + c.c. \\ & + BC^* S_{23}(z)\exp\left(-i(\omega_2 - \omega_3)t\right) + c.c.\end{aligned}$$

where

$$S_{nm}(z) = \sin\left(\frac{n\pi z}{L_z}\right)\sin\left(\frac{m\pi z}{L_z}\right)$$

i.e.,

$$\begin{aligned}|\Psi(z,t)|^2 = {}& |A|^2 + |B|^2 + |C|^2 \\ & + |AB|\cos\left[(\omega_2 - \omega_1)t + \phi_{12}\right] \\ & + |AC|\cos\left[(\omega_3 - \omega_1)t + \phi_{13}\right] \\ & + |BC|\cos\left[(\omega_3 - \omega_2)t + \phi_{23}\right]\end{aligned}$$

where the ϕ's are phase angles.

So so each of the three (angular) frequencies $\omega_2 - \omega_1 = 3\omega_1$, $\omega_3 - \omega_2 = 5\omega_1$, and $\omega_3 - \omega_1 = 8\omega_1$ will be present in the oscillations of the charge density (and hence by assumption in the emitted electromagnetic radiation). For $L_z = 1\,\text{nm}$, we have

$$\omega_1 = \frac{\hbar}{2m_o}\left(\frac{\pi}{L_z}\right)^2 = \frac{1.055\times10^{-34}}{2\times9.11\times10^{-31}}\left(\frac{\pi}{10^{-9}}\right)^2 = 5.71\times10^{14}\,\text{radians/s}$$

corresponding to a frequency of $f_1 = \omega_1/2\pi \cong 9.08\times10^{14}\,\text{Hz}$, and so the frequencies that are present in the electromagnetic radiation are

$$3f_1 = 2.73\times10^{14}\,\text{Hz},\ 5f_1 = 4.54\times10^{14}\,\text{Hz, and}\ 8f_1 = 7.27\times10^{14}\,\text{Hz.}$$

3.6.4

(i) The wavefunction is in an superposition of two eigenstates of energies E_1 and E_2 with equal real amplitudes for the two states. So we can write, at time $t = 0$ when the time-varying exponentials are all unity,

$$\Psi(z,0) = A\Phi_1 + A\Phi_2 \text{ with } |A|^2 + |A|^2 = 1, \text{ so } A = 1/\sqrt{2}$$

and hence, explicitly

$$\Psi(z,0) = \frac{1}{\sqrt{2}}\Phi_1 + \frac{1}{\sqrt{2}}\Phi_2 = \frac{1}{\sqrt{2}}\sqrt{\frac{2}{L}}\sin\left(\frac{\pi z}{L}\right) + \frac{1}{\sqrt{2}}\sqrt{\frac{2}{L}}\sin\left(\frac{2\pi z}{L}\right)$$

(ii) Since we have written the wavefunction in a superposition of energy eigenstates at $t = 0$, we can easily deduce from (i) the wavefunction at time t

$$\Psi(z,t) = \frac{1}{\sqrt{2}}\Phi_1 \exp\left(-\frac{iE_1 t}{\hbar}\right) + \frac{1}{\sqrt{2}}\Phi_2 \exp\left(-\frac{iE_2 t}{\hbar}\right)$$

$$= \frac{1}{\sqrt{2}}\sqrt{\frac{2}{L}}\sin\left(\frac{\pi z}{L}\right)\exp\left(-\frac{iE_1 t}{\hbar}\right) + \frac{1}{\sqrt{2}}\sqrt{\frac{2}{L}}\sin\left(\frac{2\pi z}{L}\right)\exp\left(-\frac{iE_2 t}{\hbar}\right)$$

(iii) By direct calculation, we have

$$\langle\Psi(z,t)|\Psi(z,t)\rangle = \int_0^L \Psi^*(z,t)\Psi(z,t)dz$$

$$= \int_0^L \left(\sqrt{\frac{1}{L}}\sin\left(\frac{\pi z}{L}\right)e^{\left(\frac{iE_1 t}{\hbar}\right)} + \sqrt{\frac{1}{L}}\sin\left(\frac{2\pi z}{L}\right)e^{\left(\frac{iE_2 t}{\hbar}\right)}\right)$$

$$\times \left(\sqrt{\frac{1}{L}}\sin\left(\frac{\pi z}{L}\right)e^{\left(\frac{-iE_1 t}{\hbar}\right)} + \sqrt{\frac{1}{L}}\sin\left(\frac{2\pi z}{L}\right)e^{\left(\frac{-iE_2 t}{\hbar}\right)}\right)dz$$

$$= \frac{1}{L}\int_0^L \left(\sin\left(\frac{\pi z}{L}\right)^2 + \sin\left(\frac{2\pi z}{L}\right)^2 + \sin\left(\frac{\pi z}{L}\right)\sin\left(\frac{2\pi z}{L}\right)e^{\left(\frac{-i(E_1 - E_2)t}{\hbar}\right)}\right.$$

$$\left. + \sin\left(\frac{\pi z}{L}\right)\sin\left(\frac{2\pi z}{L}\right)e^{\left(\frac{i(E_1 - E_2)t}{\hbar}\right)}\right)dz$$

$$= \frac{1}{L}\left(\frac{L}{2} + \frac{L}{2} + 0 + 0\right)$$

$$= 1$$

3.7.1

We are given that $E = -\dfrac{\hbar^2 k^2}{2b}$, where $b > 0$. This dispersion relation corresponds to a parabola with a peak at $k = 0$.

E(k)

k
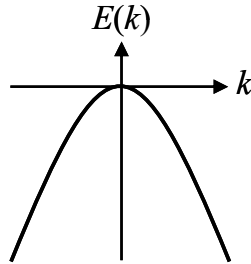
The wavepacket motion is given by the group velocity

$$v_g = \frac{\partial w}{\partial k} = \frac{1}{\hbar}\frac{\partial E}{\partial k} = -\frac{\hbar k}{b}$$

Hence we conclude

(i) For $k > 0$, $v_g < 0$, so the wavepacket moves backward (i.e., to the "left")

(i) For $k < 0$, $v_g > 0$, so the wavepacket moves forward (i.e., to the "right")

3.7.2

A. Positive group velocity. Positive effective mass.

B. Positive group velocity. Negative effective mass.

C. Negative group velocity. Negative effective mass.

D. Negative group velocity. Positive effect mass.

3.7.3

Consider first the solutions to the problem of an electron in a field F in the $+ve$ z direction, neglecting for the moment the boundary condition of the infinitely hard barrier. The solutions that we retain will only be the Ai Airy function. The Ai and Bi functions are plotted below, showing the phenomenon that the Bi function increases without bound for positive ζ. That solution increasing without bound cannot be part of the solution to this problem, because the wavefunction will be unnormalizable. Hence we drop the Bi solution, and presume that only the Ai solution is allowed.
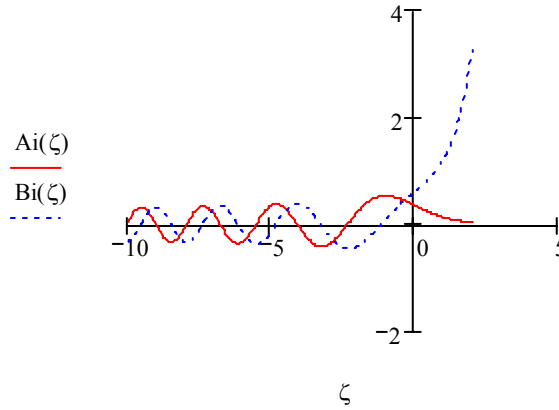
Performing the algebra to cast the Schrödinger equation into the form of the Airy differential equation, we therefore obtain the Schrödinger equation solution (within a normalization coefficient),

$$\psi_E(z) = Ai\left[\left(\frac{2m_o eF}{\hbar^2}\right)^{1/3}\left(z - \frac{E}{eF}\right)\right]$$

For this problem, it will be more convenient to express energies, E, in electron-Volts, distances, z, in Angstroms, and electric field, F, in Volts/Angstrom. With these units, we define a useful constant, a, which conveniently allows us to use these units.

$$a = \left[10^{-10}\left(\frac{2\times10^{10}m_o e}{\hbar^2}\right)^{1/3}\right] \simeq 0.64$$

As a result, with these units, with an applied field F the Airy wavefunction solution for a specific energy E (presuming for the moment that a solution to our larger quantum mechanical problem exists for such an energy) becomes

$$\psi(z,F,E) = Ai\left[aF^{1/3}\left(z - \frac{E}{F}\right)\right]$$

Now we can answer the specific questions.

(i) For our sloping potential well problem with an infinitely high barrier at $z = 0$, the solutions of the quantum well problem will be those for which the wavefunction is zero at $z = 0$. To find the situations for which the wavefunction is zero, we must first mathematically find the roots of the Airy function.

The zeros of the Ai Airy function may be found numerically as follows. Here we find the first 20 roots. As a guide, we first plot the Ai function over a sufficient range so we can see approximately where the zeros are.
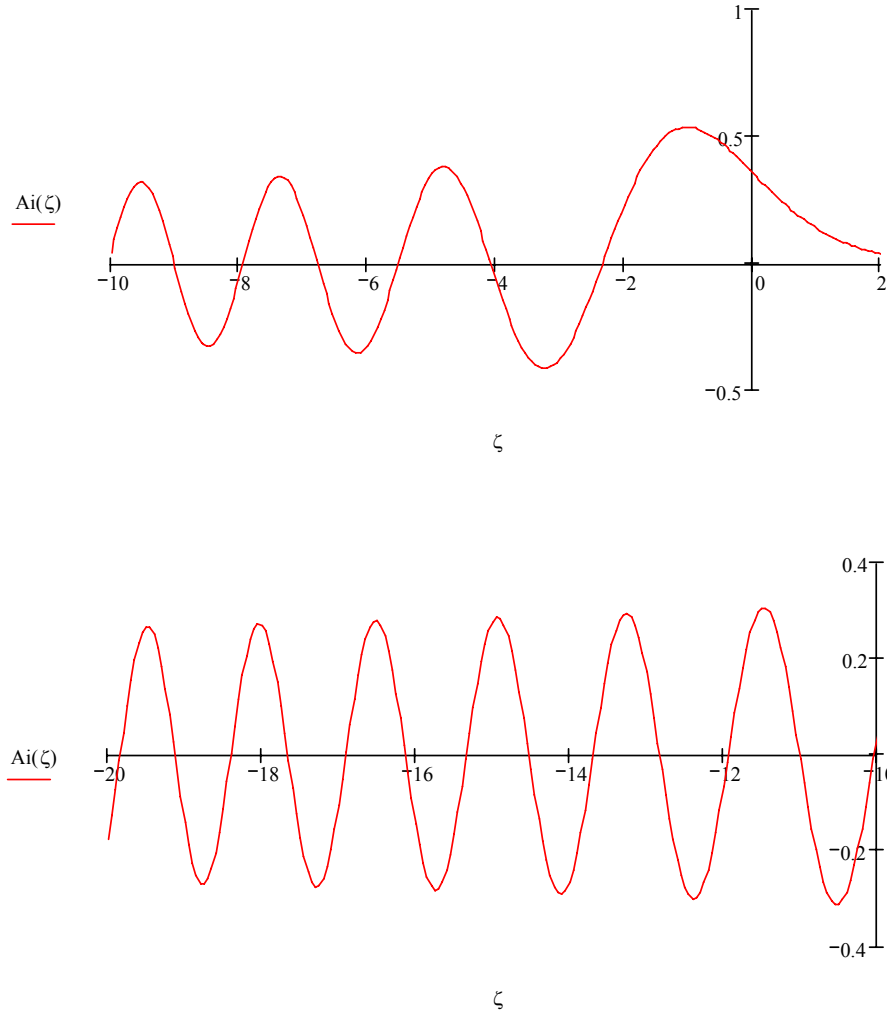
These roots R are respectively

R_1	R_2	R_3	R_4	R_5	R_6	R_7	R_8	R_9	R_{10}
-2.338	-4.088	-5.521	-6.787	-7.944	-9.023	-10.040	-11.009	-11.936	-12.829
R_{11}	R_{12}	R_{13}	R_{14}	R_{15}	R_{16}	R_{17}	R_{18}	R_{19}	R_{20}
-13.691	-14.528	-15.341	-16.133	-16.906	-17.661	-18.401	-19.126	-19.838	-20.537

So that the Airy function is zero at $z = 0$, we must have that

$$aF^{1/3}\left(0 - \frac{E}{F}\right) = \text{a root, } R, \text{ of the Ai function}$$

i.e.,
$$E = -RF^{2/3} / a$$

Hence, for a given field, we can deduce the corresponding eigenenergies (in electron-Volts), giving, for a field F of 1 V/Å (10^{10} V/m)

E_1	E_2	E_3	E_4	E_5	E_6	E_7	E_8	E_9	E_{10}
3.653	6.387	8.625	10.603	12.411	14.096	15.686	17.199	18.648	20.043
E_{11}	E_{12}	E_{13}	E_{14}	E_{15}	E_{16}	E_{17}	E_{18}	E_{19}	E
21.391	22.697	23.967	25.205	26.412	27.593	28.749	29.882	30.994	32.086

The figure below shows the explicit forms of the first three eigenfunctions.
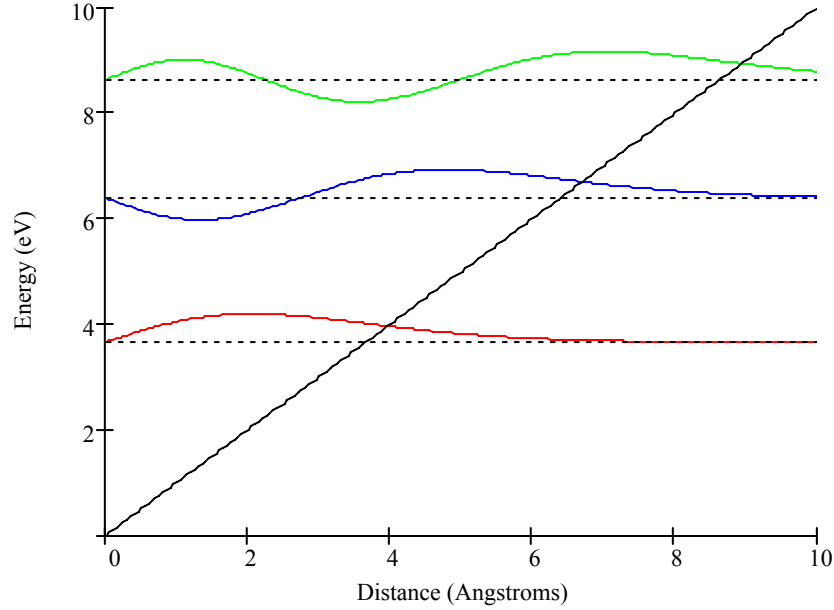
which are, mathematically,

$$\psi_1(z) = Ai\left(\left(\frac{2m_o e \times 10^{10}}{\hbar^2}\right)^{1/3}\left(z - \frac{3.653}{10^{10}}\right)\right)$$

$$\psi_2(z) = Ai\left(\left(\frac{2m_o e \times 10^{10}}{\hbar^2}\right)^{1/3}\left(z - \frac{6.387}{10^{10}}\right)\right)$$

$$\psi_3(z) = Ai\left(\left(\frac{2m_o e \times 10^{10}}{\hbar^2}\right)^{1/3}\left(z - \frac{8.625}{10^{10}}\right)\right)$$

(ii) Now we construct a wavepacket of such eigenstates. We will choose a Gaussian weighted wavepacket. We will choose a nominal energy width for the packet of $\Delta E = 2$ eV.

Note we have to add in the complex exponential time factors in making this linear superposition. We now define an appropriate constant for use in the summation, which allows use of energies in electron-Volts and time in femtoseconds.

$$b = 10^{-15}\frac{e}{\hbar} \simeq 1.518$$

We now construct the summation for the wavepacket. We center the wavepacket in energy around an energy E_o. We can if we wish take a factor $\exp(-iE_o t/\hbar)$ out of the sum, leaving only complex

exponentials oscillating at frequencies relative to the center frequency $E_o / \hbar$. Because this factor simply now multiplies the entire wavepacket wavefunction, we can actually discard it - it will make no difference to the final probability density. Hence our sum becomes

$$\Psi(z,t) = \sum_{n=1}^{20} \exp(-ibE_n t) \exp\left[\frac{-(E_n - E_o)^2}{2(\Delta E)^2} \right] \psi_n(z)$$

We can plot the result as a false plot, below. The approximately horizontal axis is time, and the approximately vertical axis is position. The color of the plot is dependent on $|\Psi(z,t)|^2$, moving from violet for small values through the spectrum to red for large values. Here we see that the wavepacket is "bouncing" off of the barrier (the "wall") in an approximately periodic pattern, and also showing interference between the incident and reflected wavepackets near the barrier. Close inspection of the wavefunctions shows that the behavior is not exactly periodic, however, with the wavepacket progressively breaking up as more cycles evolve from $t = 0$. (This is because the wavepacket is made up from a set of functions whose eigenenergies are not exactly equally spaced.)

(iii) A classical particle would trace out a position that varied parabolically in time as it moved up hill, reaching a classical turning point and then falling back to the wall. It would then "bounce" off the wall, and start its parabolic motion again. We can superimpose that classical motion on the quantum wavepacket in a pseudocolor plot.

Time (fs)
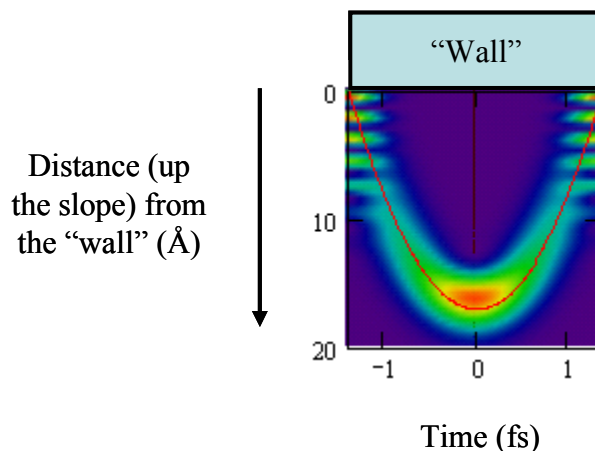
We can see by inspection from the graph of the wavepacket above that indeed the particle shows an approximately parabolic bouncing trajectory with a period of $\sim 2 \times 1.39$ fs, showing that the classical and quantum mechanical calculations agree in the center position. The quantum mechanical calculation eventually disperses – the wave-packet falls apart – and, of course, the quantum mechanical calculation is a wavepacket, not a discrete point at which the particle exists. The quantum mechanical calculation also shows interference as the wave packet bounces off of the wall.

3.8.1

Because we have decomposed the wavefunction in an orthonormal basis of energy, we have

$$\langle E \rangle = \Sigma |c_i|^2 \, E_i = \frac{1}{2} E_1 + \frac{1}{2} E_2 = \frac{5}{2} E_1$$

which does not depend on time.

3.10.1

To calculate the expectation value of energy, we need to evaluate the integral

$$< E >= \int \Psi^*(r,t)\hat{H}\Psi^*(r,t)d^3\text{r}$$

There are three approaches we can take to solving this problem. First, we can simply evaluate the result numerically using a mathematics program. Second, we can realize that the given wavefunction is actually a simple combination of harmonic oscillator energy eigenfunctions. Third, we can analytically evaluate the required integral.

The following is MATLAB code to solve this problem by the first approach. The answer it gives is 1.000000.

```
% MATLAB code for Problem 3.10.1
% Gaussian integral inside expectation value.

clear;
% Universal constants:
hbar = 1;
m0 = 1;

% a choice of a practical limit for the integral:
infinity = 5;

% Set up the space:
zstep = 0.001;
z = [-infinity:zstep:infinity];

% Define the wavefunction:
A = 1/sqrt(2*sqrt(pi));
psi = A*(1 + sqrt(2) * z).* exp(-z.^2/2);

% In the following code, we implement the Hamiltonian
% H = p^2 / 2m + V(z) = -(hbar^2 / 2m)*(d2/dz2) + z^2 / 2
% acting on the wavefunction

% derivatives of psi:
dpsi  = cat(2, diff(psi) /zstep,0);
ddpsi = cat(2, diff(dpsi)/zstep,0);

V = (z.^2)/2;
Hpsi = -(hbar^2/2*m0) * ddpsi + V.*psi;

% note that conj(psi) = psi, i.e., the wavefunction is real:
integrand = psi.* Hpsi;
expectation_of_energy = sum(integrand) * zstep
```

In the second approach, remember that the eigenfunctions of the harmonic oscillator are Hermite polynomials times a Gaussian, so we can put our wavefunction ψ in terms of the eigenfunctions of the harmonic oscillator rather easily. The first two Hermite polynomials are

$$H_0(z) = 1$$
$$H_1(z) = 2z$$

The general form of the energy eigenfunctions of the harmonic oscillator (with $\hbar = 1$ and $m = 1$) is

$$\psi_n(z) = \sqrt{\frac{1}{2^n n!\sqrt{\pi}}} \exp\left(-\frac{z^2}{2}\right)H_n(z)$$

so, explicitly, the first two energy eigenstates in these units are

$$\psi_0(z) = \frac{1}{\sqrt{\sqrt{\pi}}} \exp\left(-\frac{z^2}{2}\right) \qquad \psi_1(z) = \frac{1}{\sqrt{2\sqrt{\pi}}} \exp\left(-\frac{z^2}{2}\right)(2z)$$

Hence we can see that the given wavefunction here is

$$\psi(z) = \frac{1}{\sqrt{2}}(\psi_0(z) + \psi_1(z))$$

To calculate the expectation value is trivial now, because we have the expansion coefficients $1/\sqrt{2}$ for the first two energy eigenfunctions that together make up this wavefunction; that is, this wavefunction is just an equal superposition the first two energy eigenfunctions, so the expectation value of the energy is just the arithmetic mean of those eigenenergies. This is equal to

$$\frac{1}{2}\left(\frac{1}{2}\hbar\omega + \frac{3}{2}\hbar\omega\right) = \hbar\omega = 1 \text{ (in these units)}.$$

For the third approach of analytic evaluation of the integral, we first note the following.

$$A = \frac{1}{\sqrt{2\sqrt{\pi}}}$$

$$\psi(z) = A\left(1 + \sqrt{2}z\right)\exp(-z^2/2)$$

$$\frac{\partial\psi}{\partial z} = A\left(\sqrt{2} - z - \sqrt{2}z^2\right)\exp(-z^2/2)$$

$$\frac{\partial^2\psi}{\partial z^2} = A\left(-1 - 3\sqrt{2}z + z^2 + \sqrt{2}z^3\right)\exp(-z^2/2)$$

$$\hat{H}\psi = -\frac{1}{2}\frac{\partial^2\psi}{\partial z^2} + \frac{z^2}{2}\psi = A\left(\frac{1}{2} + \frac{3\sqrt{2}}{2}z\right)\exp(-z^2/2)$$

$$\psi^*\hat{H}\psi = A^2\exp(-z^2)\left(\frac{1}{2} + 2\sqrt{2}z + 3z^2\right)$$

The following are some useful integrals we can now use for this problem.

$$\int_{-\infty}^{\infty} \exp(-ax^2)\,dx = \sqrt{\frac{\pi}{a}}$$

$$\frac{\partial}{\partial a}\left[\int_{-\infty}^{\infty} \exp(-ax^2)\,dx = \sqrt{\frac{\pi}{a}}\right] \Rightarrow \int_{-\infty}^{\infty} x^2\exp(-ax^2)\,dx = \frac{1}{2a}\sqrt{\frac{\pi}{a}}$$

Note also that $\int_{-\infty}^{\infty} x\exp(-ax^2)\,dx = 0$ because the integrand is odd overall. Hence

$$<E> = \int_{-\infty}^{\infty} \psi^*\hat{H}\psi\,dz = A^2\int_{-\infty}^{\infty} e^{-z^2}\left(\frac{1}{2} + 2\sqrt{2}z + 3z^2\right)dz$$

$$= A^2\left(\frac{1}{2}\left(\sqrt{\pi}\right) + 2\sqrt{2}(0) + 3\left(\frac{1}{2}\sqrt{\pi}\right)\right) = \frac{1}{2\sqrt{\pi}}\left(2\sqrt{\pi}\right) = 1$$

3.11.1

Using the rules for the powers of an operator, we immediately deduce that

$$(\hat{H}^2 - \hat{H})\psi_n(r) = (E_n^2 - E_n)\psi_n(r)$$

which is an eigenvalue equation for the $\hat{H}^2 - \hat{H}$ operator. Hence, the $\psi_n(r)$ are eigenfunctions of this operator also, and the corresponding eigenvalues are $(E_n^2 - E_n)$.

3.12.1

(i) The system oscillates at a frequency corresponding to the difference between the energies of the two eigenstates.

$$\omega = \frac{E_2 - E_1}{\hbar} = \frac{1}{\hbar}\frac{\hbar^2\pi^2}{2mL^2}(2^2 - 1^2) = 3E_1 = \frac{3\hbar\pi^2}{2mL^2}$$

(ii) Here one must work out the appropriate integral for the expectation value of the momentum

$$\langle p_z(t) \rangle = \int_0^{L_z} \psi^* \hat{p}_z \psi \, dz$$

using the integral hints given. We note first that the wavefunction is

$$\psi = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{2}{L_z}} \sin kz \exp(-i\omega_1 t) + \sqrt{\frac{2}{L_z}} \sin 2kz \exp(-i\omega_2 t) \right)$$

We note next that

$$\hat{p}_z \psi = (-i\hbar\nabla)\left(\sqrt{\frac{1}{L_z}} \right)\left(\sin kz \exp(-i\omega_1 t) + \sin 2kz \exp(-i\omega_2 t) \right)$$

$$= \frac{-i\hbar k}{\sqrt{L_z}}\left(\cos kz \exp(-i\omega_1 t) + 2\cos 2kz \exp(-i\omega_2 t) \right)$$

So

$$\langle p_z(t) \rangle$$

$$= \int_0^{L_z} \left(\frac{-i\hbar k}{L_z} \right)\left(\sin kz \exp(+i\omega_1 t) + \sin 2kz \exp(+i\omega_2 t) \right)\left(\cos kz \exp(-i\omega_1 t) + 2\cos 2kz \exp(-i\omega_2 t) \right) dz$$

$$= \left(\frac{-i\hbar k}{L_z} \right)\int_0^{L_z} \left(2\sin kz \cos 2kz \exp(-i(\omega_2 - \omega_1)t) + \cos kz \sin 2kz \exp(+i(\omega_2 - \omega_1)t) \right) dz$$

$$= \frac{\hbar}{iL_z}\left(2\left(-\frac{2}{3}\right)\exp(-i(\omega_2 - \omega_1)t) + \left(\frac{4}{3}\right)\exp(+i(\omega_2 - \omega_1)t) \right) = \frac{8\hbar}{3L_z}\sin\left((\omega_2 - \omega_1)t\right)$$

(iii) If the particle is in a superposition between the first and third states of the well, then all of the integrands are odd over the allowed region and the integrals are zero. Therefore, $\langle p_z(t) \rangle = 0$. It is also possible to understand that these integrals must be zero using trigonometric identities.

$$\sin kz \cos 3kz = \frac{1}{2}\left(\sin(kz + 3kz) + \sin(kz - 3kz) \right)$$

$$k\int_0^{L_z} \sin kz \cos 3kz \, dz = \frac{1}{2}\left(-\frac{1}{4}[\cos 4kz]_0^{L_z} + \frac{1}{2}[\cos 2kz]_0^{L_z} \right) = 0$$

3.12.2

(i) Here, we note first that the given state is a momentum eigenstate; that is

$$\hat{p}\exp(i\mathbf{k}\cdot\mathbf{r}) \equiv -i\hbar\nabla\exp(i\mathbf{k}\cdot\mathbf{r}) = \hbar\mathbf{k}\exp(i\mathbf{k}\cdot\mathbf{r})$$

Since we are in an eigenstate of the momentum operator, any measurement of the momentum will always return the same value $\hbar\mathbf{k}$, and so that is the expectation value of momentum in this case.

(Note that we could attempt to evaluate the expectation value of the momentum by evaluating the integral, presuming that somehow the wavefunction $\exp(i\mathbf{k}\cdot\mathbf{r})$ could be normalized with some normalization constant A; that is

$$< \mathbf{p} > = \int_{-\infty}^{\infty} \psi^* \hat{p}\psi d^3 r = \int_{-\infty}^{\infty} \left(A^* \exp(-i\mathbf{k}\cdot\mathbf{r}) \right) \hat{p} \left(A\exp(+i\mathbf{k}\cdot\mathbf{r}) \right) d^3 r$$

$$< \mathbf{p} > = \int_{-\infty}^{\infty} \left(A^* \exp(-i\mathbf{k}\cdot\mathbf{r}) \right)(-i\hbar\nabla)\left(A\exp(+i\mathbf{k}\cdot\mathbf{r}) \right) d^3 r$$

$$< \mathbf{p} > = \int_{-\infty}^{\infty} \left(A^* \exp(-i\mathbf{k}\cdot\mathbf{r}) \right)(-i\hbar(i\mathbf{k}))\left(A\exp(+i\mathbf{k}\cdot\mathbf{r}) \right) d^3 r = \hbar\mathbf{k} \int_{-\infty}^{\infty} |\psi|^2 d^3 r = \hbar\mathbf{k}$$

though in fact, at least if we take infinite limits in our integrals, there is no such A that can normalize the wavefunction – any nonzero value for A leads to an infinite value for the normalization integral. If we imagined that our world was bounded as a finite box of some large, but not infinite size, then we could proceed in this way, with a nonzero A. The mathematical resolution of this problem of normalization of the momentum eigenfunctions in an unbounded world is to use normalization to a delta function, which is introduced in Chapter 5.)

(ii) The expectation of the momentum in an energy eigenstate of such a potential well is zero, as we can show explicitly.

$$\psi_1 = \sqrt{\frac{2}{L}} \sin\frac{\pi z}{L}$$

$$\hat{p}\psi_1 = (-i\hbar\nabla)\sqrt{\frac{2}{L}}\sin\frac{\pi z}{L} = \frac{-i\hbar\pi}{L}\sqrt{\frac{2}{L}}\cos\frac{\pi z}{L}$$

$$\int_0^L \psi_1^* \hat{p}\psi_1 \, dz = \frac{-2i\hbar\pi}{L^2}\int_0^L \sin\frac{\pi z}{L}\cos\frac{\pi z}{L}\, dz = 0$$

 (iii) The lowest energy eigenstate of the infinitely deep quantum well is an equal superposition of two eigenstates of the momentum operator, with opposite eigenvalues.

$$\psi_1 \propto \sin\frac{\pi z}{L} \propto \exp\left(i\frac{\pi z}{L}\right) - \exp\left(-i\frac{\pi z}{L}\right)$$

As a result, there is an equal probability of finding the value of the momentum to be either $\pm\hbar\frac{\pi}{L}$ which implies that the expected value must be zero. Another way of thinking about this is that it is a standing wave pattern, the sum of a left-propagating wave and a right-propagating wave with equal amplitudes.

3.12.3

(i) The time-dependent Schrödinger equation in one dimension is

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

The advantage of eigenfunctions of the time-independent Schrödinger equation is their simple time evolution (once we do start considering the time-dependent case). Recall that if $\psi_{time-ind}(z)$ is a solution to the time-independent Schrödinger equation, then a solution to the time-dependent equation is given by

$$\Psi(z,t)=\psi_{time-ind}(z)\exp(-i\omega t)$$

where $\omega = E/\hbar$ and E is the energy eigenvalue associated with $\psi_{time-ind}(z)$. Therefore, we construct the necessary wavefunction to be

$$\Psi(z,t)=\frac{1}{\sqrt{2}}\left(\psi_1(z)\exp(-i\omega_1 t)+\psi_2(z)\exp(-i\omega_2 t)\right)$$

$$=\frac{1}{\sqrt{2}}\left(\sqrt{\frac{2}{L}}\sin(kz)\exp(-i\omega_1 t)+\sqrt{\frac{2}{L}}\sin(2kz)\exp(-i\omega_2 t)\right)$$

where L is the width of the well. The square root of ½ is required for normalization of the probability density. Also $k = \pi/L$ throughout these solutions. Substituting this into the time-dependent Schrödinger equation, we have

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}\left(\frac{1}{\sqrt{2}}\left(\sqrt{\frac{2}{L}}\sin(kz)\exp(-i\omega_1 t)+\sqrt{\frac{2}{L}}\sin(2kz)\exp(-i\omega_2 t)\right)\right)$$

$$=i\hbar\frac{\partial}{\partial t}\left(\frac{1}{\sqrt{2}}\left(\sqrt{\frac{2}{L}}\sin(kz)\exp(-i\omega_1 t)+\sqrt{\frac{2}{L}}\sin(2kz)\exp(-i\omega_2 t)\right)\right)$$

i.e.,

$$\left[-\frac{\hbar^2}{2m}(-k^2)\sin(kz)\right]\exp(-i\omega_1 t)+\left[-\frac{\hbar^2}{2m}(-4k^2)\sin(2kz)\right]\exp(-i\omega_2 t)$$

$$=i\hbar\sin(kz)\left[-i\omega_1\exp(-i\omega_1 t)\right]+i\hbar\sin(2kz)\left[-i\omega_2\exp(-i\omega_2 t)\right]$$

This last equation holds true, because our definitions are such that

$$\hbar\omega_1 \equiv E_1 = \frac{\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2 = \frac{\hbar^2 k^2}{2m} \text{ and } \hbar\omega_2 \equiv E_2 = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 = \frac{4\hbar^2 k^2}{2m}$$

Hence this linear superposition is explicitly a solution of the time-dependent Schrödinger equation for a particle in such a well.

(ii)

$$\langle z \rangle = \int \Psi^*(z,t) \hat{z}\, \Psi^*(z,t)\, dz$$

$$= \int \left\{ \frac{1}{\sqrt{2}} \left[\sqrt{\frac{2}{L}} \sin(kz) \exp(-i\omega_1 t) + \sqrt{\frac{2}{L}} \sin(2kz) \exp(-i\omega_2 t) \right] \right\}^*$$

$$\times \hat{z} \left\{ \frac{1}{\sqrt{2}} \left[\sqrt{\frac{2}{L}} \sin(kz) \exp(-i\omega_1 t) + \sqrt{\frac{2}{L}} \sin(2kz) \exp(-i\omega_2 t) \right] \right\} dz$$

$$= \frac{2}{L} \int \frac{1}{\sqrt{2}} \left[\sin(kz) \exp(+i\omega_1 t) + \sin(2kz) \exp(+i\omega_2 t) \right]$$

$$\times z \frac{1}{\sqrt{2}} \left[\sin(kz) \exp(-i\omega_1 t) + \sin(2kz) \exp(-i\omega_2 t) \right] dz$$

$$= \frac{1}{L} \int z \left[\sin^2(kz) + \sin^2(2kz) + \sin(kz)\sin(2kz) 2\cos\left((\omega_1 - \omega_2)t\right) \right] dz$$

Using the results (Appendix G)

$$\int_0^\pi (x - \pi/2) \sin(nx) \sin(mx)\, dx = \frac{-4nm}{(n-m)^2 (n+m)^2}, \quad \text{for } n + m \text{ odd}$$

$$= 0, \quad \text{for } n + m \text{ even}$$

$$\int_0^\pi \sin^2(nx)\, dx = \frac{\pi}{2}$$

we can evaluate all of the integrals here. The result is that

$$\langle z \rangle = \frac{1}{L} \left\{ \frac{L^2}{4} + \frac{L^2}{4} - \frac{8}{9k^2} \left(2\cos\left[(\omega_1 - \omega_2)t \right] \right) \right\}$$

$$= \frac{L}{2} - \frac{16L}{9\pi^2} \cos\left[(\omega_1 - \omega_2)t \right] = \frac{L}{2} - \frac{16L}{9\pi^2} \cos\left(\frac{3}{2} \frac{\hbar \pi^2}{m L^2} t \right)$$

which also makes intuitive (symmetry) sense in that the position expectation value is oscillating about the center of the well.

3.12.4

$$\langle \mathbf{p} \rangle = -i\hbar \int \Psi^* (\mathbf{r}, t_o) \nabla \Psi (\mathbf{r}, t_o) d^3 \mathbf{r}$$

3.12.5

At t = 0, we are in a an energy eigenstate

$$\Psi(x,t) = \Phi_1(x,t) \text{ and } \langle E \rangle = E_1$$

Then we measure momentum. Because $\Phi_1(x,t)$ is *not* a momentum eigenstate (such an energy eigenstate in a potential is not of the form exp(ikx)), after the momentum measurement, which forces it into a momentum eigenstate, we will get a new state that must now be a superposition of energy eigenstates, not just the lowest energy eigenstate; that is, now

$$\Psi(x,t) = \sum_n c_n . \Phi_n(x,t)$$

In this superposition of energy eigenstates

$$\langle E \rangle = \sum_n |c_n|^2 E_n > E_1$$

(The lowest result we could possible have for such a sum would be for $|c_1|^2 = 1$. Any other set of c's [where we must have $\sum_n |c_n|^2 = 1$ as required by normalization] will lead to a larger result because all the other E_n are larger that E_1.)

Hence, we conclude that the result of this measurement of momentum is to increase the expected value of the energy.

3.13.1

(i)

$$\Delta x = 1 \times 10^{-10}\,\text{m}$$

$$m = 1 \times 10^{-3}\,\text{kg}$$

$$\Delta p \geq \frac{\hbar}{2}\frac{1}{\Delta x} = \frac{1.055 \times 10^{-34}\,\text{J} \cdot \text{s}}{2}\frac{1}{1 \times 10^{-10}\,\text{m}} = 5.275 \times 10^{-25}\,\text{N} \cdot \text{s}$$

$$\Delta v = \frac{\Delta p}{m} \geq \frac{5.275 \times 10^{-25}\,\text{N} \cdot \text{s}}{1 \times 10^{-3}\,\text{kg}} = 5.275 \times 10^{-22}\,\text{m/s}$$

(ii) Simply multiply by the ratio of the masses

$$\frac{m}{m_0} = \frac{1 \times 10^{-3}\,kg}{9.11 \times 10^{-31}\,kg} = 1.1 \times 10^{27}$$

$$\Rightarrow \Delta v \geq \left(5.275 \times 10^{-22}\,\text{m/s}\right) \times \left(1.1 \times 10^{27}\right) = 5.8 \times 10^{5}\,\text{m/s}$$

3.14.1

(i) The slowly-varying approximation means we can ignore $\nabla A(r)$ terms compared to A(r).

$$\mathbf{j}_p = \frac{i\hbar}{2m}\left(\Psi\nabla\Psi^* - \Psi^*\nabla\Psi\right)$$

$$\nabla\Psi = \nabla\left(A(\mathbf{r})\exp(i\mathbf{k}\cdot\mathbf{r})\right) = \left(\exp(i\mathbf{k}\cdot\mathbf{r})\nabla A(\mathbf{r}) + A(\mathbf{r})\nabla\exp(i\mathbf{k}\cdot\mathbf{r})\right)$$

$$= \exp(i\mathbf{k}\cdot\mathbf{r})\left(\nabla A(\mathbf{r}) + A(\mathbf{r})i\mathbf{k}\right) \approx A(\mathbf{r})(i\mathbf{k})\exp(i\mathbf{k}\cdot\mathbf{r})$$

$$\Rightarrow \nabla\Psi^* = A^*(\mathbf{r})(-i\mathbf{k})\exp(-i\mathbf{k}\cdot\mathbf{r})$$

$$\mathbf{j}_p = \frac{i\hbar}{2m}\left(\begin{array}{l}\left(A(\mathbf{r})\exp(i\mathbf{k}\cdot\mathbf{r})\right)\left(A^*(\mathbf{r})(-i\mathbf{k})\exp(-i\mathbf{k}\cdot\mathbf{r})\right) - \\ \left(A^*(\mathbf{r})\exp(-i\mathbf{k}\cdot\mathbf{r})\right)\left(A(\mathbf{r})(i\mathbf{k})\exp(i\mathbf{k}\cdot\mathbf{r})\right)\end{array}\right)$$

$$\mathbf{j}_p = \frac{i\hbar}{2m}\left(|A(\mathbf{r})|^2(-2i\mathbf{k})\right) = \frac{\hbar\mathbf{k}}{m}|A(\mathbf{r})|^2 = \frac{\mathbf{p}}{m}|\psi(\mathbf{r})|^2$$

(ii) Taking the potential energy to be zero for simplicity (it will not matter, we would simply end up adding it as a constant to the total energy)

$$\langle E\rangle = \int\psi^*\hat{H}\psi\,d^3r$$

$$= \int\left(A^*(\mathbf{r})\exp(-i\mathbf{k}\cdot\mathbf{r})\right)\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}\right)\left(A(\mathbf{r})\exp(i\mathbf{k}\cdot\mathbf{r})\right)d^3r$$

$$= \left(\frac{\hbar^2}{2m}(\mathbf{k}^2)\right)\int\left(A^*(\mathbf{r})\exp(-i\mathbf{k}\cdot\mathbf{r})\right)\left(A(\mathbf{r})\exp(i\mathbf{k}\cdot\mathbf{r})\right)d^3r$$

$$= \left(\frac{\hbar^2}{2m}(k^2)\right)\int\left(A^*(\mathbf{r})\right)\left(A(\mathbf{r})\right)d^3r = \left(\frac{\hbar^2 k^2}{2m}\right) = \frac{p^2}{2m}$$

assuming that the wavefunction ψ was normalized to begin with.

(iii) The above result corresponds exactly to the classical result, where the kinetic energy is

$p^2/2m \equiv (1/2)mv^2$, where v is the classical velocity.

3.14.2

(i) We can simply rederive the relation for the particle current using the new Hamiltonian, as hinted,

$$\frac{\partial}{\partial t}\left[\Psi^*\Psi\right]+\frac{i}{\hbar}\left(\Psi^*\hat{H}\Psi-\Psi\hat{H}\Psi^*\right)=0$$

$$\hat{H}\Psi=\frac{-\hbar^2}{2}\left(\frac{\partial}{\partial z}\left[\frac{1}{m(z)}\frac{\partial\Psi}{\partial z}\right]\right)+V\Psi$$

$$\hat{H}\Psi^*=\frac{-\hbar^2}{2}\left(\frac{\partial}{\partial z}\left[\frac{1}{m(z)}\frac{\partial\Psi^*}{\partial z}\right]\right)+V\Psi^*$$

$$\frac{\partial}{\partial t}\left[\Psi^*\Psi\right]+\frac{-i\hbar}{2}\left(\begin{array}{c}\Psi^*\left(\frac{\partial}{\partial z}\left[\frac{1}{m(z)}\frac{\partial\Psi}{\partial z}\right]+V\Psi\right)\\ -\Psi\left(\frac{\partial}{\partial z}\left[\frac{1}{m(z)}\frac{\partial\Psi^*}{\partial z}\right]+V\Psi\right)\end{array}\right)=0$$

$$\frac{\partial}{\partial t}\left[\Psi^*\Psi\right]+\frac{-i\hbar}{2}\left(\begin{array}{c}\Psi^*\left(\frac{\partial}{\partial z}\left[\frac{1}{m(z)}\frac{\partial\Psi}{\partial z}\right]\right)-\Psi\left(\frac{\partial}{\partial z}\left[\frac{1}{m(z)}\frac{\partial\Psi^*}{\partial z}\right]\right)\\ +\frac{1}{m(z)}\frac{\partial\Psi}{\partial z}\frac{\partial\Psi^*}{\partial z}-\frac{1}{m(z)}\frac{\partial\Psi}{\partial z}\frac{\partial\Psi^*}{\partial z}\end{array}\right)=0$$

$$\frac{\partial}{\partial t}\left[\Psi^*\Psi\right]+\frac{i\hbar}{2}\frac{\partial}{\partial z}\left(-\Psi^*\left[\frac{1}{m(z)}\frac{\partial\Psi}{\partial z}\right]+\Psi\left[\frac{1}{m(z)}\frac{\partial\Psi^*}{\partial z}\right]\right)=0$$

$$\frac{\partial}{\partial t}\left[\Psi^*\Psi\right]=-\frac{\partial}{\partial z}\left(\frac{i\hbar}{2}\left(-\Psi^*\left[\frac{1}{m(z)}\frac{\partial\Psi}{\partial z}\right]+\Psi\left[\frac{1}{m(z)}\frac{\partial\Psi^*}{\partial z}\right]\right)\right)$$

$$\Rightarrow \mathbf{j_p}=\frac{i\hbar}{2}\left(-\Psi^*\left[\frac{1}{m(z)}\frac{\partial\Psi}{\partial z}\right]+\Psi\left[\frac{1}{m(z)}\frac{\partial\Psi^*}{\partial z}\right]\right)$$

$$\mathbf{j_p}=\frac{i\hbar}{2}\frac{1}{m(z)}\left(\Psi\left[\frac{\partial\Psi^*}{\partial z}\right]-\Psi^*\left[\frac{\partial\Psi}{\partial z}\right]\right)$$

(ii) The argument is basically the same as in the book. In order to satisfy the Schrödinger equation with a finite E and finite V everywhere, it must be true that the remaining term $\frac{-\hbar^2}{2}\frac{\partial}{\partial z}\left[\frac{1}{m(z)}\frac{\partial\Psi}{\partial z}\right]$ must also be finite everywhere. This in turn requires that $\frac{1}{m(z)}\frac{\partial\Psi}{\partial z}$ be continuous everywhere. Similarly, we require that $\frac{1}{m(z)}\frac{\partial\Psi}{\partial z}$ be finite (or its derivative might be infinite), which implies the continuity of ψ.

Chapter 4 problem solutions

4.1.1

(i) $\langle 3|5 \rangle$

(ii) $G\langle 3|3 \rangle$

(iii) $\dfrac{L_z}{2}\langle 5|5 \rangle$

4.1.2

Measurement of quantity d leads to two possible outcomes

$$(1)\ |\psi_1\rangle \text{ with probability } \left(\frac{3}{5}\right)^2 = \frac{9}{25}$$

$$(2)\ |\psi_2\rangle \text{ with probability } \left(\frac{4}{5}\right)^2 = \frac{16}{25}$$

To deduce the effect of subsequent measurements of quantity c, we need to write $|\psi_1\rangle$ and $|\psi_2\rangle$ in terms of $|\phi_1\rangle$ and $|\phi_2\rangle$.

From the original expressions, we have

$$3|\phi_1\rangle + 4|\phi_2\rangle = \left(\frac{9}{5} + \frac{16}{5}\right)|\psi_1\rangle = \frac{25}{5}|\psi_1\rangle = 5|\psi_1\rangle$$

so

$$|\psi_1\rangle = \frac{3}{5}|\phi_1\rangle + \frac{4}{5}|\phi_2\rangle$$

Similarly

$$4|\phi_1\rangle - 3|\phi_2\rangle = \left(\frac{16}{5} + \frac{9}{5}\right)|\psi_2\rangle = 5|\psi_2\rangle$$

so

$$|\psi_2\rangle = \frac{4}{5}|\phi_1\rangle - \frac{3}{5}|\phi_2\rangle$$

Hence

$$\text{Case (1) (Conditional) probability of measuring } |\phi_1\rangle = \frac{9}{25}$$

$$\text{Case (2) (Conditional) probability of measuring } |\phi_1\rangle = \frac{16}{25}$$

Hence, the final total probability of measuring the system to be in the state $|\phi_1\rangle$ is

$$P(|\psi_1\rangle) = \frac{9}{25} \times \frac{9}{25} + \frac{16}{25} \times \frac{16}{25}$$

$$= \frac{81}{625} + \frac{256}{625} = \frac{337}{625}$$

4.2.1

(i) These functions are rather obviously orthogonal because one is even and the other odd over the interval. Explicitly

$$\langle \psi_1 | \psi_2 \rangle = \int_{-1}^{1} \left(\frac{1}{\sqrt{2}} \right) \left(\sqrt{\frac{3}{2}} x \right) dx = \int (even)(odd) \, dx = 0$$

These functions are also normalized, that is

$$\langle \psi_1 | \psi_1 \rangle = \int_{-1}^{1} \left(\frac{1}{\sqrt{2}} \right)^2 dx = \frac{1}{2} \int_{-1}^{1} dx = \frac{1}{2} \left[x \big|_{-1}^{1} \right] = 1$$

$$\langle \psi_2 | \psi_2 \rangle = \int_{-1}^{1} \left(\sqrt{\frac{3}{2}} x \right)^2 dx = \frac{3}{2} \int_{-1}^{1} x^2 dx = \frac{3}{2} \left[\frac{x^3}{3} \Big|_{-1}^{1} \right] = 1$$

and hence they form an orthonormal set of functions.

(ii) Consider a general function in this space $f(x) = ax + b$. We can construct this function from our functions ψ_1, ψ_2 in the following manner

$$f(x) = c_1 \psi_1 + c_2 \psi_2 = c_1 \left(\frac{1}{\sqrt{2}} \right) + c_2 \left(\sqrt{\frac{3}{2}} x \right) = b + ax$$

$$c_1 = \sqrt{2} b; \quad c_2 = \sqrt{\frac{2}{3}} a$$

(iii) Note that, in this case, the values of the c's are given by

$$c_1 = b\sqrt{2} = 3\sqrt{2} = 4.242$$

$$c_2 = a\sqrt{\frac{2}{3}} = 2\sqrt{\frac{2}{3}} = 1.633$$
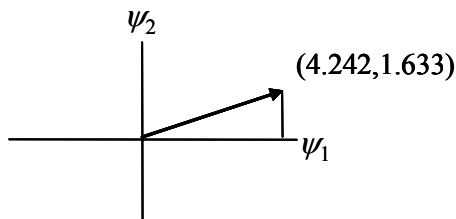
4.6.1

(i) $\langle f | g \rangle$

complex number

(ii) $\langle f | \hat{A}$

row vector

(iii) $| f \rangle \langle g |$

matrix

(iv) $\hat{A} | f \rangle \langle g |$

matrix

(v) $\hat{A}^\dagger | f \rangle \left(| f \rangle \right)^\dagger$

matrix

4.8.1

Consider an operator $\hat{A}$, and evaluate the sum of squares of its matrix elements evaluated on a basis $|\psi_m\rangle$. We have for this sum

$$S = \sum_{m,n} \left| \langle \psi_m | \hat{A} | \psi_n \rangle \right|^2 = \sum_{m,n} \langle \psi_m | \hat{A} | \psi_n \rangle \langle \psi_n | \hat{A}^\dagger | \psi_m \rangle$$

Introduce the identity operator on a new basis $|\phi_p\rangle$

$$\hat{I} = \sum_p |\phi_p\rangle\langle\phi_p|$$

Inserting this operator, we have

$$S = \sum_{m,n,p} \langle \psi_m | \hat{A} | \phi_p \rangle \langle \phi_p | \psi_n \rangle \langle \psi_n | \hat{A}^\dagger | \psi_m \rangle$$

Removing the identity operator in $|\psi_n\rangle$

$$S = \sum_{m,p} \langle \psi_m | \hat{A} | \phi_p \rangle \langle \phi_p | \hat{A}^\dagger \psi_m \rangle$$

Introducing another identity operator in $|\phi_p\rangle$, this time with the index q

$$S = \sum_{m,p,q} \langle \psi_m | \hat{A} | \phi_p \rangle \langle \phi_p | \hat{A}^\dagger | \phi_q \rangle \langle \phi_q | \psi_m \rangle$$

Interchanging complex numbers in the sum gives

$$S = \sum_{m,p,q} \langle \phi_q | \psi_m \rangle \langle \psi_m | \hat{A} | \phi_p \rangle \langle \phi_p | \hat{A}^\dagger | \phi_q \rangle$$

Removing the identity operator in $|\psi_m\rangle$ gives the desired result, which is the sum of the modulus squared matrix elements on the new basis, and is equal to the sum S we started with, that is

$$S = \sum_{p,q} \langle \phi_q | \hat{A} | \phi_p \rangle \langle \phi_p | \hat{A}^\dagger | \phi_q \rangle \equiv \sum_{p,q} \left| \langle \phi_q | \hat{A} | \phi_p \rangle \right|^2$$

4.10.1

(i) We find eigenvalues in the usual way by finding those conditions for which the determinant below is zero, i.e.,

$$\det\left(\hat{M}_{old} - m\hat{I}\right) = 0$$

$$\det\begin{pmatrix} -m & i \\ -i & -m \end{pmatrix} = m^2 - 1 = 0 \Rightarrow m = \pm 1$$

To find the eigenvectors, we just apply the matrix to a generalized vector and then solve the eigenvalue equation.

$$\begin{bmatrix} 0 & i \\ -i & 0 \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = m\begin{bmatrix} a \\ b \end{bmatrix}$$

$$\begin{bmatrix} 0 & i \\ -i & 0 \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} a \\ b \end{bmatrix} \Rightarrow \begin{cases} ib = a \\ -ia = b \end{cases} \Rightarrow \psi_1 = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -i \end{bmatrix}$$

$$\begin{bmatrix} 0 & i \\ -i & 0 \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = -\begin{bmatrix} a \\ b \end{bmatrix} \Rightarrow \begin{cases} ib = -a \\ -ia = -b \end{cases} \Rightarrow \psi_{-1} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ i \end{bmatrix}$$

The normalization of these eigenvectors has led to the $1/\sqrt{2}$ factors. Note that we could multiply either of these eigenvectors by any unit complex constant, and they would still be normalized eigenvectors.

(ii) We want to find a matrix $\hat{U}$, such that it transforms the eigenvectors found above into the simple eigenvectors given in the statement of the problem. With the simple eigenvectors we desire in the end here, it is easiest to think of this particular problem backwards, constructing $\hat{U}^\dagger$, which is the matrix that turns the $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$ vectors into the $\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -i \end{bmatrix}$ and $\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ i \end{bmatrix}$ vectors, respectively. That matrix simply has the vectors $\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -i \end{bmatrix}$ and $\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ i \end{bmatrix}$ as its columns, that is,

$$U^\dagger = \left(\frac{1}{\sqrt{2}}\right)\begin{bmatrix} 1 & 1 \\ -i & i \end{bmatrix}$$

It is easily verified that, for example,

$$\hat{U}^\dagger\begin{bmatrix} 1 \\ 0 \end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -i \end{bmatrix}$$

The Hermitian adjoint of this matrix is then the one that will transform the "old" eigenvectors into the new basis (and in general transforms from the old basis to the new one), that is,

$$\hat{U} = \left(\hat{U}^\dagger\right)^\dagger = \begin{bmatrix} 1 & i \\ 1 & -i \end{bmatrix}$$

(iii) With our unitary matrices

$$U = \left(\frac{1}{\sqrt{2}}\right)\begin{bmatrix} 1 & i \\ 1 & -i \end{bmatrix} \text{ and } U^\dagger = \left(\frac{1}{\sqrt{2}}\right)\begin{bmatrix} 1 & 1 \\ -i & i \end{bmatrix}$$

we can now formally transform our operator $\hat{M}$, obtaining

$$\hat{M}_{new} = \hat{U}\hat{M}_{old}\hat{U}^\dagger = \left(\frac{1}{\sqrt{2}}\right)\begin{bmatrix} 1 & i \\ 1 & -i \end{bmatrix}\begin{bmatrix} 0 & i \\ -i & 0 \end{bmatrix}\left(\frac{1}{\sqrt{2}}\right)\begin{bmatrix} 1 & 1 \\ -i & i \end{bmatrix}$$

$$= \frac{1}{2}\begin{bmatrix} 1 & i \\ 1 & -i \end{bmatrix}\begin{bmatrix} 1 & -1 \\ -i & -i \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 2 & 0 \\ 0 & -2 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Hence, as desired, we have diagonalized this matrix by transforming it to the basis corresponding to its eigenvectors.

Just to see what the matrix itself would be on its eigenvector basis is actually trivial, because on that basis a matrix will always just have its eigenvalues on the leading diagonal and all other entries zero.

4.10.2

We will call the old axes $|\psi_1\rangle$ and $|\psi_2\rangle$ and the new axes $|\phi_1\rangle$ and $|\phi_2\rangle$, respectively. Plotting these two axes on a diagram gives the following figure.
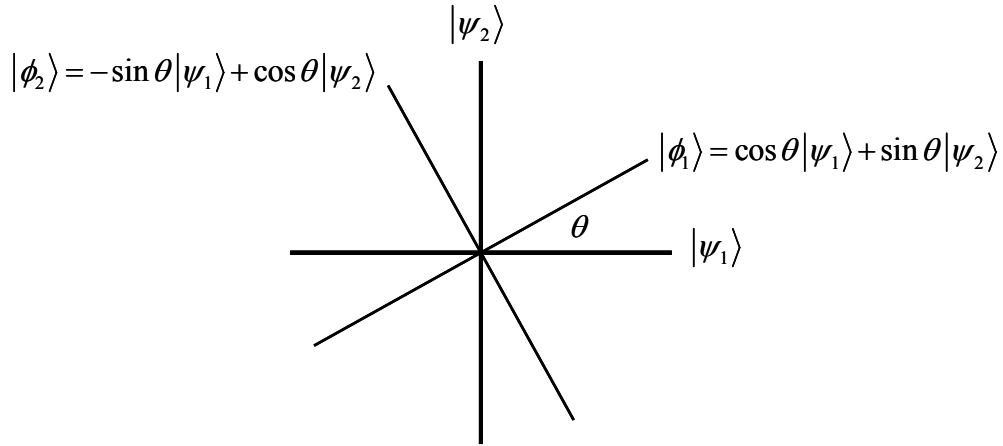
On this figure we have marked the forms for $|\phi_1\rangle$ and $|\phi_2\rangle$ in terms of $|\psi_1\rangle$ and $|\psi_2\rangle$ that we can deduce from simple geometry. From these forms, we can deduce

$$\langle\psi_1|\phi_1\rangle = \cos\theta$$
$$\langle\psi_2|\phi_1\rangle = \sin\theta$$
$$\langle\psi_1|\phi_2\rangle = -\sin\theta$$
$$\langle\psi_2|\phi_2\rangle = \cos\theta$$

All of these quantities happen to be real, so we have $\langle\psi_1|\phi_1\rangle = \langle\phi_1|\psi_1\rangle$ and similarly for the other matrix elements. So we have for the unitary matrix to transform a vector from the "old" $|\psi_1\rangle$ and $|\psi_2\rangle$ basis to the "new" basis $|\phi_1\rangle$ and $|\phi_2\rangle$

$$\hat{U} = \begin{bmatrix} \langle\phi_1|\psi_1\rangle & \langle\phi_1|\psi_2\rangle \\ \langle\phi_2|\psi_1\rangle & \langle\phi_2|\psi_2\rangle \end{bmatrix} = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix}$$

4.10.3

(i) Note that these new basis functions are just the equal sum and difference of our original basis functions. Hence we have

(4.24, 1.63)
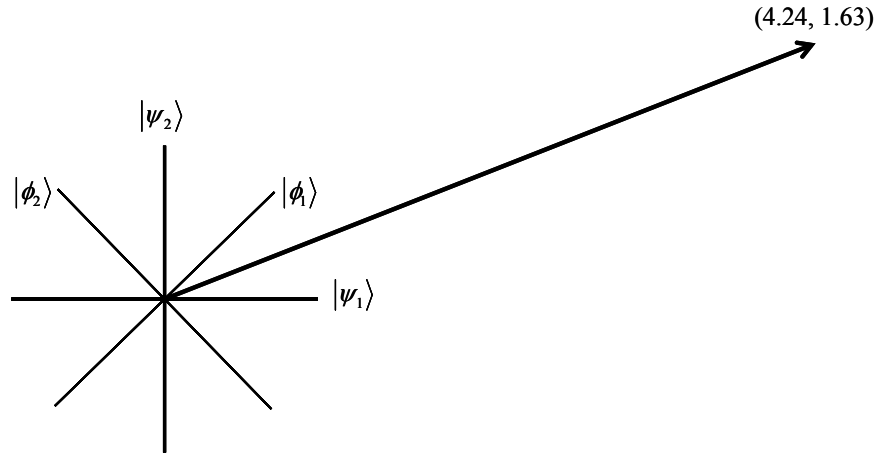
(ii) Represent ψ_1 as $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and ψ_2 as $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$. Then the matrix that transforms from one basis to another is

$$\left(\frac{1}{\sqrt{2}}\right)\begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} = \begin{bmatrix} \dfrac{1}{\sqrt{2}} & \dfrac{1}{\sqrt{2}} \\ -\dfrac{1}{\sqrt{2}} & \dfrac{1}{\sqrt{2}} \end{bmatrix}$$

(iii)

$$\left(\frac{1}{\sqrt{2}}\right)\begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}^{\dagger} = \left(\frac{1}{\sqrt{2}}\right)\begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}$$

So

$$\left(\frac{1}{\sqrt{2}}\right)\begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}^{\dagger}\left(\frac{1}{\sqrt{2}}\right)\begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} = \hat{I}$$

and hence the matrix is unitary.

(iv) In the old basis, the function can be represented as $\begin{bmatrix} 3\sqrt{2} \\ 2\sqrt{\dfrac{2}{3}} \end{bmatrix}$. It is trivial to convert this into the

new basis. All we do is multiply by the matrix above.

$$\begin{bmatrix} d_1 \\ d_2 \end{bmatrix} = \left(\frac{1}{\sqrt{2}}\right)\begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}\begin{bmatrix} 3\sqrt{2} \\ 2\sqrt{\dfrac{2}{3}} \end{bmatrix} = \begin{bmatrix} 3 + \dfrac{2}{\sqrt{3}} \\ -3 + \dfrac{2}{\sqrt{3}} \end{bmatrix}$$

(v) The resulting vector will be in the same place as the original vector (shown in the figure with coordinates relative the original axes), even if now expressed using different basis functions.

4.10.4

(i) To find the eigenvalues note that $\hat{A}x = \lambda x \implies (\hat{A} - \lambda \hat{I})x = 0$ for an arbitrary x.

For this to be true for arbitrary x, the matrix $(\hat{A} - \lambda \hat{I})$ should not be invertible, i.e. its determinant should be zero. This condition gives us a characteristic polynomial in λ whose solutions are the eigenvalues.

In this case,

$$\det\left(\hat{\sigma}_z - \lambda \hat{I}\right) = \det\begin{bmatrix} 1-\lambda & 0 \\ 0 & -1-\lambda \end{bmatrix} = \lambda^2 - 1 = 0$$

$$\implies \lambda = \pm 1$$

The eigenvectors can be found by using

$$\hat{\sigma}_z \left| \psi_1 \right\rangle = \lambda_1 \left| \psi_1 \right\rangle$$

i.e.,

$$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = 1\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \implies x_1 = x_1 \quad \text{and} \quad -x_2 = x_2 \implies x_2 = 0 \quad \text{and} \quad x_1 = c$$

where c is any complex constant, which we will choose to be 1 here. Note that an eigenfunction is defined only up to some constant factor, i.e., some constant times an eigenfunction is still the same eigenfunction, so this factor is arbitrary.

To find the second eigenfunction we use the same procedure with the second eigenvalue

$$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = -1\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \implies x_1 = -x_1 \quad \text{and} \quad x_2 = x_2 \implies x_1 = 0 \quad \text{and} \quad x_2 = c$$

where c is any complex constant, which we will choose to be 1 here. The above illustrates the procedure for calculating eigenvalues and functions by hand. We obtained the simple result in this case

$$\lambda_1 = 1, \quad \lambda_2 = -1, \quad \psi_{z1} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \psi_{z2} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

(ii) To find the eigenvalues

$$\det\left(\hat{\sigma}_z - \lambda \hat{I}\right) = \det\begin{bmatrix} -\lambda & 1 \\ 1 & -\lambda \end{bmatrix} = \lambda^2 - 1 = 0 \implies \lambda = \pm 1$$

To find the eigenvectors

$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = 1\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \implies x_2 = x_1 \quad \text{and} \quad x_2 = x_1 \implies x_2 = x_1 = c = 1$$

and

$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = -1\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \Rightarrow x_2 = -x_1 \quad \text{and} \quad x_2 = -x_1 \Rightarrow -x_2 = x_1 = c = 1$$

To normalize the eigenfunctions, we need a factor of $\dfrac{1}{\sqrt{2}}$

$$\lambda_1 = 1, \quad \lambda_2 = -1, \quad \psi_{x1} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad \psi_{x2} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

(iii)

$$\sum_i |\psi_{xi}\rangle\langle\psi_{xi}| = \frac{1}{2}\begin{bmatrix} 1 \\ 1 \end{bmatrix}\begin{bmatrix} 1 & 1 \end{bmatrix} + \frac{1}{2}\begin{bmatrix} 1 \\ -1 \end{bmatrix}\begin{bmatrix} 1 & -1 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} + \frac{1}{2}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \hat{I}$$

(iv) We know we can write the matrix for an operator in the x eigenbasis in the following way

$$\hat{A} \equiv \begin{bmatrix} \langle\psi_{x1}|\hat{A}|\psi_{x1}\rangle & \langle\psi_{x1}|\hat{A}|\psi_{x2}\rangle \\ \langle\psi_{x2}|\hat{A}|\psi_1\rangle & \langle\psi_{x2}|\hat{A}|\psi_{x2}\rangle \end{bmatrix}$$

We already know $\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z$ in the z basis. Hence to express any operator in the x basis all we would need to know are $|\psi_{x1}\rangle$ and $|\psi_{x2}\rangle$ in the z basis – which we have from part (ii) above.

Thus in the x eigenbasis, writing $\hat{\sigma}_x = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$, we have

$$A_{11} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \end{bmatrix}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix} = 1 \qquad A_{12} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \end{bmatrix}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix} = 0$$

$$A_{21} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & -1 \end{bmatrix}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix} = 0 \qquad A_{22} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & -1 \end{bmatrix}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix} = -1$$

so $\hat{\sigma}_x = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$

Similarly, writing $\hat{\sigma}_y = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$, we have

$$A_{11} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \end{bmatrix}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix} = 0 \qquad A_{12} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \end{bmatrix}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix} = i$$

$$A_{21} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & -1 \end{bmatrix}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix} = -i \qquad A_{22} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & -1 \end{bmatrix}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix} = 0$$

so $\hat{\sigma}_y = \begin{bmatrix} 0 & i \\ -i & 0 \end{bmatrix}$

Similarly, writing $\hat{\sigma}_z = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$, where

$$A_{11} = \frac{1}{\sqrt{2}}[1 \quad 1]\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix} = 0 \qquad A_{12} = \frac{1}{\sqrt{2}}[1 \quad 1]\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix} = 1$$

$$A_{21} = \frac{1}{\sqrt{2}}[1 \quad -1]\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix} = 1 \qquad A_{22} = \frac{1}{\sqrt{2}}[1 \quad -1]\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix} = 0$$

so $\hat{\sigma}_z = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$

So in the x eigenbasis the Pauli matrices are

$$\hat{\sigma}_x = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad \hat{\sigma}_y = \begin{bmatrix} 0 & i \\ -i & 0 \end{bmatrix}, \quad \hat{\sigma}_z = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

4.10.5

With the definition of $\hat{W}$, then we have

$$\hat{W}^\dagger = \sum_{p,q} \left(a_{pq} |\phi_p\rangle\langle\psi_q| \right)^\dagger = \sum_{p,q} a_{pq}^* |\psi_q\rangle\langle\phi_p|$$

So

$$\hat{W}^\dagger\hat{W} = \sum_{i,j,p,q} a_{pq}^* a_{ij} |\psi_q\rangle\langle\phi_p|\phi_i\rangle\langle\psi_j| = \sum_{i,j,q} a_{iq}^* a_{ij} |\psi_q\rangle\langle\psi_j|$$

Hence, if $\sum_i a_{iq}^* a_{ij} = \delta_{qj}$, then

$$\hat{W}^\dagger\hat{W} = \sum_{j,q} \delta_{qj} |\psi_q\rangle\langle\psi_j| = \sum_{j} |\psi_j\rangle\langle\psi_j| = \hat{I}$$

and so $\hat{W}$ is unitary.

4.10.6

We know that

$$\exp\left[-\frac{i\hat{H}t}{\hbar}\right] \equiv \left[1 + \left(-\frac{i\hat{H}t}{\hbar}\right) + \frac{1}{2!}\left(-\frac{i\hat{H}t}{\hbar}\right)^2 + \ldots\right]$$

The right hand side is a sum of matrices. Now we take the Hermitian adjoint of the entire sum, which is the same as taking it term by term because the Hermitian adjoint of the sum is just a sum of the Hermitian adjoints.

Also note that $\left(\hat{H}^n\right)^\dagger = \left(\hat{H}^\dagger\right)^n$, which we can prove using the relation $\left(AB\right)^\dagger = B^\dagger A^\dagger$. So we have

$$\left[\exp\left[-\frac{i\hat{H}t}{\hbar}\right]\right]^\dagger = \left[1 + \left(\frac{i\hat{H}^\dagger t}{\hbar}\right) + \frac{1}{2!}\left(\frac{i\hat{H}^\dagger t}{\hbar}\right)^2 + \ldots\right] = \exp\left[\frac{i\hat{H}^\dagger t}{\hbar}\right]$$

Since we know that H is Hermitian, $H^\dagger = H$ and so

$$\left[\exp\left[-\frac{i\hat{H}t}{\hbar}\right]\right]^\dagger = \exp\left[\frac{i\hat{H}t}{\hbar}\right]$$

$$\exp\left[-\frac{i\hat{H}t}{\hbar}\right] \times \left[\exp\left[-\frac{i\hat{H}t}{\hbar}\right]\right]^\dagger = \exp\left[-\frac{i\hat{H}t}{\hbar}\right] \times \exp\left[\frac{i\hat{H}t}{\hbar}\right] = \exp\left[\frac{i\hat{H}t}{\hbar} - \frac{i\hat{H}t}{\hbar}\right] = \exp[0] = I$$

which is the identity matrix. (The "0" in exp[0] is technically the zero operator.) Hence the time-evolution operator is unitary.

4.11.1

Remember the definitions of unitary and Hermitian. Unitary means that a matrix multiplied by its adjoint will equal the identity matrix. Hermitian means that a matrix equals its adjoint.

Number	Matrix	Unitary?	Hermitian?
(i)	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	YES	YES
(ii)	$\begin{bmatrix} 1 & i \\ -i & 1 \end{bmatrix}$	NO	YES
(iii)	$\begin{bmatrix} i & 0 \\ 0 & i \end{bmatrix}$	YES	NO
(iv)	$\begin{bmatrix} 0 & 1 \\ i & 0 \end{bmatrix}$	YES	NO

4.11.2

$$\left(AB\right)_{ij} = ij^{th} \text{ element of } AB = \sum_n A_{in} B_{nj}$$

$$\left(AB\right)_{ij}^{\dagger} = \left[\left(AB\right)_{ji}\right]^{*} = \sum_n A_{jn}^{*} B_{ni}^{*} = \sum_n B_{ni}^{*} A_{jn}^{*} = \sum_n \left(B^{\dagger}\right)_{in} \left(A^{\dagger}\right)_{nj} = \left(B^{\dagger} A^{\dagger}\right)_{ij}$$

Hence, since the elements of these matrices $\left(AB\right)^{\dagger}$ and $B^{\dagger} A^{\dagger}$ are identical, then by definition these two matrices are identical.

4.11.3

(i).

$$p_x = -i\hbar \frac{\partial}{\partial x}$$

$$p_{ij} = \langle \psi_i | \hat{p} | \psi_j \rangle = \int\limits_{-\infty}^{\infty} \psi_i^* p \psi_j dx = \int\limits_{-\infty}^{\infty} \psi_i^* \left(-i\hbar \frac{\partial}{\partial x} \right) \psi_j dx$$

$$= -i\hbar \int\limits_{-\infty}^{\infty} \psi_i^* \frac{\partial \psi_j}{\partial x} dx = -i\hbar \left[\psi_i^* \psi_j |_{-\infty}^{\infty} - \int\limits_{-\infty}^{\infty} \psi_j \frac{\partial \psi_i^*}{\partial x} dx \right]$$

$$= i\hbar \int\limits_{-\infty}^{\infty} \psi_j \frac{\partial \psi_i^*}{\partial x} dx = \int\limits_{-\infty}^{\infty} \psi_j \left(i\hbar \frac{\partial}{\partial x} \right) \psi_i^* dx$$

$$= \left(\int\limits_{-\infty}^{\infty} \psi_j^* \left(-i\hbar \frac{\partial}{\partial x} \right) \psi_i \, dx \right)^* = p_{ji}^*$$

(ii) The operator $\frac{d}{dx}$ is NOT Hermitian. This is exactly the same argument as in part (i) except a that we are left with an extra minus sign. Explicitly

$$\int\limits_{-\infty}^{\infty} \psi_i^* \left(\frac{\partial}{\partial x} \right) \psi_j dx = \int\limits_{-\infty}^{\infty} \psi_i^* \frac{\partial \psi_j}{\partial x} dx = \left[\psi_i^* \psi_j |_{-\infty}^{\infty} - \int\limits_{-\infty}^{\infty} \psi_j \frac{\partial \psi_i^*}{\partial x} dx \right] = -\int\limits_{-\infty}^{\infty} \psi_j \frac{\partial \psi_i^*}{\partial x} dx = \int\limits_{-\infty}^{\infty} \psi_j \left(-\frac{\partial}{\partial x} \right) \psi_i^* dx$$

$$= \left(\int\limits_{-\infty}^{\infty} \psi_j^* \left(-\frac{\partial}{\partial x} \right) \psi_i \, dx \right)^*$$

(iii) The operator $\frac{d^2}{dx^2}$ is Hermitian. Integrating by parts twice gives us the answer. This time there are two minus signs that cancel out (since there are two integrations by parts) and the operator is real.

$$\int\limits_{-\infty}^{\infty} \psi_i^* \left(\frac{\partial^2}{\partial x^2} \right) \psi_j dx = \int\limits_{-\infty}^{\infty} \psi_i^* \frac{\partial^2 \psi_j}{\partial x^2} dx = \left[\psi_i^* \frac{\partial \psi_j}{\partial x} \Big|_{-\infty}^{\infty} - \int\limits_{-\infty}^{\infty} \frac{\partial \psi_j}{\partial x} \frac{\partial \psi_i^*}{\partial x} dx \right]$$

$$= -\int\limits_{-\infty}^{\infty} \frac{\partial \psi_j}{\partial x} \frac{\partial \psi_i^*}{\partial x} dx = -\left[\frac{\partial \psi_i^*}{\partial x} \psi_j \Big|_{-\infty}^{\infty} - \int\limits_{-\infty}^{\infty} \psi_j \frac{\partial^2 \psi_i^*}{\partial x^2} dx \right]$$

$$= \int\limits_{-\infty}^{\infty} \psi_j \left(\frac{\partial^2}{\partial x^2} \right) \psi_i^* dx = \left(\int\limits_{-\infty}^{\infty} \psi_j \left(\frac{\partial^2}{\partial x^2} \right) \psi_i^* dx \right)^*$$

(iv) The Hamiltonian operator (if $V(x)$ is real) is Hermitian. We can consider the terms separately by linearity. The derivative term is Hermitian because we just proved that in part (iii). The potential term is Hermitian because it is a real-valued function

$$V_{ij} = \int\limits_{-\infty}^{\infty} \psi_i^* V \psi_j dx = \left(\int\limits_{-\infty}^{\infty} \psi_i V^* \psi_j^* dx \right)^* = \left(\int\limits_{-\infty}^{\infty} \psi_i V \psi_j^* dx \right)^*$$

$$= \left(\int\limits_{-\infty}^{\infty} \psi_j^* V \psi_i \, dx \right)^* = V_{ji}^*$$

4.11.4

Let $\hat{A}$ be a Hermitian operator. Then $\hat{A} = \hat{A}^\dagger$ by definition. Let $\hat{B} = \hat{U}^\dagger \hat{A} \hat{U}$ be the operator transformed by the unitary operator $\hat{U}$. Formally evaluating the Hermitian adjoint of $\hat{B}$

$$\hat{B}^\dagger = \left(\hat{U}^\dagger \hat{A} \hat{U} \right)^\dagger = \left(\hat{U} \right)^\dagger \left(\hat{A} \right)^\dagger \left(\hat{U}^\dagger \right)^\dagger = \hat{U}^\dagger \hat{A}^\dagger \hat{U} = \hat{U}^\dagger \hat{A} \hat{U} = \hat{B}$$

Hence the transformed operator is still Hermitian.

4.11.5

Suppose the operator $\hat{A}$ has eigenfunctions $|\psi_n\rangle$ with corresponding eigenvalues α_n. Consider any state ψ expanded in these eigenfunctions

$$|\psi\rangle = \sum c_n |\psi_n\rangle$$

Then we have

$$\hat{A}|\psi\rangle = \sum c_n \hat{A}|\psi_n\rangle = \sum c_n \alpha_n |\psi_n\rangle$$

Note that this is the same as letting the operator have the assumed form

$$\hat{A} = \sum_i \alpha_i |\psi_i\rangle\langle\psi_i|$$

which we can check by showing that the result of operating with the operator in this form on our arbitrary state ψ

$$\hat{A}|\psi\rangle = \left(\sum_i \alpha_i |\psi_i\rangle\langle\psi_i|\right)\left(\sum_n c_n |\psi_n\rangle\right) = \sum_{i,n} \alpha_i c_n |\psi_i\rangle\langle\psi_i|\psi_n\rangle$$

$$\hat{A}|\psi\rangle = \sum_{i,n} \alpha_i c_n |\psi_i\rangle\delta_{in} = \sum_n \alpha_n c_n |\psi_n\rangle$$

As for the inverse of the operator $\hat{A}$, we can see that, since $\hat{A}$ is now a diagonal operator in this representation, the diagonal operator with the reciprocals of the eigenvalues of $\hat{A}$ as its diagonal elements will be the inverse, that is

$$\hat{A}^{-1} = \sum_i (\alpha_i)^{-1} |\psi_i\rangle\langle\psi_i|$$

We can confirm that this is, in fact, the inverse of A

$$\hat{A}^{-1}\hat{A} = \left(\sum_i (\alpha_i)^{-1} |\psi_i\rangle\langle\psi_i|\right)\left(\sum_j \alpha_j |\psi_j\rangle\langle\psi_j|\right)$$

$$\hat{A}^{-1}\hat{A} = \sum_{i,j} (\alpha_i)^{-1} \alpha_j |\psi_i\rangle\langle\psi_i|\psi_j\rangle\langle\psi_j|$$

$$\hat{A}^{-1}\hat{A} = \sum_{i,j} (\alpha_i)^{-1} \alpha_j |\psi_i\rangle\delta_{ij}\langle\psi_j| = \sum_i (\alpha_i)^{-1} \alpha_i |\psi_i\rangle\langle\psi_i|$$

$$\hat{A}^{-1}\hat{A} = \sum_i |\psi_i\rangle\langle\psi_i| = \hat{I}$$

4.11.6

In its eigenfunction basis, an operator is written as

$$\hat{A} = \sum_i \alpha_i |\psi_i\rangle\langle\psi_i|$$

where the α_i are the eigenvalues, so the trace of this operator, i.e., the sum of the diagonal elements, is, when evaluated in the eigenfunction basis,

$$Tr\left(\hat{A}\right) = \sum_j \langle\psi_j|\hat{A}|\psi_j\rangle = \sum_j \langle\psi_j|\left(\sum_i \alpha_i |\psi_i\rangle\langle\psi_i|\right)|\psi_j\rangle = \sum_j \alpha_j$$

i.e., the sum of the eigenvalues. But the trace is independent of the representation (as proved in the book), and is always equal to the sum of the diagonal elements in any representation, so the sum of the diagonal elements of an operator is always equal to the sum of the eigenvalues of the operator.

4.11.7

We want to show that

$$\int g^*(x)\hat{M}f(x)dx = \int \left\{\hat{M}g(x)\right\}^* f(x)\, dx$$

where in the integral form we are only allowed to have the operator operating to the right.

We expand on the given basis, that is,

$$g(x) = \sum_i g_i \left|\psi_i\right\rangle$$

and

$$f(x) = \sum_j f_j \left|\psi_j\right\rangle$$

Then

$$\int g^*(x)\hat{M}f(x)dx = \sum_{i,j} g_i^* f_j \int \psi_i^*(x)\hat{M}\psi_j(x)\, dx$$

$$= \sum_{i,j} g_i^* f_j M_{ij} = \sum_{i,j} g_i^* f_j M_{ji}^*$$

$$= \sum_{i,j} g_i^* f_j \left[\int \psi_j^*(x)\hat{M}\psi_i(x)\, dx\right]^*$$

$$= \sum_{i,j} g_i^* f_j \int \left\{\hat{M}\psi_i(x)\right\}^* \psi_j(x)\, dx$$

$$= \int \left\{\hat{M}\sum_i g_i\psi_i(x)\right\}^* \sum_j f_j\psi_j(x)\, dx$$

$$= \int \left\{\hat{M}g(x)\right\}^* f(x)\, dx$$

as required.

4.11.8

For any operator $\hat{M}$, we would have

$$\left(\langle f|\hat{M}|f\rangle\right)^{*} \equiv \left(\langle f|\hat{M}|f\rangle\right)^{\dagger} = \left(\hat{M}|f\rangle\right)^{\dagger}\left(\langle f|\right)^{\dagger} = \langle f|\hat{M}^{\dagger}|f\rangle$$

But $\hat{M}$ is Hermitian, so

$$\langle f|\hat{M}^{\dagger}|f\rangle = \langle f|\hat{M}|f\rangle$$

Hence, we have proved that

$$\left(\langle f|\hat{M}|f\rangle\right)^{*} = \langle f|\hat{M}|f\rangle$$

If a quantity is equal to its own complex conjugate, it must be real. Hence $\langle f|\hat{M}|f\rangle$ is real for any Hermitian operator $\hat{M}$.

4.12.1

By looking at the formula and remembering that the column vector for the function f looks like

$$|f\rangle = \begin{bmatrix} \vdots \\ f(x-\delta x) \\ f(x) \\ f(x+\delta x) \\ \vdots \end{bmatrix}$$

then the matrix for the second derivative must be the following

$$\frac{d^2}{dx^2} = \frac{1}{(\delta x)^2} \begin{bmatrix} \ddots & 1 & 0 & 0 & \iddots \\ 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ \iddots & 0 & 0 & 1 & \ddots \end{bmatrix}$$

Checking that this works, we have

$$\frac{d^2}{dx^2}|f\rangle = \frac{1}{(\delta x)^2} \begin{bmatrix} \ddots & 1 & 0 & 0 & \iddots \\ 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ \iddots & 0 & 0 & 1 & \ddots \end{bmatrix} \begin{bmatrix} \vdots \\ f(x-\delta x) \\ f(x) \\ f(x+\delta x) \\ \vdots \end{bmatrix}$$

$$\frac{d^2}{dx^2}|f\rangle = \frac{1}{(\delta x)^2} \begin{bmatrix} \vdots \\ f(x-\delta x) - 2f(x) + f(x+\delta x) \\ \vdots \end{bmatrix}$$

which is the correct form (as $\delta x \to 0$) for the second derivative.

Chapter 5 problem solutions

5.1.1

$$\left[\hat{\sigma}_x, \hat{\sigma}_y\right] = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} - \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix} - \begin{bmatrix} -i & 0 \\ 0 & i \end{bmatrix} = 2i\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = 2i\hat{\sigma}_z$$

$$\left[\hat{\sigma}_y, \hat{\sigma}_z\right] = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} - \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & i \\ i & 0 \end{bmatrix} - \begin{bmatrix} 0 & -i \\ -i & 0 \end{bmatrix} = 2i\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = 2i\hat{\sigma}_x$$

$$\left[\hat{\sigma}_z, \hat{\sigma}_x\right] = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} - \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} - \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} = 2\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} = 2i\hat{\sigma}_y$$

5.1.2

We consider two Hermitian operators; that is

$$A = A^\dagger, B = B^\dagger$$

Now let us consider the operator formed from the product of these two, namely AB. The Hermitian adjoint of this operator is

$$(AB)^\dagger = B^\dagger A^\dagger = BA$$

The operator AB can only be Hermitian if it equals its adjoint. But from the above algebra we see that its adjoint equals BA. Therefore, it can only be Hermitian if $AB = BA$, which means they commute.

5.1.3

Remembering that $\hat{A}$ and $\hat{B}$ are Hermitian. We write the commutator of $\hat{A}$ and $\hat{B}$ formally as

$$\left[\hat{A}, \hat{B}\right] = \hat{C}$$

for some operator $\hat{C}$. Then

$$\hat{C}^\dagger = \left(\left[\hat{A}, \hat{B}\right]\right)^\dagger = \left(\hat{A}\hat{B} - \hat{B}\hat{A}\right)^\dagger = \left(\hat{A}\hat{B}\right)^\dagger - \left(\hat{B}\hat{A}\right)^\dagger$$

$$= \hat{B}^\dagger\hat{A}^\dagger - \hat{A}^\dagger\hat{B}^\dagger = \hat{B}\hat{A} - \hat{A}\hat{B} = -\left[\hat{A}, \hat{B}\right] = -\hat{C}$$

Any such operator $\hat{C}$ is therefore not Hermitian, since its Hermitian adjoint is the negative of itself, which can only be true if $\hat{C}$ is the zero operator.

5.2.1

We are given that $\partial \hat{A}/\partial t = 0$, and we know that the expectation value of $\hat{A}$ is given by $\langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle$. Consider the time derivative of the expectation value, which is

$$\frac{\partial}{\partial t} \langle \hat{A} \rangle = \left(\frac{\partial}{\partial t} \langle \psi | \right) \hat{A} | \psi \rangle + \langle \psi | \frac{\partial \hat{A}}{\partial t} | \psi \rangle + \langle \psi | \hat{A} \left(\frac{\partial}{\partial t} | \psi \rangle \right)$$

$$= \left(\left\langle \frac{\partial \psi}{\partial t} \right| \right) \hat{A} | \psi \rangle + \langle \psi | \hat{A} \left(\frac{\partial}{\partial t} | \psi \rangle \right)$$

since $\partial \hat{A}/\partial t = 0$. Also we know from the general form of Schrödinger's equation that

$$\hat{H} \equiv i\hbar \frac{\partial}{\partial t}$$

which implies that

$$\frac{\partial}{\partial t} = \frac{1}{i\hbar} \hat{H}$$

So

$$\langle \psi | A \left(\frac{\partial}{\partial t} | \psi \rangle \right) = \langle \psi | \frac{1}{i\hbar} \hat{A} \hat{H} | \psi \rangle$$

and

$$\left(\left\langle \frac{\partial \psi}{\partial t} \right| \right) \hat{A} | \psi \rangle = \left\langle \frac{1}{i\hbar} \hat{H} \psi \middle| \hat{A} | \psi \rangle = \langle \psi | \left(\frac{1}{i\hbar} \hat{H} \right)^{\dagger} \hat{A} | \psi \rangle = -\langle \psi | \frac{1}{i\hbar} \hat{H}^{\dagger} \hat{A} | \psi \rangle$$

Now using the fact that $\hat{H}$ is Hermitian and $\hat{A}$ and $\hat{H}$ commute

$$\left(\left\langle \frac{\partial \psi}{\partial t} \right| \right) \hat{A} | \psi \rangle = -\langle \psi | \frac{1}{i\hbar} \hat{H} \hat{A} | \psi \rangle = -\langle \psi | \hat{A} \left(\frac{\partial}{\partial t} | \psi \rangle \right)$$

Hence $\partial \langle \hat{A} \rangle / \partial t = 0$

5.2.2

Noting that $\langle f | \hat{A} | f \rangle = \overline{A}$, where $\overline{A}$ is a real number because $\hat{A}$ is a Hermitian operator, and that, because it is a number, $\overline{A}$ can be moved about in multiplicative expressions,

$$\langle f | \left(\hat{A} - \overline{A} \right)^2 | f \rangle = \langle f | \hat{A}^2 + \overline{A}^2 - 2\overline{A}\hat{A} | f \rangle = \langle f | \hat{A}^2 + \overline{A}^2 - 2\overline{A}^2 | f \rangle = \langle f | \hat{A}^2 - \overline{A}^2 | f \rangle$$

5.2.3

(i) Remember that $x, y, z, \hat{p}_x, \hat{p}_y,$ and $\hat{p}_z$ are all Hermitian. It is also important to note that $[x, \hat{p}_x] = i\hbar$, but that $[y, \hat{p}_x] = [z, \hat{p}_x] = [y, \hat{p}_z] = 0$, and so on. So

$$\hat{L}_x^\dagger = (y\hat{p}_z - z\hat{p}_y)^\dagger = (y\hat{p}_z)^\dagger - (z\hat{p}_y)^\dagger = \hat{p}_z^\dagger y^\dagger - \hat{p}_y^\dagger z^\dagger$$
$$= \hat{p}_z y - \hat{p}_y z = y\hat{p}_z - z\hat{p}_y = \hat{L}_x$$

(ii) We know that

$$\left[\hat{A}, \hat{B}\right] = i\hat{C} \Rightarrow (\Delta A)^2 (\Delta B)^2 \geq \frac{(<C>)^2}{4}$$

So the problem is reduced to finding the commutator of $\hat{L}_x$ and $\hat{L}_y$. The rest is just algebra, using the commutators defined above in part (i).

$$\left[\hat{L}_x, \hat{L}_y\right] = \hat{L}_x\hat{L}_y - \hat{L}_y\hat{L}_x = (y\hat{p}_z - z\hat{p}_y)(z\hat{p}_x - x\hat{p}_z) - (z\hat{p}_x - x\hat{p}_z)(y\hat{p}_z - z\hat{p}_y)$$
$$= (y\hat{p}_z z\hat{p}_x - y\hat{p}_z x\hat{p}_z - z\hat{p}_y z\hat{p}_x + z\hat{p}_y x\hat{p}_z) - (z\hat{p}_x y\hat{p}_z - z\hat{p}_x z\hat{p}_y - x\hat{p}_z y\hat{p}_z + x\hat{p}_z z\hat{p}_y)$$
$$= y\hat{p}_z z\hat{p}_x + z\hat{p}_y x\hat{p}_z - z\hat{p}_x y\hat{p}_z - x\hat{p}_z z\hat{p}_y$$
$$= \left((y\hat{p}_x - x\hat{p}_y)(\hat{p}_z z) + (\hat{p}_y x - \hat{p}_x y)(z\hat{p}_z)\right)$$
$$= \left((y\hat{p}_x - x\hat{p}_y)(\hat{p}_z z) + (\hat{p}_y x - \hat{p}_x y)(i\hbar + \hat{p}_z z)\right) = i\hbar(\hat{p}_y x - \hat{p}_x y)$$
$$= i\hbar\hat{L}_z$$

$$\Rightarrow (\Delta L_x)^2 (\Delta L_y)^2 \geq \frac{\hbar^2}{4}(\langle L_z\rangle)^2$$

5.4.1

For the operator $\hat{U}$ to be unitary, we require that the Hermitian adjoint is the inverse, which will be the case if

$$\hat{U}^{\dagger}\hat{U}|f\rangle = |f\rangle$$

for an arbitrary function $|f\rangle \equiv f(z)$. For the given operator and its adjoint, we have

$$\hat{U}^{\dagger}\hat{U}|f\rangle = \frac{1}{2\pi}\int \exp(ikz')\int \exp(-ikz) f(z) dz dk$$

$$= \frac{1}{2\pi}\iint \exp\left[-ik(z-z')\right] dk \, f(z) dz$$

$$= \int \delta(z'-z) f(z)$$

$$= f(z')$$

$$= |f\rangle$$

Note incidentally in the above argument that we do need two different z variables (z and z'). We integrate over the first argument, z, in operating on $|f\rangle$ with $\hat{U}$ as we change from a z representation to a k representation. Then we integrate over k as we operate with $\hat{U}^{\dagger}$ to change from a k representation back to a z representation, in terms of a formally different variable z'. What we call the variable that indexes the different elements of the vector $|f\rangle$ does not matter – all that matters is the sequence and values of the elements in the vector – so the vector $|f\rangle$ is the same whether the variable indexing the values is called z or z', or anything else. The net result of this combined operation $\hat{U}^{\dagger}\hat{U}$ on the vector $|f\rangle$ is to give us the same vector we started with.

We can repeat an exactly similar argument for $\hat{U}\hat{U}^{\dagger}|h\rangle = |h\rangle$ for an arbitrary function $|h\rangle \equiv h(k)$, and hence we can formally prove that $\hat{U}^{\dagger}$ is the inverse of $\hat{U}$, and vice versa. Hence $\hat{U}$ is unitary.

5.4.2

Consider first the commutator $[\hat{z}, \hat{p}_z]$ operating on an arbitrary function $|f\rangle$ in the position representation. We have

$$[\hat{z}, \hat{p}_z]|f\rangle = -i\hbar z \frac{\partial f(z)}{\partial z} + i\hbar \frac{\partial}{\partial z}\{zf(z)\}$$

$$= -i\hbar z \frac{\partial f(z)}{\partial z} + i\hbar z \frac{\partial f(z)}{\partial z} + i\hbar f(z)\frac{\partial z}{\partial z}$$

$$= i\hbar|f\rangle$$

and so we can state

$$[\hat{z}, \hat{p}_z] = i\hbar$$

Now consider the comparable result in the momentum representation for some arbitrary function $|g\rangle$ in the momentum representation, where we note that the value of the momentum is $p_z = \hbar k$ and that the position operator is

$$\hat{z} = i \frac{\partial}{\partial k}$$

We have

$$[\hat{z}, \hat{p}_z]|g\rangle = i\hbar \frac{\partial}{\partial k}\{kg(k)\} - i\hbar k \frac{\partial g(k)}{\partial k}$$

$$= i\hbar k \frac{\partial g(k)}{\partial k} + i\hbar g(k)\frac{\partial k}{\partial k} - i\hbar k \frac{\partial g(k)}{\partial k}$$

$$= i\hbar|g\rangle$$

and hence in this representation we obtain the identical result $[\hat{z}, \hat{p}_z] = i\hbar$.

5.4.3

We follow similar algebra to that used to change the position operator from the position representation to the momentum representation, but starting with z momentum operator $\hat{p}_{zold} = (-i\hbar)(\partial/\partial z)$ as the momentum operator in the "old" (i.e., position) representation. We operate with this momentum operator, formally transformed by the unitary transformation between the coordinate systems, on an arbitrary function $|f\rangle$ in the momentum representation

$$
\begin{aligned}
\hat{p}_{znew}|f\rangle &= \hat{U}\hat{p}_{zold}\hat{U}^\dagger|f\rangle \\
&= \frac{-i\hbar}{2\pi}\int \exp(-ikz)\int \frac{\partial}{\partial z}\exp(ik'z)f(k')\,dk'dz \\
&= \frac{-i\hbar}{2\pi}\int\int ik'\exp\left[i(k'-k)z\right]f(k')\,dk'dz \\
&= \frac{\hbar}{2\pi}\int\int k'\exp\left[i(k'-k)z\right]dz\,f(k')\,dk' \\
&= \hbar\int k'\delta(k'-k)f(k')\,dk' \\
&= \hbar k f(k) \\
&\equiv p_z|f\rangle
\end{aligned}
$$

Hence, the operating with the momentum operator in the "new" (i.e., momentum) representation is equivalent to multiplying by the value p_z of the momentum.

Chapter 6 problem solutions

6.2.1

We will construct a finite matrix approximation to the actual Hamiltonian as a 2×2 matrix. Using the known solutions to the problem of a potential well without field, we have, in our dimensionless units, from Eq. (6.11)

$$|\psi_1\rangle = \sqrt{2}\sin(\pi\xi)$$
$$|\psi_2\rangle = \sqrt{2}\sin(2\pi\xi)$$

Our perturbing Hamiltonian for 3 units of field in our dimensionless units is, from Eqs. (6.7) and (6.9)

$$\hat{H}_p = 3\left(\xi - \frac{1}{2}\right)$$

Hence

$$\langle\psi_1|\hat{H}_p|\psi_2\rangle = 3\int_0^1 2\left(\xi - \frac{1}{2}\right)\sin(\pi\xi)\sin(2\pi\xi)d\xi$$
$$= -6\left(\frac{8}{9\pi^2}\right) = -\frac{16}{3\pi^2}$$
$$= \langle\psi_1|H_p|\psi_2\rangle$$

Since $|\psi_1\rangle$ and $|\psi_2\rangle$ are orthogonal eigenfunctions of $\hat{H}_o$, the unperturbed Hamiltonian, by orthogonality

$$\langle\psi_2|\hat{H}_o|\psi_1\rangle = 1\langle\psi_2|\psi_1\rangle = 0$$
$$\langle\psi_1|\hat{H}_o|\psi_2\rangle = 4\langle\psi_2|\psi_1\rangle = 0$$

So

$$\langle\psi_1|\hat{H}_o + \hat{H}_p|\psi_2\rangle = \langle\psi_2|\hat{H}_o + \hat{H}_p|\psi_1\rangle = -\frac{8}{3\pi^2}$$

Also

$$\langle\psi_1|\hat{H}_p|\psi_2\rangle = \langle\psi_2|\hat{H}_p|\psi_1\rangle = 0$$

by symmetry so

$$\hat{H} = \hat{H}_o + \hat{H}_p = \begin{bmatrix} 1 & -\dfrac{16}{3\pi^2} \\ -\dfrac{16}{3\pi^2} & 4 \end{bmatrix}$$

where the top left element is formally $\langle\psi_1|\hat{H}|\psi_1\rangle$. To find the eigenvalues, we formally write the eigen equation for some arbitrary vector(s) with elements a and b to be determined, i.e., we write

$$\hat{H}\begin{bmatrix} a \\ b \end{bmatrix} = E \begin{bmatrix} a \\ b \end{bmatrix}$$

so

$$\begin{bmatrix} 1-E & -\dfrac{16}{3\pi^2} \\ -\dfrac{16}{3\pi^2} & 4-E \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = 0$$

which requires the determinant of the matrix is zero because it must be a singular matrix, i.e.,

$$(1-E)(4-E) - \left(\frac{16}{3\pi^2}\right)^2 = 0$$

i.e.,

$$E^2 - 5E + 4 - \left(\frac{16}{3\pi^2}\right)^2 = 0$$

Hence

$$E = \frac{5 \pm \sqrt{25 - 4\left(4 - \left(\dfrac{16}{3\pi^2}\right)^2\right)}}{2} = \frac{5 \pm \sqrt{9 + \dfrac{1024}{9\pi^4}}}{2} = \frac{5 \pm 3.1887}{2}$$

$$= 0.9056 \ \text{ or } \ 4.094$$

which are the eigenenergies in dimensionless units in this model.

The corresponding eigenvectors are deduced as follows.

For $E = 0.9056$, we have

$$\begin{bmatrix} 0.0944 & -0.5404 \\ -0.5404 & 3.0944 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = 0$$

i.e.,

$$0.0944a - 0.5404b = 0$$

$$(\text{and } -0.5404a + 3.0944b = 0)$$

i.e.,

$$b = \frac{0.0944}{0.5404}a = 0.1747a$$

Normalizing by a factor

$$\frac{1}{\sqrt{1 + (0.1747)^2}} = 0.9851$$

we have, for the eigenstate

$$|\phi_1\rangle = 0.9851|\psi_1\rangle + 0.1721|\psi_2\rangle$$

For $E = 4.094$, we have

$$\begin{bmatrix} -3.094 & -0.5404 \\ -0.5404 & -0.094 \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = 0$$

i.e.,

$$3.094a + 0.5404b = 0$$

i.e.,.

$$b = \frac{-3.094}{0.5404}a = -5.725a$$

Normalizing by a factor

$$\frac{1}{\sqrt{1+(5.725)^2}} = 0.17206$$

we have for the eigenstate

$$|\phi_2\rangle = 0.17206|\psi_1\rangle - 0.9851|\psi_2\rangle$$

Note that these numbers are actually all in reasonable agreement with the numbers calculated numerically for the case of three members of the basis set.
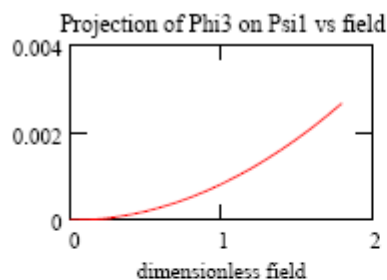
6.2.2

This problem can be solved by the finite matrix method or by perturbation theory. The results we quote here are by the finite matrix method using 5 basis functions. Negligible change was observed in going to 19 basis functions.
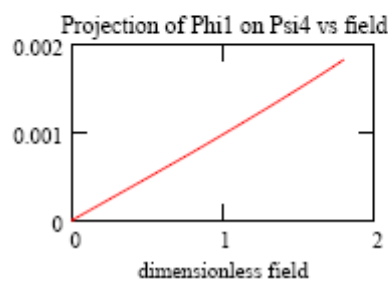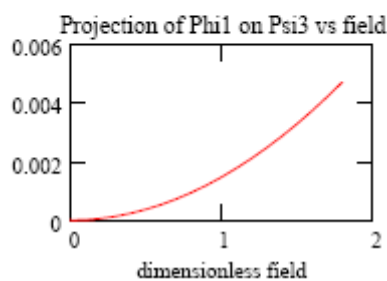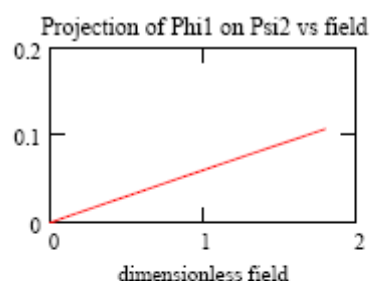
(i) We plot the results here as a function of the dimensionless field, which runs from 0 to 1.776 units as the actual field runs from 0 to 10 V/micron. One unit of energy on these plots is ~ 56 meV.

Energy separation: first & second

Energy separation: first & third
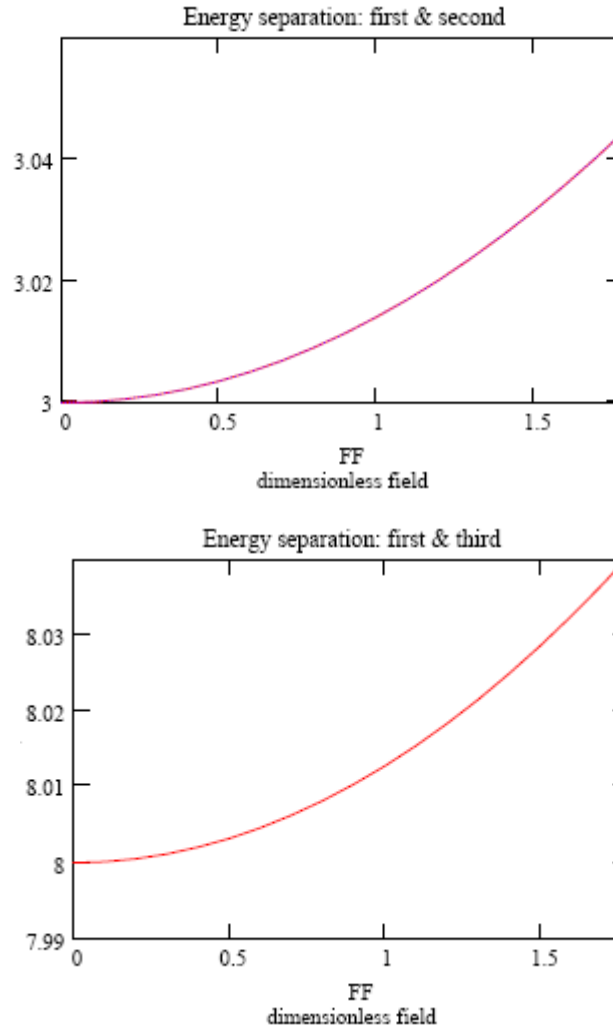
(ii) For the various coefficients, calling the unperturbed functions psi and the new eigenfunction solutions in the presence of field phi, we calculate the overlap integrals as shown in the graphs.

Projection of Phi1 on Psi1 vs field

Projection of Phi1 on Psi2 vs field
dimensionless field

Projection of Phi1 on Psi3 vs field
dimensionless field

Projection of Phi1 on Psi4 vs field
dimensionless field

Projection of Phi2 on Psi1 vs field
dimensionless field

Projection of Phi2 on Psi2 vs field
dimensionless field

Projection of Phi2 on Psi3 vs field
dimensionless field

Projection of Phi2 on Psi4 vs field

Projection of Phi3 on Psi1 vs field
dimensionless field

Projection of Phi3 on Psi2 vs field
dimensionless field

Projection of Phi3 on Psi3 vs field
dimensionless field

Projection of Phi3 on Psi4 vs field
dimensionless field

(iii) The transition rate from level 1 to level 2 is shown in the following graph
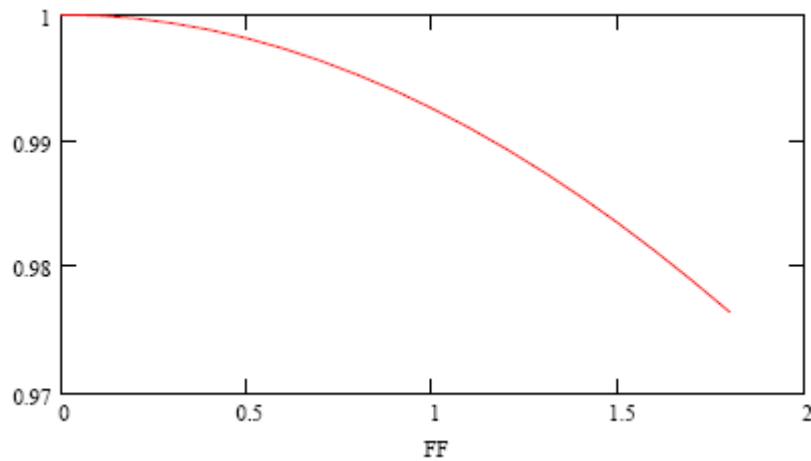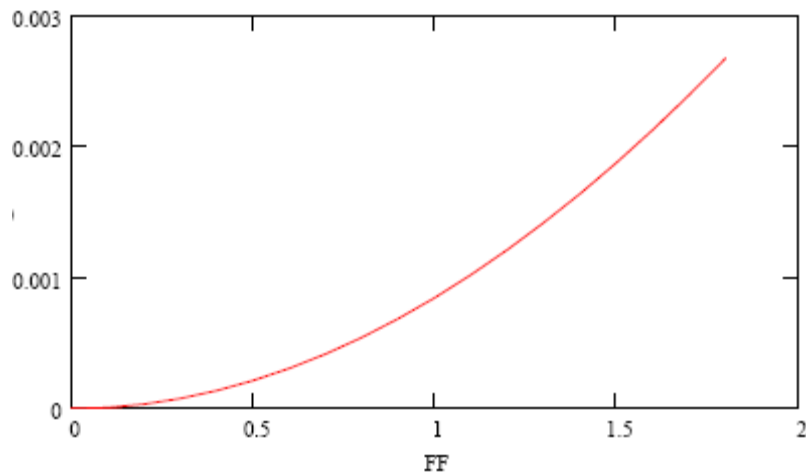

The transition rate from level 1 to level 3 is shown in the following graph.

(iv) The 1 to 3 transition is not 10% as strong as the zero field 1 – 2 transition for the given range of fields. Thus only the 1 to 2 transition is usable in this device. The energy spread for the 1 – 2 transition was from 3 units of energy to 3.04 units of energy. The corresponding wavelength range is from 7.358 microns (without field) to 7.261 microns with field, a range of roughly 100 nm.

See the following Mathcad worksheet for detailed calculations.

Problem 6.2.2 Solution Mathcad worksheet

Constants

$q := 1.6 \cdot 10^{-19} C$ $mo := 9.1 \cdot 10^{-31} kg$ $hbar := 1.055 \cdot 10^{-34} J \cdot s$ $Angstrom := 1 \cdot 10^{-10} m$

$meff := 0.067 \cdot mo$ $Lz := 100 \, Angstrom$ $c := 3 \cdot 10^{8} \frac{m}{s}$ $eV := \left(1.6 \cdot 10^{-19}\right) J$

$Eo := \dfrac{hbar^{2} \cdot \left(\dfrac{\pi}{Lz}\right)^{2}}{2 \cdot meff}$ $Fo := \dfrac{Eo}{q \cdot Lz}$ $Fo = 5.63 \times 10^{6} \dfrac{V}{m}$ $Fmax := 10^{7} \dfrac{V}{m}$ $\dfrac{Fmax}{Fo} = 1.776$

$Eo = 0.056 \, eV$ $Eo = 0.09 \, 10^{-19} \cdot J$

Finite Basis Subsets

We will use the finite basis subset method first:

(i) Calculate the energy separations between the first and second energy levels and between the first and third energy levels over the stated range of fields, and plot these on a graph.

Using dimensionless variables as before, we have the total Hamiltonian including the perturbation in Eq, (6.7).

The Hamiltonian and eigenfunctions of the unperturbed system in these units become

$Ho(i, j) := i^{2} \cdot \delta(i, j)$ $\psi(m, \zeta) := \left(\sqrt{2}\right) \cdot \left(\sin(\pi \cdot m \cdot \zeta)\right)$

The matrix elements of the full Hamiltonian are

$H(i, j, f) := \left[\displaystyle\int_{0}^{1} f \cdot \psi(i, \zeta) \cdot (\zeta - 0.5) \cdot \psi(j, \zeta) \, d\zeta \right] + Ho(i, j)$

We will make a p by p matrix from the above element definition, calculate the eigenvalues and eigenvectors of this matrix, and put them all together into one big matrix. Since Mathcad does not necessarily generate the eigenvalues in ascending order, we will sort the values and their corresponding vectors. System(p,F) will be the matrix containing the eigenvalues and vectors. p is the number of bases to include in our finite basis set calculation and F is the field. **We can later increase p as much as we like to see the improvement in our calculation as we add more basis functions**.

$$\text{System}(p,F) := \begin{vmatrix} \text{for } ii \in 1..p \\ \quad \text{for } jj \in 1..p \\ \qquad \left(H1_{ii,\,jj} \leftarrow H(ii,jj,F)\right) \\ \text{evals} \leftarrow \text{eigenvals}(H1) \\ \text{evects} \leftarrow \text{eigenvecs}(H1) \\ \text{esystem} \leftarrow \text{csort}\!\left(\text{augment}\!\left(\text{eigenvals}(H1),\text{eigenvecs}(H1)^T\right),1\right) \\ \text{esystem} \end{vmatrix}$$

So to clarify the format of the output above: if we want to use 5 basis functions, for a relative field of 3, we have the system matrix below: here each row has the eigenvalue in the first column and the new eigenvector projection on each of the initial 5 basis functions on the other columns.

$$\text{System}(5,3) = \begin{pmatrix} 0.904 & 0.985 & 0.174 & 0.013 & 3.344 \times 10^{-3} & 4.822 \times 10^{-4} \\ 4.027 & -0.175 & 0.978 & 0.115 & 5.246 \times 10^{-3} & 2.721 \times 10^{-3} \\ 9.017 & 7.357 \times 10^{-3} & -0.116 & 0.99 & 0.085 & 2.781 \times 10^{-3} \\ 16.011 & -3.005 \times 10^{-3} & 3.95 \times 10^{-3} & -0.085 & 0.994 & 0.066 \\ 25.04 & 1.8 \times 10^{-4} & -2.691 \times 10^{-3} & 2.565 \times 10^{-3} & -0.066 & 0.998 \end{pmatrix}$$
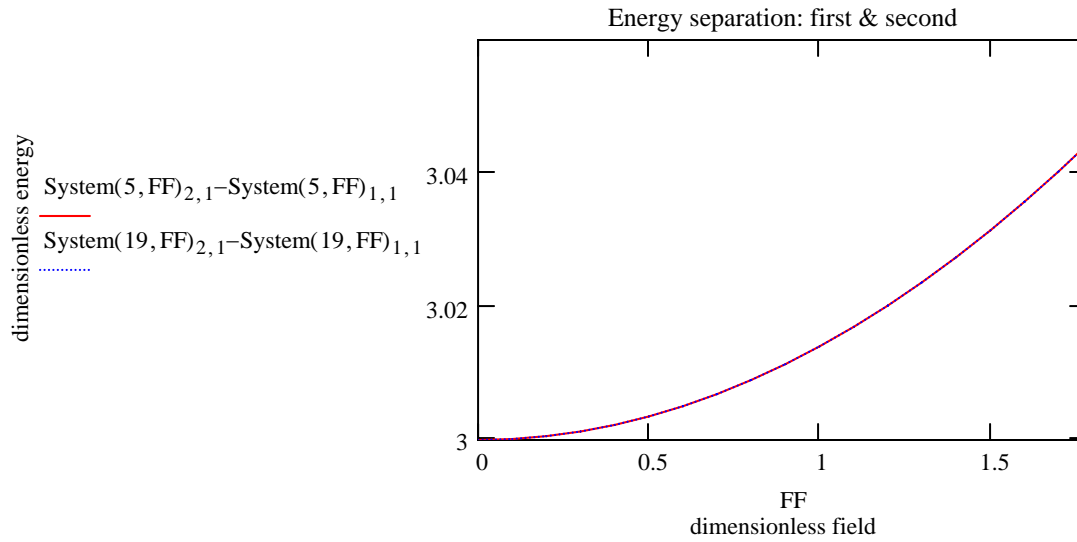
As a check we look at the 0 field case to make sure we get what we expect:

$$\text{System}(5,0) = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 & 0 \\ 4 & 0 & 1 & 0 & 0 & 0 \\ 9 & 0 & 0 & 1 & 0 & 0 \\ 16 & 0 & 0 & 0 & 1 & 0 \\ 25 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

Now we plot the energy separations between the first and second and first and third energy levels over the range of fields. In dimensionless units this is roughly over 0 to 1. **To check whether we are justified in taking just 5 basis functions we compare to the case where we take 19 basisfunctions. We see that the curves for 5 and 19 basis functions overlap, and we know that the finite basis method essentially converges to the exact solution as we take more basis functions, so we are justified in taking 5 basis functions.**

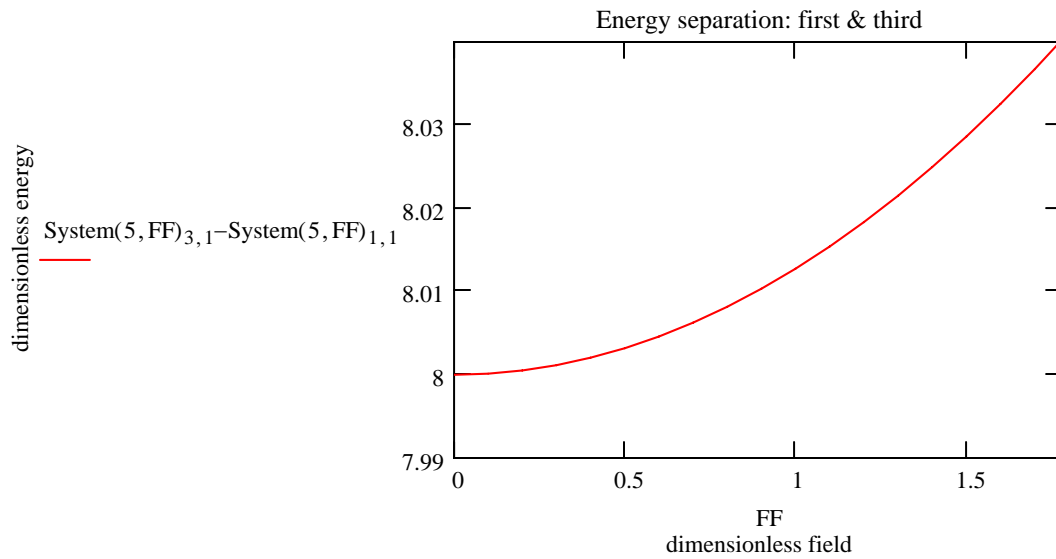Normalized field ranges from 0 to 1.776 (see constants section)

Energy separation: first & second

dimensionless energy

$System(5, FF)_{2,1} - System(5, FF)_{1,1}$

$System(19, FF)_{2,1} - System(19, FF)_{1,1}$

3.04

3.02

3

0   0.5   1   1.5

FF
dimensionless field

The energy spread here is from 3Eo to 3.04Eo.

In Joules that is: $3 \cdot Eo = 0.27 \, J \, 10^{-19}$ to $3.04 \cdot Eo = 0.274 \, J \, 10^{-19}$

In eV that is: $3 \cdot Eo = 0.169 \, eV$ to $3.04 \cdot Eo = 0.171 \, eV$

Energy separation: first & third

dimensionless energy

8.03

8.02

$System(5, FF)_{3,1} - System(5, FF)_{1,1}$

8.01

8

7.99

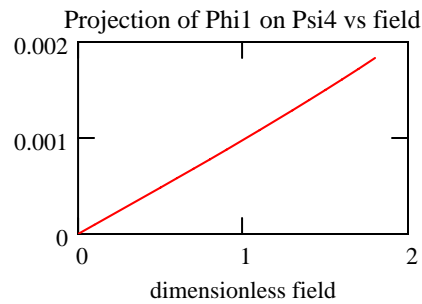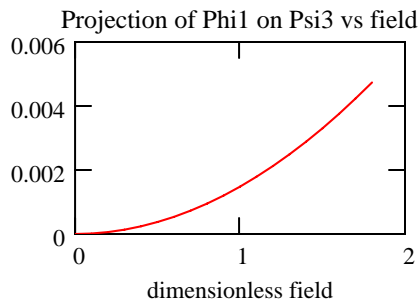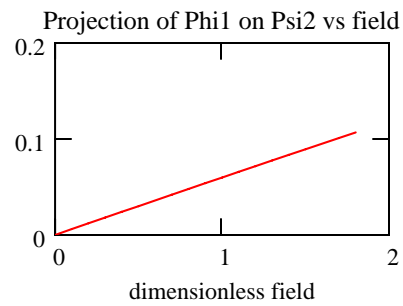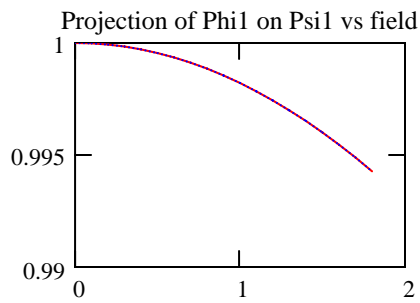0   0.5   1   1.5

FF
dimensionless field

The energy spread here is from 8Eo to 8.04Eo

In Joules that is: $8 \cdot Eo = 0.721 \, J \, 10^{-19}$ $8.04 \cdot Eo = 0.724 \, J \, 10^{-19}$

In eV that is: $8 \cdot Eo = 0.45 \, eV$ to $8.04 \cdot Eo = 0.453 \, eV$

(II) As a function of field plot the projection of the first three new eigenfunctions on the first four old basis functions.

We already have this information in the system matrix above so now we just plot it. Lets call the new functions phi and the old functions psi. We also check the first one with 19 basis functions again to make sure we are accurate

Projection of Phi1 on Psi1 vs field

Projection of Phi1 on Psi2 vs field

Projection of Phi1 on Psi3 vs field

Projection of Phi1 on Psi4 vs field

Plotting the same for the second and third functions:
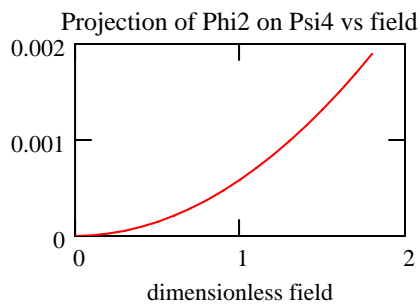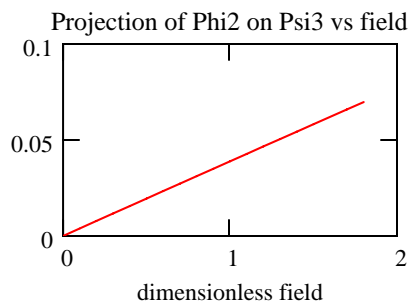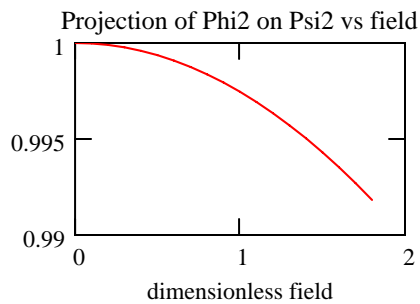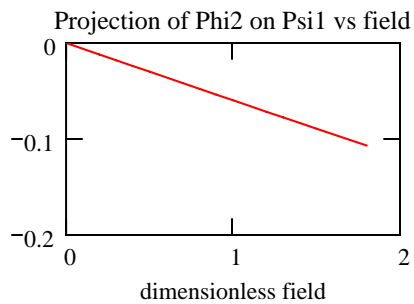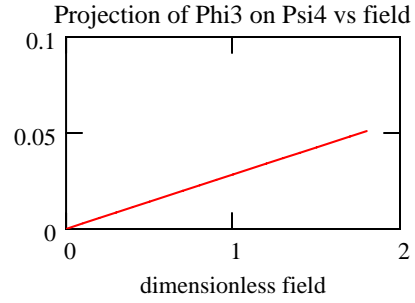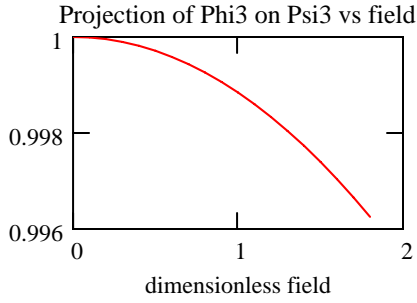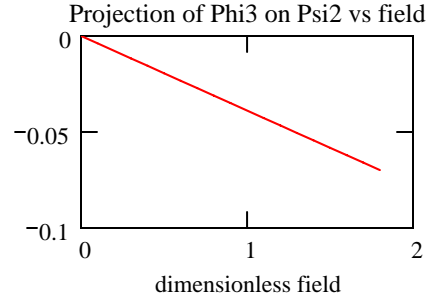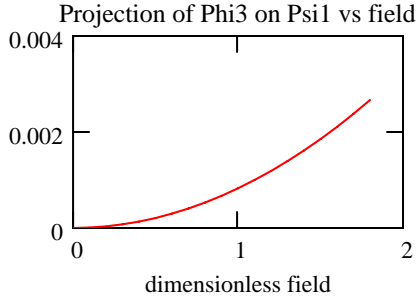
Projection of Phi2 on Psi1 vs field

Projection of Phi2 on Psi2 vs field

Projection of Phi2 on Psi3 vs field

Projection of Phi2 on Psi4 vs field

Projection of Phi3 on Psi1 vs field

Projection of Phi3 on Psi2 vs field

Projection of Phi3 on Psi3 vs field

Projection of Phi3 on Psi4 vs field

(iii) We know how to calculate transition rates, we will calculate them relative to the zero field first- second transition.

$$\text{TR\_nofield}(i,j) := \left[\left|\left|\int_0^1 \psi(i,\zeta)\cdot(\zeta - 0.5)\cdot\psi(j,\zeta)\, d\zeta\right|\right|\right]^2 \quad \text{TR\_nofield}(1,2) = 0.032$$

For the rates with the field on we use the above formula except with the new eigenfunctions instead

$$\text{Phi1}(FF,p,\zeta) := \sum_{a=1}^{p} \left(\text{System}(5,FF)_{1,\,a+1}\cdot\psi(a,\zeta)\right)$$

$$\text{Phi2}(FF,p,\zeta) := \sum_{a=1}^{p} \left(\text{System}(5,FF)_{2,\,a+1}\cdot\psi(a,\zeta)\right)$$

$$\text{Phi3}(FF,p,\zeta) := \sum_{a=1}^{p} \left(\text{System}(5,FF)_{3,\,a+1}\cdot\psi(a,\zeta)\right)$$

$$\text{TR\_one\_two}(p,FF) := \frac{\left[\left|\left|\int_0^1 \text{Phi1}(FF,p,\zeta)\cdot(\zeta - 0.5)\cdot\text{Phi2}(FF,p,\zeta)\, d\zeta\right|\right|\right]^2}{\text{TR\_nofield}(1,2)}$$
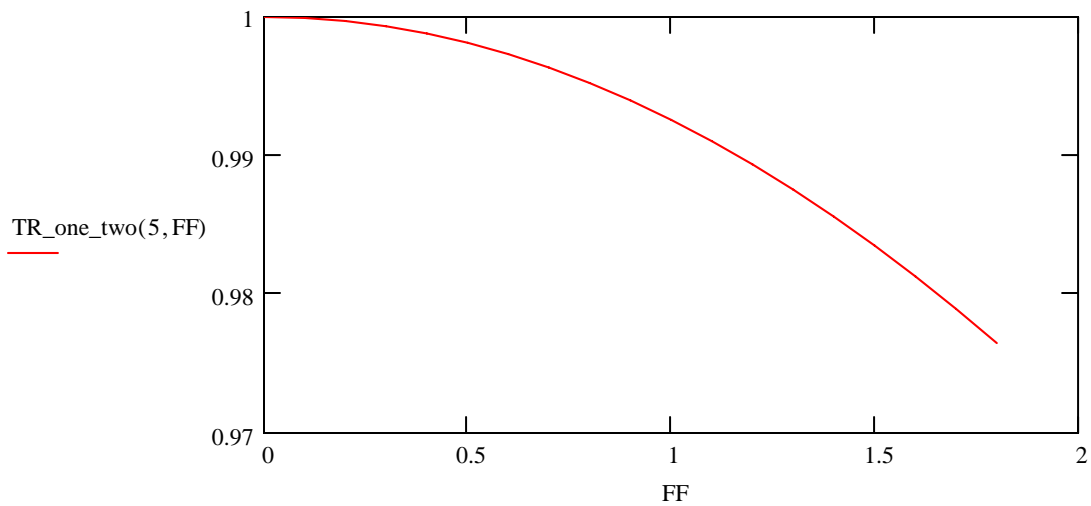
$$\text{TR\_one\_three}(p, FF) := \frac{\left[\left|\left|\int_0^1 \text{Phi1}(FF, p, \zeta) \cdot (\zeta - 0.5) \cdot \text{Phi3}(FF, p, \zeta) \, d\zeta\right|\right|\right]^2}{\text{TR\_nofield}(1, 2)}$$
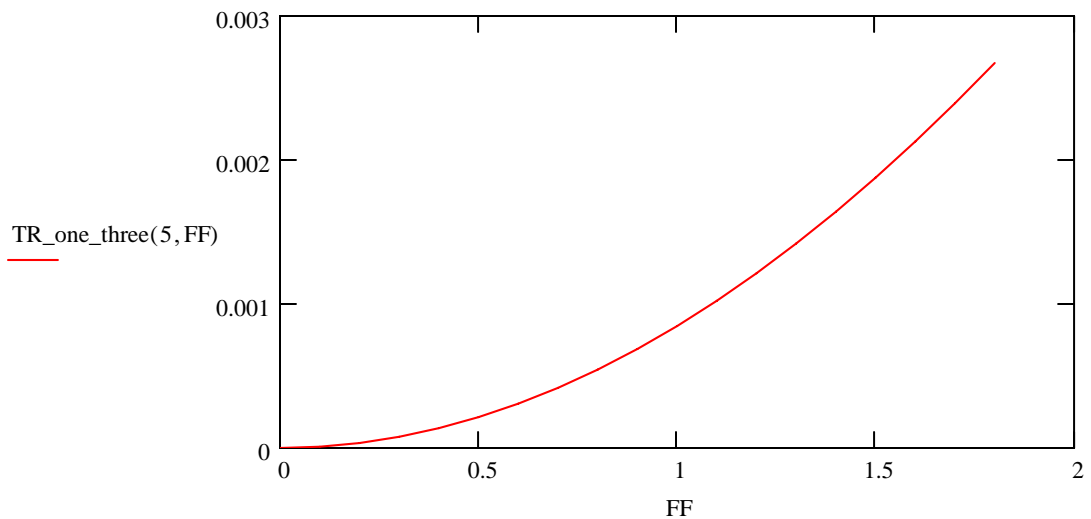
(iv)

The one to three transition is not 10% as strong as the zero field one to two transition for the given range of fields. Thus only the one to two transition is usable in this device. Let us calculate what range of tuning this gives us: From the plot in part (i) the energy difference changes from 3 to 3.015 in units of Eo

The energy spread for the 1->2 transition was from 3Eo to 3.04Eo.

The wavelengths corresponding to these energy differences are

$$wave1 := hbar \cdot 2 \cdot \pi \cdot \frac{c}{3 \cdot Eo}$$ $wave1 = 7.35824 \times 10^{-6} \, m$ $hbar \cdot 2 \cdot \pi = 6.629 \frac{kg \, m^2}{s} 10^{-34}$

$$wave2 := hbar \cdot 2 \cdot \pi \cdot \frac{c}{3.04 \cdot Eo}$$ $wave2 = 7.261 \times 10^{-6} \, m$

$$Tune\_range := wave1 - wave2 = \left(9.682 \times 10^{-8} \, m \right)$$ roughly 100nm

<u>Perturbation Theory</u>

Now we solve the problem using perturbation theory. Since we know the finite basis results above are quite close to the exact solutions, we will compare our results to the finite basis method to figure out when we have a good enough approximation in perturbation theory.

(i) Calculate the energy separations between the first and second electron levels and between the first and third energy levels over the stated range of fields, and plot these on a graph.

Using dimensionless variables as before we write the terms of the perturbing hamiltonian leaving. Here we leave out the field which is just a constant multiplying this expression. See Eq. (6.53).

$$Hp(i,j) := \int_0^1 \psi(i,\zeta) \cdot (\zeta - 0.5) \cdot \psi(j,\zeta) \, d\zeta$$

The zeroth order energies are:

$$E_0(j) := j^2$$

In our notation here, the argument respresents which original wavefunction we are correcting while the subscript is the order of the correction.

For the first order energy corrections (which are all zero by symmetry) for example our notation is:

$$E_1(j) := Hp(j,j)$$ first order correction in energy of jth state. Note here the multiplication by Fo is left out to be added in later.

$Hp(1,1) = 0$ $Hp(2,2) = 0$ $Hp(3,3) = 0$

Second-order corrections in the energies maybe more meaningful here

We will have to take a sum over a certain number of terms; let us call that number pp

$$E_2(j, pp) := \sum_{i=1}^{pp} \text{if}\left[i = j, 0, \frac{(|Hp(i, j)|)^2}{E_0(j) - E_0(i)} \right]$$ second order correction in energy of jth state

So now, for example, the correction in the energy of the first eigenfunction if we sum over 10 states :

$E_2(1, 10) = -0.01083$ and over 20 states is: $E_2(1, 10) = -0.01083$

Similarly we calculate the energy correction in the second and third states.

$E_2(2, 20) = 3.229 \times 10^{-3}$ $E_2(3, 20) = 1.924 \times 10^{-3}$

The above corrections are proportional to field squared. So the total energies (correct to second order) are:

$$Etot(m, FF) := E_0(m) + \left(FF^2\right) \cdot E_2(m, 20)$$

Now we plot as a function of field the spacing of first and second and the first and third levels. The solid line in the plots below shows the perturbation theory calculation. The dashed line is the finite basis subset. Since they agree quite well, we do not need to consider higher order energy corrections.
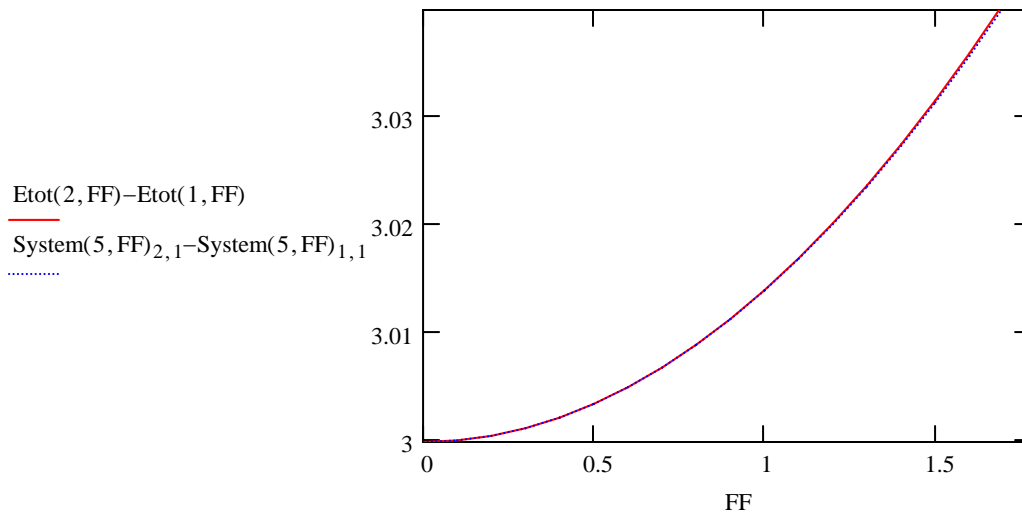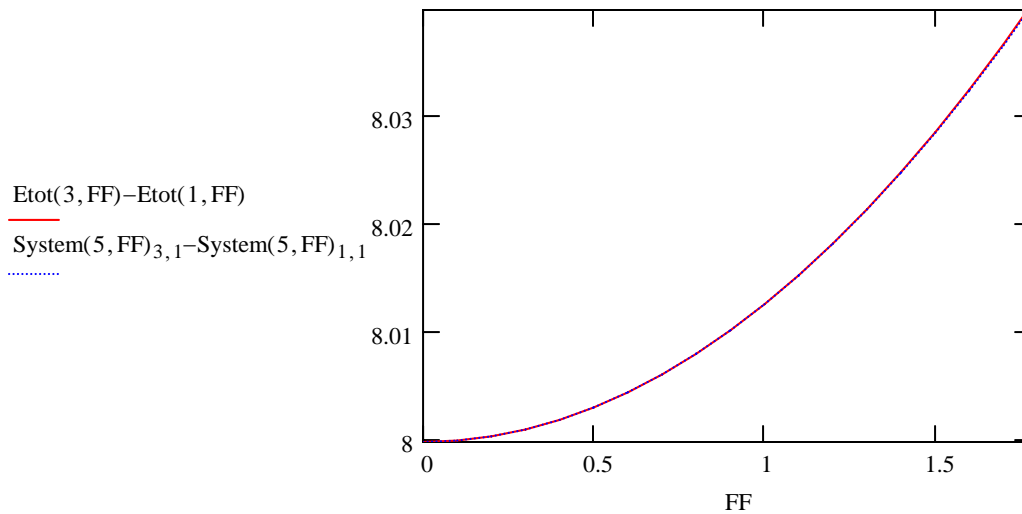
Etot(2, FF)−Etot(1, FF)

System(5, FF)$_{2,1}$−System(5, FF)$_{1,1}$

$$\text{Etot}(3,\text{FF})-\text{Etot}(1,\text{FF})$$

$$\text{System}(5,\text{FF})_{3,1}-\text{System}(5,\text{FF})_{1,1}$$

(ii) As a function of field plot the projection of the first three new eigenfunctions on the first four old basis functions.

The first order correction to the wavefunctions has the following amplitudes:

$$A_1(i,j) := \frac{\text{Hp}(i,j)}{E_0(j) - E_0(i)}$$

This is the ith coefficient in the first order correction of the jth wavefunction

The second order correction to the wavefunctions has the following amplitudes (this is just Eq. (6.46) without the second term which is zero in this case):

$$A_2(i,j,pp) := \left[\sum_{n=1}^{pp} \text{if}\left[n = j, 0, \frac{\text{Hp}(i,n)\cdot\text{Hp}(n,j)}{\big(E_0(j) - E_0(i)\big)\cdot\big(E_0(j) - E_0(n)\big)} \right] \right]$$

(Note the if(cond,x,y) statement returns x if the logical condition cond is true (non-zero), y otherwise.)

Now we calculate the lowest non-zero amplitudes for each of the three wavefunctions.

First state:

$$A_1(2,1) = 0.06$$

this is the (lowest non-zero order) correction in the projection of the new 1st state on the old 2nd state.

$$A_1(3,1) = 0$$

since the first order correction in the projection of the new 1st state on the old 3rd state is zero we go to the next higher order.

$$A_2(3,1,10) = 1.484 \times 10^{-3} \qquad A_2(3,1,20) = 1.484 \times 10^{-3}$$

(not much difference whehter we take the sum over 10 or 20 functions)

$A_1(4,1) = 9.607 \times 10^{-4}$ this is the lowest non-zero order correction in the projection of the new 1st state on the old 4th state.

We also calculate the sum we would need to normalize with:

$$\text{Norm1(FF)} := \left[\left(A_1(4,1) \cdot \text{FF} \right)^2 + \left(A_2(3,1,10) \cdot \text{FF}^2 \right)^2 + \left(A_1(2,1) \cdot \text{FF} \right)^2 + 1 \right]^{0.5}$$

By definition, the field dependence of the first order coefficients is linear and of the second order is quadratic Now we plot this.
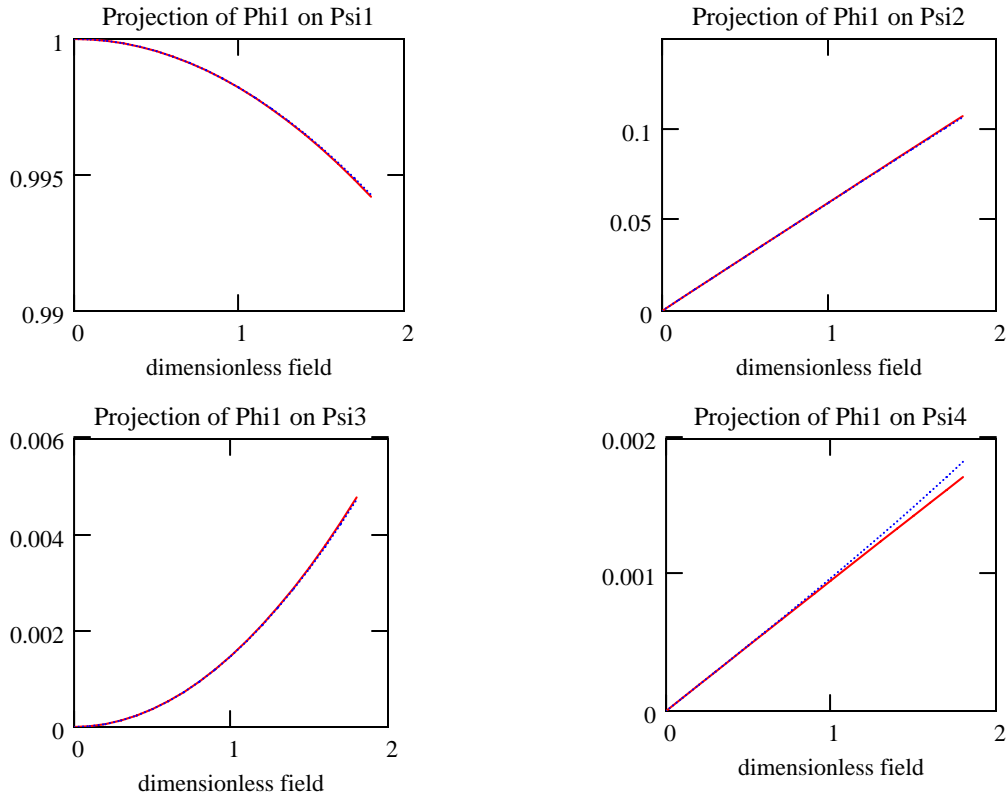
As before, the finite basis method calculation of the corresponding coefficients is also plotted (dashed line). Note that the projections on the 2nd and 4th wavefunctions vary linearly while that on the 3rd has a quadratic / second order dependence. The first also has a quadratic dependence if you normalize, as done here.

Second state:

$A_1(1,2) = -0.06$ this is the lowest non-zero order correction in the projection of the new 2nd state on the old 1st state.

$A_1(3,2) = 0.039$ this is the lowest non-zero order correction in the projection of the new 2nd state on the old 3rd state.

$A_1(4,2) = 0$ $A_2(4,2,10) = 5.863 \times 10^{-4}$ $A_2(4,2,20) = 5.863 \times 10^{-4}$

$A_2(4,2,10) = 5.863 \times 10^{-4}$ his is the lowest non-zero order correction in the projection of the new 2nd state on the old 4th state.

$$\text{Norm2(FF)} := \left[\left(A_1(1,2) \cdot FF \right)^2 + \left(A_1(3,2) \cdot FF \right)^2 + \left(A_2(4,2,10) \cdot FF^2 \right)^2 + 1 \right]^{0.5}$$

Again, by definition the field dependence of first order coefficients is linear and of the second order is quadratic. Now we plot this.

Projection of Phi2 on Psi1

Projection of Phi2 on Psi2

Projection of Phi2 on Psi3

Projection of Phi2 on Psi4
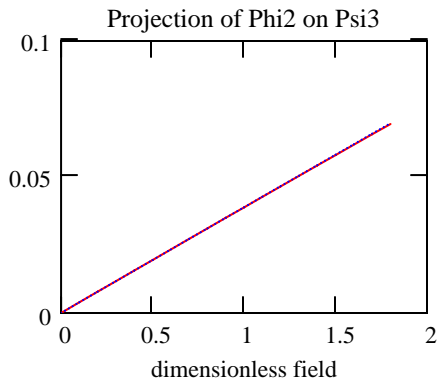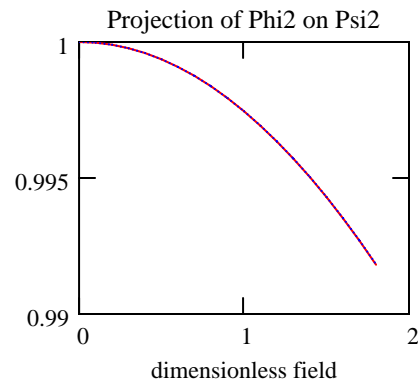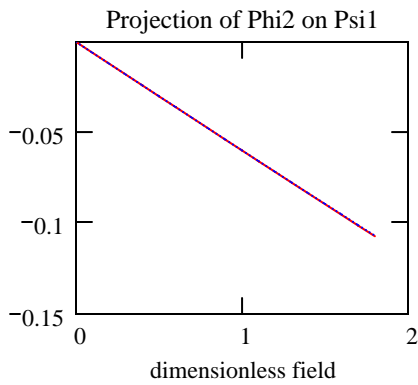
Third state:

$A_1(1,3) = 0$ $A_2(1,3,10) = 8.246 \times 10^{-4}$ this is the lowest non-zero order correction in the projection of the new 3rd state on the old 1st state.

$A_1(2,3) = -0.039$ lowest non-zero order correction in the projection of the new 3rd state on the old 2nd state.

$A_1(4,3) = 0.028$ lowest non-zero order correction in the projection of the new 3rd state on the old 4th state.

$$\text{Norm3(FF)} := \left[\left(A_2(1,3,10) \cdot FF^2 \right)^2 + \left(A_1(2,3) \cdot FF \right)^2 + \left(A_1(4,3) \cdot FF \right)^2 + 1 \right]^{0.5}$$
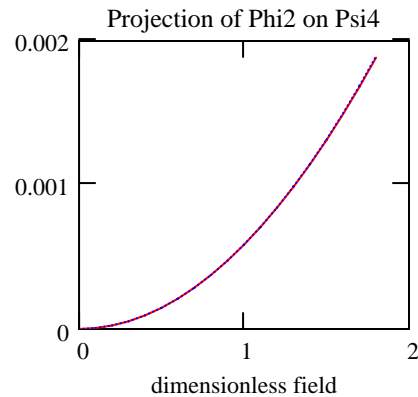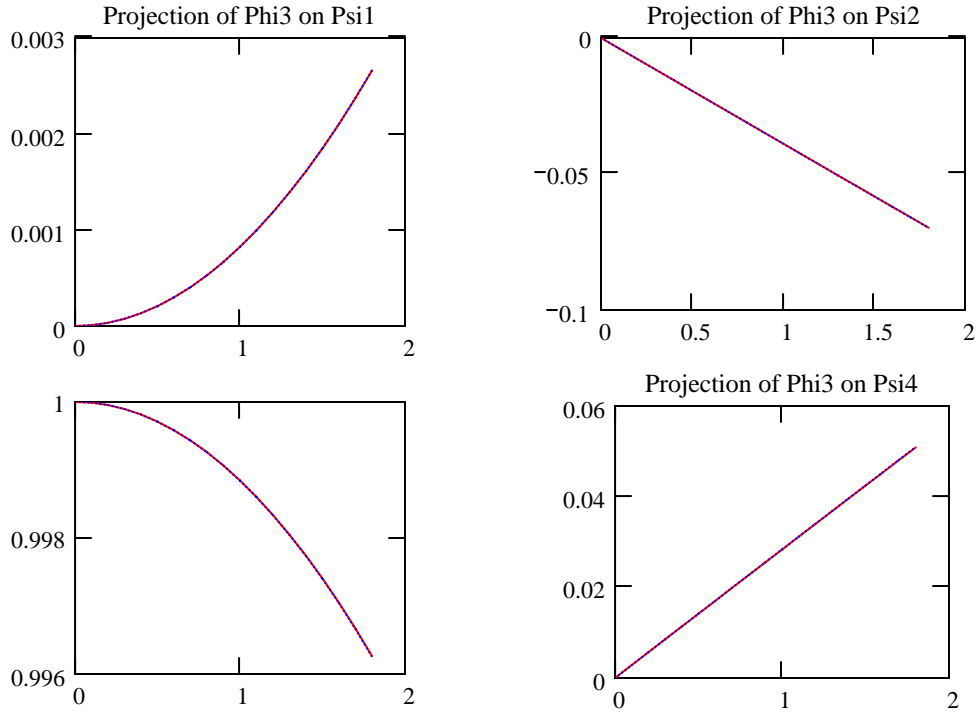
Projection of Phi3 on Psi1

Projection of Phi3 on Psi2

Projection of Phi3 on Psi4

(iii) We know how to calculate transition rates; we will calculate them relative to the zero field first-second transition.

The perturbed wavefunctions are:

$$\text{PHI\_pert1}(\zeta, \text{FF}) := \frac{\psi(1,\zeta) + A_1(2,1)\cdot\text{FF}\cdot\psi(2,\zeta) + A_2(3,1,10)\cdot\text{FF}^2\cdot\psi(3,\zeta) + A_1(4,1)\cdot\text{FF}\cdot\psi(4,\zeta)}{\text{Norm1}(\text{FF})}$$

$$\text{PHI\_pert2}(\zeta, \text{FF}) := \frac{\psi(1,\zeta)\cdot\left(A_1(1,2)\cdot\text{FF}\right) + \psi(2,\zeta) + A_1(3,2)\cdot\text{FF}\cdot\psi(3,\zeta) + A_2(4,2,10)\cdot\text{FF}^2\cdot\psi(4,\zeta)}{\text{Norm2}(\text{FF})}$$

$$\text{PHI\_pert3}(\zeta, \text{FF}) := \frac{\left[\psi(1,\zeta)\cdot\left(A_2(1,3,10)\cdot\text{FF}^2\right) + A_1(2,3)\cdot\text{FF}\cdot\psi(2,\zeta) + \psi(3,\zeta) + A_1(4,3)\cdot\text{FF}\cdot\psi(4,\zeta)\right]}{\text{Norm3}(\text{FF})}$$

$$\text{TR\_one\_two\_pert}(\text{FF}) := \frac{\left[\left|\left|\int_0^1 \text{PHI\_pert1}(\zeta,\text{FF})\cdot(\zeta - 0.5)\cdot\text{PHI\_pert2}(\zeta,\text{FF})\,d\zeta\right|\right|\right]^2}{\text{TR\_nofield}(1,2)}$$

$$\text{TR\_one\_three\_pert}(\text{FF}) := \frac{\left[\left|\left|\int_0^1 \text{PHI\_pert1}(\zeta,\text{FF})\cdot(\zeta - 0.5)\cdot\text{PHI\_pert3}(\zeta,\text{FF})\,d\zeta\right|\right|\right]^2}{\text{TR\_nofield}(1,2)}$$
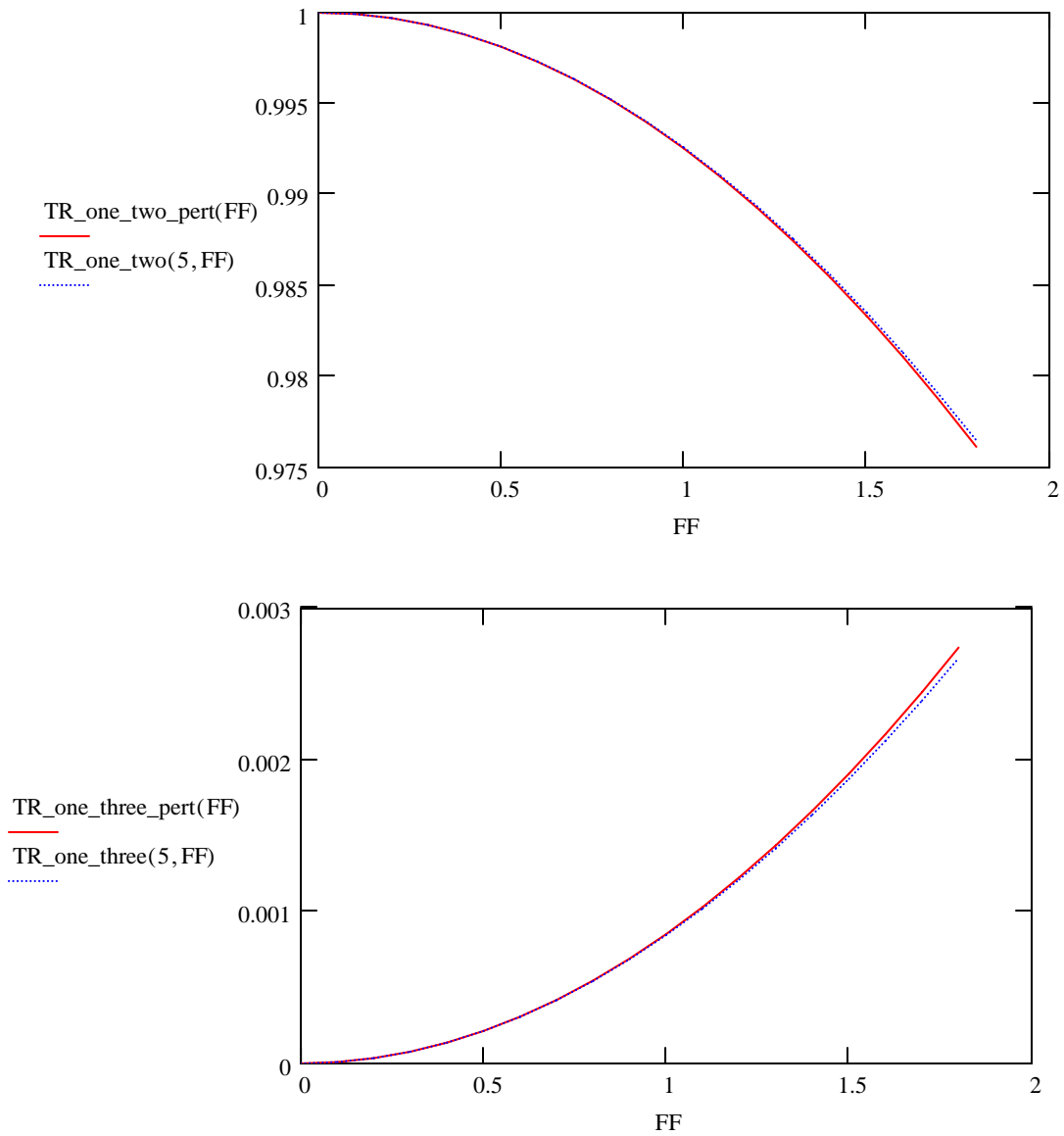
As usual the dashed curve is the finite basis subset method curve plotted again here for comparison. We see that for both transitions' results for perturbation theory agree quite well with the finite basis method which we know to be accurate.

Part (iv) is the same as done in the finite basis section. No further calculation is required.

6.3.1

(i) The perturbing Hamiltonian here is $H_p = eF\left(z - \dfrac{L_z}{2}\right)$, where we have chosen the zero for the potential in the middle of the well. We consider level n in the potential well, and its shift with applied electric field. There will be no linear shift, by symmetry (or verified by first order perturbation theory, since $\langle \psi_n | z | \psi_n \rangle = 0$).

The second order shift is

$$E_n^{(2)} \simeq \sum_{q \neq n} \frac{\left| \langle \psi_q | H_p | \psi_n \rangle \right|^2}{E_n - E_q}$$

The matrix elements are

$$\langle \psi_q | H_p | \psi_n \rangle = eF \left\langle \psi_q \left| z - \frac{L_z}{2} \right| \psi_n \right\rangle = eF \left\langle \psi_q \left| z - \frac{L_z}{2} \right| \psi_n \right\rangle (q \neq n)$$

$$= \frac{2}{L_z} \int_0^{L_z} \sin\left(\frac{\pi q z}{L_z} \right) \left(z - \frac{L_z}{2} \right) \sin\left(\frac{\pi n z}{L_z} \right) dz = \frac{2}{L_z} \left(\frac{L_z}{\pi} \right)^2 \int_0^{\pi} \left(\zeta - \frac{\pi}{2} \right) \sin(q\zeta) \sin(n\zeta) d\zeta$$

where

$$\zeta = \frac{\pi z}{L_z}$$

Using the expression

$$\int_0^{\pi} \left(\zeta - \frac{\pi}{2} \right) \sin(q\zeta) \sin(n\zeta) d\zeta = -\frac{4qn}{(n-q)^2 (n+q)^2} \text{ for n + q odd}$$

$$= 0 \text{ for } n+q \text{ even}$$

we have

$$\langle \psi_q | z | \psi_n \rangle = -\frac{8 L_z}{\pi^2} \frac{qn}{(n-q)^2 (n+q)^2} \text{ for } n+q \text{ odd}$$

$$= 0 \text{ for } n+q \text{ even}$$

Hence, for $n = 2$, we have matrix elements

$$\langle \psi_1 | z | \psi_2 \rangle = -\frac{8 L_z}{\pi^2} \frac{2}{1 \times 9} = -\frac{16}{9} \frac{L_z}{\pi^2} = -1.778 \frac{L_z}{\pi^2}$$

$$\langle \psi_3 | z | \psi_2 \rangle = -\frac{8 L_z}{\pi^2} \frac{6}{1 \times 25} = -\frac{48}{25} \frac{L_z}{\pi^2} = -1.920 \frac{L_z}{\pi^2}$$

$$\langle \psi_4 | z | \psi_2 \rangle = 0$$

$$\langle \psi_5 | z | \psi_2 \rangle = -\frac{8 L_z}{\pi^2} \frac{10}{9 \times 49} = -\frac{80}{9 \times 49} \frac{z}{\pi^2} \frac{L_z}{\pi^2} = -0.181 \frac{L_z}{\pi^2}$$

$$\langle \psi_6 | z | \psi_2 \rangle = 0$$

$$\langle \psi_7 | z | \psi_2 \rangle = -\frac{8L_z}{\pi^2} \frac{14}{25 \times 81} \frac{L_z}{\pi^2} = -\frac{112}{25 \times 81} \frac{L_z}{\pi^2} = -0.055 \frac{L_z}{\pi^2}$$

so, with E_1 as the energy of the unperturbed first state,

$$E_2^{(2)} \simeq \left(\frac{eFL_z}{\pi^2}\right)^2 \frac{1}{E_1} \left[\frac{(1.778)^2}{3} - \frac{(1.92)^2}{5} - \frac{(0.181)^2}{21} - \frac{(0.055)^2}{45} + \dots \right]$$

$$\simeq \left(\frac{eFL_z}{\pi^2}\right)^2 \frac{1}{E_1} [1.053 - 0.737 - 0.002 - 0.000 + \dots]$$

$$\simeq \left(\frac{eFL_z}{\pi^2}\right)^2 \frac{1}{E_1} [0.296]$$

where

$$E_1 = \frac{\hbar^2}{2m} \left(\frac{\pi}{L_z}\right)^2 = \frac{1.055 \times 1.055 \times 10^{-68} \times \pi^2}{2 \times 0.07 \times 9.1095 \times 10^{-31} \times 1.602 \times 10^{-19} \times 10^{-16}} \text{ eV} = 53.76 \text{ meV}$$

and where m is the appropriate mass (the electron mass for an electron in a potential well). Hence, writing out the entire expression, the shift with field, from second order perturbation theory, is

$$E_2^{(2)} \simeq 0.296 \left(\frac{eFL_z}{\pi^2}\right)^2 \frac{1}{E_1}$$

$$= \frac{0.296}{\pi^4} \frac{(eFL_z)^2}{E_1}$$

(ii) Explicitly for the GaAs case, we therefore have, in electron volts

$$E_2^{(2)} = \frac{0.296}{\pi^4} \times \frac{(0.1)^2}{0.05376} = 0.565 \text{ meV}$$

This energy is increasing (relative to the energy at the center of the well).

6.3.2

Use perturbation theory with $H_p = u(z - L_z / 2)^2$

Recall that

$$E_n^{(0)} = \frac{n^2 \hbar^2 \pi^2}{2mL_z^2} \text{ and } |\psi_n\rangle = \sqrt{\frac{2}{L_z}} \sin(\frac{n\pi z}{L_z})$$

$$E_1^{(1)} = \langle \psi_1 | \hat{H}_p | \psi_1 \rangle = \int_0^{L_z} \sqrt{\frac{2}{L_z}} \sin(\frac{\pi z}{L_z}) u(z - L_z / 2)^2 \sqrt{\frac{2}{L_z}} \sin(\frac{2\pi z}{L_z}) dz$$

Using standard results for integration, we then obtain

$$E_1^{(1)} = \frac{uL_z^2}{12} \left(1 - \frac{6}{\pi^2} \right)$$

and

$$E_2^{(1)} = \frac{uL_z^2}{12} \left(1 - \frac{6}{4\pi^2} \right)$$

Hence the transition energy is

$$\left(E_2^{(0)} + E_2^{(1)} \right) - \left(E_1^{(0)} + E_1^{(1)} \right) = \frac{3\hbar^2 \pi^2}{2mL_z^2} + \frac{3uL_z^2}{8\pi^2}$$

6.3.3

(i) and (ii) With applied field F, the wavefunctions will be perturbed.

$$\left|\phi_m\right\rangle = \left|\psi_m\right\rangle + \left|\phi_m^{(1)}\right\rangle + \dots$$

$$\left|\phi_m\right\rangle = \left|\psi_m\right\rangle + \sum_{n \neq m} \frac{\left\langle\psi_n\left|H_p\right|\psi_m\right\rangle}{E_m - E_n}\left|\psi_n\right\rangle + \dots$$

Now we can just apply the equation for the polarization P.

$$P = q\left\langle\phi\left|z - z_0\right|\phi\right\rangle$$

$$P = q\left[\begin{array}{l} \left\langle\psi_m\left|z - z_0\right|\psi_m\right\rangle + \left\langle\psi_m\left|z - z_0\right|\phi_m^{(1)}\right\rangle \\ + \left\langle\phi_m^{(1)}\left|z - z_0\right|\psi_m\right\rangle + \left\langle\phi_m^{(1)}\left|z - z_0\right|\phi_m^{(1)}\right\rangle \end{array} \right]$$

We can throw out the first term (defined as zero due to symmetry of the initial wavefunction) and the last term (since it is second order in the perturbed wavefunction).

$$P = q\left[\left\langle\psi_m\left|z - z_0\right|\phi_m^{(1)}\right\rangle + \left\langle\phi_m^{(1)}\left|z - z_0\right|\psi_m\right\rangle\right]$$

$$P = q\left[\begin{array}{l} \left\langle\psi_m\left|z - z_0\right|\left[\sum_{n \neq m} \frac{\left\langle\psi_n\left|H_p\right|\psi_m\right\rangle}{E_m - E_n}\left|\psi_n\right\rangle\right]\right\rangle + \\ \left[\sum_{n \neq m} \left(\frac{\left\langle\psi_n\left|H_p\right|\psi_m\right\rangle}{E_m - E_n}\right)^* \left\langle\psi_n\right|\right]\left|z - z_0\right|\psi_m\right\rangle \end{array} \right]$$

$$P = q\left[\begin{array}{l} \left[\sum_{n \neq m} \frac{\left\langle\psi_n\left|H_p\right|\psi_m\right\rangle}{E_m - E_n}\left\langle\psi_m\left|z - z_0\right|\psi_n\right\rangle\right] + \\ \left[\sum_{n \neq m} \left(\frac{\left\langle\psi_n\left|H_p\right|\psi_m\right\rangle}{E_m - E_n}\right)^* \left\langle\psi_n\left|z - z_0\right|\psi_m\right\rangle\right] \end{array} \right]$$

Substituting in for the perturbing Hamiltonian,

$$P = q \left[\begin{array}{c} \left[\displaystyle\sum_{n \neq m} \dfrac{\left\langle \psi_n \left| -qF(z-z_0) \right| \psi_m \right\rangle}{E_m - E_n} \left\langle \psi_m \left| z-z_0 \right| \psi_n \right\rangle \right] + \\[4mm] \left[\displaystyle\sum_{n \neq m} \left(\dfrac{\left\langle \psi_n \left| -qF(z-z_0) \right| \psi_m \right\rangle}{E_m - E_n} \right)^* \left\langle \psi_n \left| z-z_0 \right| \psi_m \right\rangle \right] \end{array} \right]$$

$$P = -q^2 F \left[\begin{array}{c} \left[\displaystyle\sum_{n \neq m} \dfrac{\left\langle \psi_n \left| z-z_0 \right| \psi_m \right\rangle}{E_m - E_n} \left\langle \psi_m \left| z-z_0 \right| \psi_n \right\rangle \right] + \\[4mm] \left[\displaystyle\sum_{n \neq m} \dfrac{\left\langle \psi_m \left| z-z_0 \right| \psi_n \right\rangle}{E_m - E_n} \left\langle \psi_n \left| z-z_0 \right| \psi_m \right\rangle \right] \end{array} \right]$$

$$P = -q^2 F \left[2 \left[\sum_{n \neq m} \dfrac{\left\langle \psi_n \left| z-z_0 \right| \psi_m \right\rangle}{E_m - E_n} \left\langle \psi_m \left| z-z_0 \right| \psi_n \right\rangle \right] \right]$$

$$P = -q^2 F \left[2 \left[\sum_{n \neq m} \dfrac{\left| \left\langle \psi_n \left| z-z_0 \right| \psi_m \right\rangle \right|^2}{E_m - E_n} \right] \right]$$

(iii) First order perturbation theory gives zero for the energy correction. Going to second order,

$$E_m^{(2)} = \sum_{n \neq m} \frac{\left| \left\langle \psi_n \left| \hat{H}_p \right| \psi_m \right\rangle \right|^2}{E_m - E_n} = \sum_{n \neq m} \frac{\left| \left\langle \psi_n \left| -qF(z-z_0) \right| \psi_m \right\rangle \right|^2}{E_m - E_n}$$

$$E_m^{(2)} = q^2 F^2 \sum_{n \neq m} \frac{\left| \left\langle \psi_n \left| (z-z_0) \right| \psi_m \right\rangle \right|^2}{E_m - E_n}$$

(iv)

$$\Delta E = q^2 F^2 \sum_{n \neq m} \frac{\left| \left\langle \psi_n \left| (z-z_0) \right| \psi_m \right\rangle \right|^2}{E_m - E_n}$$

$$P = -q^2 F \left[2 \left[\sum_{n \neq m} \frac{\left| \left\langle \psi_n \left| z-z_0 \right| \psi_m \right\rangle \right|^2}{E_m - E_n} \right] \right]$$

$$P = \frac{-2}{F} \left[q^2 F^2 \sum_{n \neq m} \frac{\left| \left\langle \psi_n \left| (z-z_0) \right| \psi_m \right\rangle \right|^2}{E_m - E_n} \right] = \frac{-2}{F} \Delta E$$

$$\Delta E = -\frac{1}{2} PF$$

6.4.1

(i) The three degenerate "first excited" states of a cubic quantum box are, with the coordinate origin in the middle of the box,

$$\psi_1(x,y,z) = \left(\frac{2}{L}\right)^{3/2} \sin\left(\frac{2\pi x}{L}\right)\cos\left(\frac{\pi y}{L}\right)\cos\left(\frac{\pi z}{L}\right)$$

$$\psi_2(x,y,z) = \left(\frac{2}{L}\right)^{3/2} \cos\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi y}{L}\right)\cos\left(\frac{\pi z}{L}\right)$$

$$\psi_3(x,y,z) = \left(\frac{2}{L}\right)^{3/2} \cos\left(\frac{\pi x}{L}\right)\cos\left(\frac{\pi y}{L}\right)\sin\left(\frac{2\pi z}{L}\right)$$

(ii) With the potential energy

$$V_p = eFz \equiv \hat{H}_p$$

acting as the perturbing Hamiltonian, where F is the electric field, we have, for the various matrix elements

$$H_{11} = H_{22} = H_{33} = H_{12} = H_{21} = 0$$

by parity in the z direction,

$$H_{13} = H_{31} = 0$$

by parity in the x direction, and

$$H_{23} = H_{32} = 0$$

by parity in the y direction.

Hence, we are left with a first-order degenerate perturbing matrix of the zero matrix (all the matrix elements are zero), so there is no first-order degenerate perturbation correction to the energies in this case.

(iii) With the potential energy

$$V_p = \alpha z^2 = \hat{H}_p$$

acting as the perturbing Hamiltonian,

$$H_{11} = \left(\frac{2}{L}\right)^3 \alpha \int_{-\frac{L}{2}}^{\frac{L}{2}} \int_{-\frac{L}{2}}^{\frac{L}{2}} \int_{-\frac{L}{2}}^{\frac{L}{2}} \sin^2\left(\frac{2\pi x}{L}\right)\cos^2\left(\frac{\pi y}{L}\right) z^2 \cos^2\left(\frac{\pi z}{L}\right) dx\,dy\,dz = A$$

$$= H_{22}$$

$$H_{33} = \left(\frac{2}{L}\right)^3 \alpha \int_{-\frac{L}{2}}^{\frac{L}{2}} \int_{-\frac{L}{2}}^{\frac{L}{2}} \int_{-\frac{L}{2}}^{\frac{L}{2}} \cos^2\left(\frac{\pi x}{L}\right)\cos^2\left(\frac{\pi y}{L}\right) z^2 \sin^2\left(\frac{2\pi z}{L}\right) dx\,dy\,dz = B$$

Also $H_{12} = H_{21} = H_{13} = H_{31} = 0$ by parity in the x direction, and $H_{23} = H_{32} = 0$ by parity in the y direction. Hence, the degenerate perturbation eigen equation (Eq. 6.67) becomes

$$
\begin{bmatrix} A & 0 & 0 \\ 0 & A & 0 \\ 0 & 0 & B \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = E^{(1)} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix}
$$

where formally

$$
\psi = a_1\psi_1 + a_2\psi_2 + a_3\psi_3
$$

Because the matrix is diagonal, there is no mixing of the original degenerate basis set by the perturbation.

The resulting perturbed states are

ψ_1 with additive energy correction A

ψ_2 with additive energy correction A

ψ_3 with additive energy correction B

Formally evaluating, we have

$$
A = \frac{\alpha 2}{L} \int_{-L/2}^{L/2} \sin^2(\frac{2\pi x}{L}) dx \, \frac{2}{L} \int_{-L/2}^{L/2} \cos^2(\frac{\pi y}{L}) dy \, \frac{2}{L} \int_{-L/2}^{L/2} z^2 \cos^2(\frac{\pi z}{L}) dz
$$

The first two integrals with their $2/L$ factors become unity because the wavefunctions are normalized. Then we are left with

$$
A = \alpha \frac{2}{L} \int_{-L/2}^{L/2} z^2 \cos^2(\frac{\pi z}{L}) dz = \alpha \frac{2}{L} \frac{L^3}{\pi^3} \int_{-\pi/2}^{\pi/2} \theta^2 \cos^2 \theta \, d\theta
$$

where

$$
\theta = \frac{\pi z}{L}, \text{ i.e., } z = \frac{L\theta}{\pi}
$$

Since

$$
\int_{-\pi/2}^{\pi/2} \theta^2 \cos^2 \theta \, d\theta = \frac{\pi^3}{24} - \frac{\pi}{4}
$$

then

$$
A = \alpha \frac{2L^2}{\pi^3} \left[\frac{\pi^3}{24} - \frac{\pi}{4} \right] = \alpha L^2 \left[\frac{1}{12} - \frac{1}{2\pi^2} \right]
$$

Similarly, evaluating B gives

$$
B = \alpha \frac{2}{L} \int_{-L/2}^{L/2} z^2 \sin^2(\frac{2\pi z}{L}) dz
$$

$$
= \alpha \frac{2}{L} \frac{L^3}{\pi^3} \int_{-\pi/2}^{\pi/2} \theta^2 \sin^2(2\theta) dz
$$

Since

$$\int_{-\pi/2}^{\pi/2} \theta^2 \sin^2(2\theta)d\theta = \frac{\pi^3}{24} - \frac{\pi}{16}$$

$$B = \alpha L^2 \left[\frac{1}{12} - \frac{1}{8\pi^2} \right]$$

Hence, finally we find that the degeneracy is partially lifted with the ψ_3 state at a higher energy than the two degenerate states ψ_1 and ψ_2 (for positive α), whose energy is also raised by a positive amount (for positive α).

6.5.1

Taking the same approach as for two wells, with the same notation, we obtain a Hamiltonian matrix

$$\hat{H} = \begin{pmatrix} E_1 & \Delta E & 0 \\ \Delta E & E_1 & \Delta E \\ 0 & \Delta E & E_1 \end{pmatrix}$$

where ΔE is the overlap integral in one barrier. The eigenvalues are obtained from setting the determinant to zero as usual

$$\begin{vmatrix} E_1 - E & \Delta E & 0 \\ \Delta E & E_1 - E & \Delta E \\ 0 & \Delta E & E_1 - E \end{vmatrix} = 0$$

i.e.,

$$(E_1 - E)\left[(E_1 - E)^2 - \Delta E^2\right] - \Delta E\left[\Delta E(E_1 - E)\right]$$
$$= (E_1 - E)\left[(E_1 - E)^2 - 2\Delta E^2\right]$$
$$= (E_1 - E)\left(E_1 - E + \sqrt{2}\Delta E\right)\left(E_1 - E - \sqrt{2}\Delta E\right) = 0$$

There are now three possible solutions for E, namely

$$E = E_1 - \sqrt{2}\left|\Delta E\right|, E_1, E_1 + \sqrt{2}\left|\Delta E\right|$$

The resulting normalized eigenvectors are

$$\psi_1 = \frac{1}{4}\begin{bmatrix} 1 \\ \sqrt{2} \\ 1 \end{bmatrix}, \ \psi_2 = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}, \ \psi_3 = \frac{1}{4}\begin{bmatrix} 1 \\ -\sqrt{2} \\ 1 \end{bmatrix}$$

or, expressed in terms of the isolated well wavefunctions, ψ_{left}, ψ_{middle}, and ψ_{right},

$$\psi_1 = \frac{1}{4}\psi_{left} + \frac{1}{2\sqrt{2}}\psi_{middle} + \frac{1}{4}\psi_{right} \ \text{(no zeros)}$$

$$\psi_2 = \frac{1}{\sqrt{2}}\psi_{left} - \frac{1}{\sqrt{2}}\psi_{right} \ \text{(one zero, in the middle)}$$

$$\psi_3 = \frac{1}{4}\psi_{left} - \frac{1}{2\sqrt{2}}\psi_{middle} + \frac{1}{4}\psi_{right} \ \text{(two zeros, one in each barrier)}$$

6.5.2

(i) At $t = 0$, $\psi = \psi_{left} = \dfrac{1}{\sqrt{2}}\left(\psi_+ + \psi_-\right)$, so at a later time

$$\psi = \frac{1}{\sqrt{2}}\left[\psi_+ \exp\left(-i(E + \Delta E)t/\hbar\right) + \psi_- \exp\left(-i(E - \Delta E)t/\hbar\right)\right]$$

For the probability density, we have

$$|\psi|^2 = \frac{1}{2}\left[|\psi_+|^2 + |\psi_-|^2 + \psi_-^*\psi_+ \exp\left(-i(2\Delta E)t/\hbar\right) + \psi_-\psi_+^* \exp\left(-i(-2\Delta E)t/\hbar\right)\right]$$

i.e.,
$$|\psi|^2 = \frac{1}{2}\left(|\psi_+|^2 + |\psi_-|^2 + \psi_-\psi_+\left(2\cos\left((2\Delta E)t/\hbar\right)\right)\right)$$

(ii) The probability density moves back and forth between the two wells. At $t = 0$, it is essentially in the left well, and after a time $t_\pi = \pi\dfrac{\hbar}{2\Delta E}$ the probability density is essentially in the right well.

6.6.1

The finite basis subset method will only ever give a solution that is a linear combination of the finite set of basis functions used. If that set includes, or can exactly represent, the energy eigenstate with the lowest energy eigenvalue, then it is possible that the finite basis subset method will return that state as the result, in which case we can have this method return the exact energy value for the lowest energy eigenstate. Otherwise, the method will return a larger answer because any other linear combination will have a larger value for its energy expectation value because of the variational principle.

Formally, since the energy eigenfunctions for the problem of interest $|\psi_{Em}\rangle$ form a complete set (with energy eigenvalues E_m), we can expand each of the members of the finite basis subset $|\psi_{fbn}\rangle$ in them; that is,

$$|\psi_{fbn}\rangle = \sum_m a_{nm} |\psi_{Em}\rangle$$

Consider, then, some normalized linear combination $|\psi_{FB}\rangle$ of this finite set

$$|\psi_{FB}\rangle = \sum_n b_n |\psi_{fbn}\rangle = \sum_n \sum_m b_n a_{nm} |\psi_{Em}\rangle = \sum_m c_m |\psi_{Em}\rangle$$

where

$$c_m = \sum_n b_n a_{nm}$$

and

$$\sum_m |c_m|^2 = 1$$

by normalization.

Then, for the expectation value of the Hamiltonian $\hat{H}$ in this state we have

$$\langle \psi_{FB} | \hat{H} | \psi_{FB} \rangle = \sum_{p,m} c_p^* c_m \langle \psi_{Ep} | \hat{H} | \psi_{Em} \rangle = \sum_m |c_m|^2 E_m \geq E_1$$

where E_1 is the lowest energy eigenvalue. This last step is the standard step in the variational argument; the smallest the last sum can be, given the normalization condition above, is if $|c_1|^2 = 1$. Any other choice means that there is a finite amount of a higher energy in the sum, which makes the sum necessarily larger.

In this argument, we have not really used the finiteness of the basis subset; we have only had to allow that this set may be a different set of functions from the actual energy eigenfunctions (though it does not have to be a different set).

6.6.2

(i) Solving for the first two states.

We use the finite matrix method, using the eigenfunctions of the infinite well problem as the basis set, and evaluating the integrals numerically to construct the Hamiltonian matrix. In the computer program to calculate this, we have the number of the basis functions used (and hence the dimension of the matrix) as a variable, and we keep increasing that until we have at least apparently converged to the answer within 5%. In this case, we ended up using a 6 x 6 matrix. (We also can check this by perturbation theory.)

Finding the eigenvalues of this matrix gives, for the first energy eigenvalue

$$E_1 = 0.07098 \text{ eV}$$

and for the second energy eigenvalue

$$E_2 = 0.167 \text{ eV}$$

with corresponding eigenvectors

$$|\phi_1\rangle = \begin{bmatrix} 0.995 \\ 0 \\ 0.095 \\ 0 \\ -0.030 \\ 0 \end{bmatrix} \quad |\phi_2\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Note that the first eigenfunction, though predominantly still the first basis state, has measurable admixtures of the third and fifth basis states, whereas the second eigenfunction is essentially entirely the unperturbed second basis state.

(A second-order perturbation calculation gives 0.06986 eV for the first level, which confirms we can have reasonable grounds for believing we have a result within 5% for this first level.)

We plot the wavefunctions below, including the perturbation calculation of the first level. Note that, though not identical, the two methods (finite basis subset and perturbation) give very similar results for the first eigenfunction. The second eigenfunction is essentially the unperturbed second basis function.

1st state (finite matrix)
1st state (perturbation)
2nd state (finite matrix)
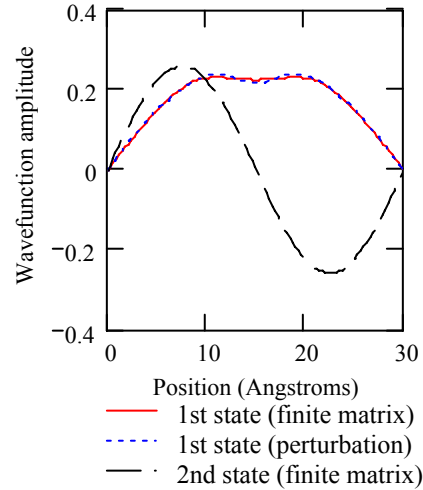
(ii) Polarizability

To calculate polarizability, we will need to do a perturbation theory calculation. In this case, however, we want to regard the perturbation as the potential from the applied electric field, not the potential step inserted in the well. A key point in doing this calculation is to use wavefunctions calculated in the first part as the basis set for calculations in this second part. As always, a good choice for the basis functions for solving the problem is the energy eigenfunctions from the unperturbed problem. In the finite matrix model above, we calculated a set of 6 functions that are approximate solutions to the problem without field. We will use these here as the new basis set. One might argue that this is not a very complete basis set, but we know from perturbation theory that eigenstates corresponding to energy levels that are far away in energy from the state of interest have little effect on the result because of the energy denominators that enter in the perturbation calculations. Indeed, if there is one state that is close and for which the relevant matrix element is substantial, that may dominate the calculation.

With our perturbing Hamiltonian in the form

$$\hat{H}_{pF} = eF\left(z - L_z / 2\right)$$

we find first that the first order perturbation theory correction is zero (by symmetry), and so we have to go to second order. The result of this calculation is, for unit field (squared)

$$\Delta E_1 = -364.277 F^2$$

where the fields are in V/Å, and the energies are in electron-volts. Hence we have

$$\alpha = 728.553 \ \text{eV/(V/Å)}^2$$

To check this out in terms of the size of the effect, note that the energy of the first state in this system is $\sim$ 70 meV. A field corresponding to 1/10 th of this energy over the thickness (30 Å) of this structure is a field of 2.333 x 10^{-3} V/Å leads to a shift of $\sim$ 2 meV, which seems a reasonable magnitude of shift for such a problem.

See the following Mathcad worksheet for detailed calculations.

Problem 6.6.2 Solution Mathcad worksheet

Setting up the problem

We consider the potential structure shown below.
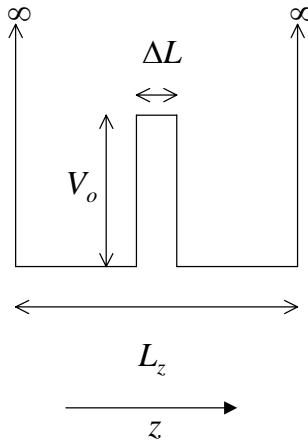
We set the specific values for the parameters. We will use Angstroms for the distance units, and electron volts for the energy units.

$$Lz := 30 \qquad \Delta L := 0.5 \quad Vo := 1$$

The relevant fundamental constants are, in the usual MKS units,

$$hbar := 1.055 \cdot 10^{-34} \qquad mo := 9.1095 \cdot 10^{-31} \qquad q := 1.602 \cdot 10^{-19}$$

In the Angstrom and electron volt units, the Hamiltonian becomes, within the well, with

$$A := hbar \cdot \frac{hbar}{2 \cdot q \cdot mo \cdot 10^{-20}} \qquad A = 3.813$$

$$\hat{H} = -A\frac{d^2}{dz^2} + V_o \mathrm{rect}\left[\frac{(L_z - \Delta L)}{2}, \frac{(L_z + \Delta L)}{2}\right]$$

where the rect(a,b) function (rectangle function) is the function that is unity between a and b and zero elsewhere.

We will use as a basis here, in the first part of the problem, the energy eigenfunctions of the infinitely deep potential well of thickness Lz. This is a typical choice, using the eigenfunctions of the unperturbed problem as the basis. Hence our basis functions are

$$\psi(z, n) := \sqrt{\frac{2}{Lz}} \cdot \sin\left(n \cdot \pi \cdot \frac{z}{Lz}\right)$$

With this choice, we are taking the position origin to be at the left of the structure.

We also need formally to tell the program that we want all vector and matrix indices to start at 1 rather than zero

$$ORIGIN \equiv 1$$

We will also suppress here any very small results in matrix elements by suppressing scientific notation in the display of the results. Very small negative results show up as -0.

(i) Solving for the first two states

Finite basis subset approach

The matrix elements of the Hamiltonian can be written as

$$H(i,j) := -A \cdot \int_0^{Lz} \psi(z,i) \cdot \frac{d^2}{dz^2} \psi(z,j) \, dz + Vo \cdot \int_{\frac{(Lz-\Delta L)}{2}}^{\frac{(Lz+\Delta L)}{2}} \psi(z,i) \cdot \psi(z,j) \, dz$$

We will construct the Hamiltonian, using as the basis subset the first p eigenfunctions of the unperturbed problem, and we choose p here. The final p chosen here is chosen to be high enough to give apparent convergence to the desired accuracy (~5%), and agreement with the perturbation calculation below for the first energy level within ~5%.

$$p := 6$$

We now formally construct the Hamiltonian matrix. We start by defining integer range variables for the calculation.

$$i := 1, 2 .. p \qquad j := 1, 2 .. p$$

$$Hamiltonian_{i,j} := H(i,j)$$

For our chosen parameter values, this matrix then is, numerically,

$$Hamiltonian = \begin{pmatrix} 0.075 & 0 & -0.033 & 0 & 0.033 & 0 \\ -0 & 0.167 & 0 & -0 & 0 & 0 \\ -0.033 & 0 & 0.41 & 0 & -0.033 & 0 \\ -0 & -0 & -0 & 0.669 & 0 & -0 \\ 0.033 & 0 & -0.033 & 0 & 1.079 & 0 \\ -0 & 0 & -0 & -0 & -0 & 1.506 \end{pmatrix}$$

Note that this matrix is Hermitian as expected. (In this particular case, all the elements are real.) Now we find the eigenvalues of this matrix.

$$E := \text{eigenvals}(\text{Hamiltonian})$$

$$E = \begin{pmatrix} 0.071 \\ 1.081 \\ 0.411 \\ 1.506 \\ 0.167 \\ 0.669 \end{pmatrix}$$

Note, incidentally, that the eigenvalues, and the corresponding eigenvectors, are not in order in the result returned by the program. This will not cause any problems, but needs to be remembered.

The lowest energy eigenvalue is therefore

$$E_1 = 0.07098$$ electron volts

Note that this solution says that the energy of the first eigenstate has been pushed to higher energy.

The second energy eigenvalue is, in this particular case

$$E_5 = 0.167$$ electron volts

Note that this is numerically unchanged from the unperturbed case.

For the corresponding eigenvectors, we have

$$\phi 1 := \text{eigenvec}\left(\text{Hamiltonian}, E_1\right) \qquad \phi 2 := \text{eigenvec}\left(\text{Hamiltonian}, E_5\right)$$

$$\phi 1 = \begin{pmatrix} 0.995 \\ 0 \\ 0.095 \\ 0 \\ -0.03 \\ 0 \end{pmatrix} \qquad \phi 2 = \begin{pmatrix} 0 \\ 1 \\ -0 \\ 0 \\ -0 \\ -0 \end{pmatrix}$$

Note that the first eigenfunction, though predominantly still the first basis state, has measurable admixtures of the third and fifth basis states, whereas the second eigenfunction is essentially entirely the unperturbed second basis state.

For the convenience of the program we also formally calculate all of the eigenvectors, expressed as a matrix, with the eigenvectors as the columns, in the same order from left to right as the eigenvalues are from top to bottom in the above vector E.

$$\phi\text{kets} := \text{eigenvecs}(\text{Hamiltonian})$$

$$\phi\text{kets} = \begin{pmatrix} 0.995 & 0.035 & -0.093 & 0 & 0 & -0 \\ 0 & 0 & 0 & 0 & 1 & -0 \\ 0.095 & -0.051 & 0.994 & 0 & -0 & 0 \\ 0 & 0 & 0 & -0 & 0 & 1 \\ -0.03 & 0.998 & 0.054 & 0 & -0 & -0 \\ 0 & 0 & 0 & 1 & -0 & 0 \end{pmatrix}$$

The wavefunctions themselves are, explicitly,

$$\phi\text{fb}(z, j) := \sum_{n = 1}^{p} \phi\text{kets}_{n, j} \cdot \psi(z, n)$$

We will graph these below

Perturbation theory approach

We can check the above result for the first level energy and wavefunction by using a perturbation approach. The perturbing Hamiltonian is

$$\hat{H}_p = V_o \text{rect}\left[\frac{(L_z - \Delta L)}{2}, \frac{(L_z + \Delta L)}{2}\right]$$

The energies of state m of the unperturbed problem are

$$\text{Eu}(i) := A \cdot \left(i \cdot \frac{\pi}{Lz}\right)^2$$

Hence the sums for n not equal to m or i not equal to m reduce to sums starting at n = 2 or i = 2. Also, we already know what Eu(1), the energy of the first unperturbed state, is.

$$\text{Eu}(1) = 0.042 \quad \text{electron volts}$$

For future comparison, we can calculate the second level of the "unperturbed" problem. We find

$$\text{Eu}(2) = 0.167 \quad \text{electron volts}$$

For the perturbation theory calculation, we will need the matrix elements of the perturbing Hamiltonian, which are

$$Hp(i,j) := Vo \cdot \int_{\frac{(Lz-\Delta L)}{2}}^{\frac{(Lz+\Delta L)}{2}} \psi(z,i) \cdot \psi(z,j) \, dz$$

We will define a practical upper limit for our summations

$q := 10$

We calculate the first order correction to the energy.

$E1 := Hp(1,1)$ $E1 = 0.033$

The second order correction to the energy is

$$E2 := \sum_{i=2}^{q} \frac{(|Hp(i,1)|)^2}{Eu(1) - Eu(i)}$$

which gives

$E2 = -5.2873 \times 10^{-3}$

The pertubation result for the energy is therefore, to second order

$Esecond := Eu(1) + E1 + E2$ $\boxed{Esecond = 0.06986}$

This agrees well with the finite basis subset approach above, so we can reasonably conclude that

$\boxed{\text{The energy of the first state is } \sim 0.07 \text{ eV}}$

The energy of the second level has not been changed compared to the unperturbed state, which is consistent with the fact that the wavefunction is apparently also essentially unperturbed, and hence we can state that

$\boxed{\text{the energy of the second state is } \sim 0.167 \text{ eV}}$

Now let us calculate the first order correction to the wave function. The first order coefficients are

$$a1(i) := \frac{Hp(i,1)}{Eu(1) - Eu(i)}$$

so the ket from this first order perturbation calculation has elements (considering the first 6)

$\phi ketp_1 := 1$ $\phi ketp_2 := a1(2)$ $\phi ketp_3 := a1(3)$ $\phi ketp_4 := a1(4)$ $\phi ketp_5 := a1(5)$ $\phi ketp_6 := a1(6)$

$$\phi ketp = \begin{pmatrix} 1 \\ 0 \\ 0.1 \\ 0 \\ -0.033 \\ 0 \end{pmatrix}$$

For comparison, the finite basis subset version is

$$\phi1 = \begin{pmatrix} 0.995 \\ 0 \\ 0.095 \\ 0 \\ -0.03 \\ 0 \end{pmatrix}$$

which is in quite good agreement. We note that the even coefficients are all zero. This can be deduced from the symmetry of the wavefunction and the potential. The complete wavefunction including the first order perturbation correction is therefore,

$$\phi p1(z) := \psi(z,1) + \sum_{i\,=\,2}^{q} a1(i)\,\psi(z,i)$$

Now we can graph both of the approximations to the lowest wavefunction, and the second wavefunction obtained from the finite basis set approach. First we need to define a range variable for plotting

$$delta := \frac{Lz}{100} \qquad\qquad zrange := 0, delta..Lz$$

Position (Angstroms)
—— 1st state (finite matrix)
·········· 1st state (perturbation)
------ 2nd state (finite matrix)

Note that, though not identical, the two methods (finite basis subset and perturbation) give very similar results for the first eigenfunction. The second eigenfunction is essentially the unperturbed second basis function.

(ii) Polarizability

To calculate polarizability, we will need to do a perturbation theory calculation. In this case, however, we want to regard the perturbation as the potential from the applied electric field, not the potential step inserted in the well. A key point in doing this calculation is to use wavefunctions calculated in the first part as the basis set for calculations in ths second part. As always, a good choice for the basis functions for solving the problem is the energy eigenfunctions from the unperturbed problem. In the finite basis subset model above, we calculated a set of 6 functions that are approximate solutions to the problem without field. We will use these here as the new basis set. One might argue that this is not a very complete basis set, but we know from perturbation theory that eigenstates corresponding to energy levels that are far away in energy from the state of interest have little effect on the result because of the energy denominators that enter in the perturbation calculations. Indeed, if there is one state that is close and for which the relevant matrix element is substantial, that may dominate the calculation. Hence we use as our basis set the functions ϕfb(z,j) calculated above in the finite basis subset method, with corresponding energies E_j.

The unperturbed Hamiltonian is now

$$\hat{H}_o = -A\frac{d^2}{dz^2} + V_o \text{rect}\left[\frac{(L_z - \Delta L)}{2}, \frac{(L_z + \Delta L)}{2}\right]$$

and the perturbing Hamiltonian is now

$$H_{pF} = qF\left(z - L_z/2\right)$$

It will be more convenient for us to calculate the perturbation per unit field, HpoF=HpF/F, and to calculate energies in electron volts, so we can also drop the factor q (the electronic charge). Also, since our distance units in this problem are Angstroms, we are implicitly using field units of volts/Angstrom. Hence, the matrix elements of the perturbation are, per unit field

$$\text{HpoF}_{i,j} := \int_0^{Lz} \phi\text{fb}(z,i)\left(z - \frac{Lz}{2}\right) \cdot \phi\text{fb}(z,j)\, dz$$

which gives

$$\text{HpoF} = \begin{pmatrix} -0 & -0 & -0 & 0.003 & -5.915 & -0.816 \\ -0 & -0 & -0 & -5.99 & -0.44 & -5.705 \\ -0 & -0 & -0 & -0.911 & -5.329 & -6.204 \\ 0.003 & -5.99 & -0.911 & -0 & -0 & -0 \\ -5.915 & -0.44 & -5.329 & -0 & -0 & -0 \\ -0.816 & -5.705 & -6.204 & -0 & -0 & 0 \end{pmatrix}$$

Note, incidentally, that the eigenvalues and eigenvectors returned by the finite basis subset method were not ordered. The first eigenvalue and eigenvector corresponded to the first (lowest energy) state, but it was the fourth eigenvalue and eigenvector that corresponded to the second

(second lowest energy) state. We see here, therefore, that the largest matrix element associated with the first state (i.e., those in the first row or column) is the matrix element for interaction with the second state of the system (fourth eigenvector) as one might expect.

Now let us check by calculating the first order correction, EF1 to the energy. We have (per unit field)

$$\text{EF1} := \text{HpoF}_{1,1} \qquad \text{EF1} = -0$$

For the second order correction, we have, per unit field squared

$$\text{EF2} := \sum_{i=2}^{p} \frac{\left(\left|\text{HpoF}_{i,1}\right|\right)^2}{E_1 - E_i} \qquad \text{EF2} = -364.277$$

By the definition of polarizability, we have

$$\alpha := -2 \cdot \text{EF2}$$

That is

$$\alpha = 728.553$$

To check this out in terms of the size of the effect, note that the energy of the first state in this system is ~ 70 meV. A field corresponding to 1/10 th of this energy over the thickness (30 Angstroms) of this structure is a field of

$$\text{Ftest} := \frac{0.07}{\text{Lz}} \qquad \text{Ftest} = 2.333 \times 10^{-3} \quad \text{Volts per Angstrom}$$

which would give a shift of

$$\text{Eshift} := \frac{\alpha \cdot \text{Ftest}^2}{2} \qquad \text{Eshift} = 1.983 \times 10^{-3} \quad \text{electron volts}$$

that is, about 2 meV, which intuitively seems a reasonable magnitude of shift for such a problem.

Chapter 7 problem solutions

7.1.1

(i) Recall that, for a potential well with infinitely high walls and a particle of mass (or effective mass) m_{eff}, the energy and wavefunction for the nth level are given by, respectively,

$$E_n^{(0)} = \frac{n^2 \hbar^2 \pi^2}{2 m_{eff} L_z^2} \quad \text{and} \quad \left|\psi_n^{(0)}\right\rangle = \sqrt{\frac{2}{L_z}} \sin(\frac{n\pi z}{L_z})$$

Because the electron is initially in the lowest state of this well, the unperturbed state is $\left|\psi_1^{(0)}\right\rangle$, i.e., in the expansion for the unperturbed wavefunction

$$a_1^{(0)} = 1 \quad \text{and} \quad a_n^{(0)} = 0 \quad \text{where } n > 1 \tag{1}$$

To find the probability of finding the electron in the second state, we need to know the coefficient of the second (unperturbed) wavefunction in the expansion representing the perturbed wavefunction. Here, we look at only the first order change in that coefficient. It can be found by integrating

$$\dot{a}_2^{(1)}(t) = \frac{1}{i\hbar} \sum_n a_n^{(0)} \exp\left(i\omega_{2n}t\right)\left\langle \psi_2 \middle| \hat{H}_p(t) \middle| \psi_n \right\rangle$$

Using (1), we have

$$\dot{a}_2^{(1)}(t) = \frac{1}{i\hbar} a_1^{(0)} \exp\left(i\omega_{21}t\right)\left\langle \psi_2 \middle| \hat{H}_p(t) \middle| \psi_1 \right\rangle$$

Now, using the usual electric dipole energy of an electron in an electric field of strength F, we have, using our given form of the electric field with time

$$\hat{H}_p(t) = eF(t)\left(z - \frac{L_z}{2}\right) = eF_o \sin\left(\pi t / \Delta t\right)\left(z - \frac{L_z}{2}\right)$$

where we have chosen the potential origin in the middle of the well. So

$$\left\langle \psi_2 \middle| \hat{H}_p(t) \middle| \psi_1 \right\rangle = eF_o \sin\left(\pi t / \Delta t\right) \int_0^{L_z} \sqrt{\frac{2}{L_z}} \sin(\frac{2\pi z}{L_z})\left(z - \frac{L_z}{2}\right)\sqrt{\frac{2}{L_z}} \sin(\frac{\pi z}{L_z}) dz$$

With a change of variable to $\zeta = \pi z / L_z$

$$\int_0^{L_z} \sqrt{\frac{2}{L_z}} \sin(\frac{2\pi z}{L_z})\left(z - \frac{L_z}{2}\right)\sqrt{\frac{2}{L_z}} \sin(\frac{\pi z}{L_z}) dz = \frac{2}{L_z}\left(\frac{L_z}{\pi}\right)^2 \int_0^{\pi}\left(\zeta - \frac{\pi}{2}\right)\sin\left(2\zeta\right)\sin\left(\zeta\right) d\zeta$$

$$= \frac{2}{L_z}\left(\frac{L_z}{\pi}\right)^2\left(-\frac{8}{9}\right) = \frac{-16 L_z}{9\pi^2}$$

where we have used a standard result for the integral (see Appendix G of the book). That is,

$$\left\langle \psi_2 \middle| \hat{H}_p(t) \middle| \psi_1 \right\rangle = eF_o \sin\left(\pi t / \Delta t\right)\left(-\frac{16 L_z}{9\pi^2}\right)$$

Now integrating over time to get the desired coefficient

$$a_2^{(1)}(t) = \int_0^{\Delta t} \frac{1}{i\hbar} a_1^{(0)} \exp(i\omega_{21}t)\langle\psi_2|\hat{H}_p(t)|\psi_1\rangle dt$$

$$= \int_0^{\Delta t} \frac{1}{i\hbar} \exp(i\omega_{21}t) eF_o \sin(\pi t/\Delta t)\left(-\frac{16L_z}{9\pi^2}\right)dt$$

$$= \frac{1}{i\hbar} eF_o\left(-\frac{16L_z}{9\pi^2}\right)\int_0^{\Delta t} \exp(i\omega_{21}t)\sin(\pi t/\Delta t)\,dt$$

$$= \frac{-1}{2\hbar} eF_o\left(-\frac{16L_z}{9\pi^2}\right)\int_0^{\Delta t} \exp(i\omega_{21}t)\left(\exp(i\pi t/\Delta t) - \exp(-i\pi t/\Delta t)\right)dt$$

$$= \frac{1}{i\hbar} eF_o\left(\frac{16L_z}{9\pi}\right)\frac{\Delta t\left(1+\exp\left(i\dfrac{3E_1^{(0)}}{\hbar}\Delta t\right)\right)}{\left(\left(\dfrac{3E_1^{(0)}}{\hbar}\Delta t\right)^2 - \pi^2\right)}$$

(There are several relatively straightforward algebraic steps between the last two lines.) The probability of finding the electron in the second level is therefore

$$\left|a_2^{(1)}(t)\right|^2 = \left(\frac{16eF_oL_z\Delta t}{9\pi\hbar}\right)^2 \frac{4\cos^2\left(\dfrac{3E_1^{(0)}}{2\hbar}\Delta t\right)}{\left(\left(\dfrac{3E_1^{(0)}}{\hbar}\Delta t\right)^2 - \pi^2\right)^2}$$

where we used the identity $2\cos^2(\theta/2) = 1 + \cos\theta$.

(ii) For a GaAs semiconductor structure with $m_{eff} = 0.07m_o$ and width $L_z = 10$ nm, we have

$$\frac{E_1^{(0)}}{\hbar} = \frac{\hbar\pi^2}{2m_{eff}L_z^2} = \frac{1.055\times10^{-34}\times\pi^2}{2\times0.07\times9.109\times10^{-31}\times10^{-16}} = 8.16\times10^{13}\text{ s}^{-1}$$

so for $\Delta t = 100$ fs, $\dfrac{3E_1^{(0)}}{2\hbar}\Delta t \simeq 12.25$ and hence

$$\cos\left(\frac{3E_1^{(0)}}{2\hbar}\Delta t\right) \simeq 0.950 \text{ and } \cos^2\left(\frac{3E_1^{(0)}}{2\hbar}\Delta t\right) \simeq 0.89$$

Using the result above and substituting in 0.01 for the probability $\left|a_2^{(1)}(t)\right|^2$, we have

$$F_o = \sqrt{\left|a_2^{(1)}(t)\right|^2} \frac{\left(\left(\frac{3E_1^{(0)}}{\hbar}\Delta t\right)^2 - \pi^2\right)}{2\left|\cos\left(\frac{3E_1^{(0)}}{2\hbar}\Delta t\right)\right|} \frac{9\pi\hbar}{16eL_z\Delta t}$$

$$= 0.1 \times \frac{589.4}{1.87} \times \frac{9\pi \times 1.055 \times 10^{-34}}{16 \times 1.602 \times 10^{-19} \times 10^{-8} \times 10^{-13}} = 3.67 \times 10^7 \text{ V/m}$$

which is therefore the minimum field required.

(iii) For a full cycle pulse the only mathematical difference is

$$a_2^{(1)}(t) = \frac{-1}{2\hbar} eF_o\left(-\frac{16L_z}{9\pi^2}\right) \int_0^{\Delta t} \exp(i\omega_{21}t)_o \left(\exp(2\pi it/\Delta t) - \exp(-2\pi it/\Delta t)\right)dt$$

$$= \frac{1}{i\hbar} eF_o\left(\frac{16L_z}{9\pi}\right) \frac{\Delta t\left(1 - \exp\left(i\frac{3E_1^{(0)}}{\hbar}\Delta t\right)\right)}{\left(\left(\frac{3E_1^{(0)}}{\hbar}\Delta t\right)^2 - \pi^2\right)}$$

so the probability of finding the electron in the second level is

$$\left|a_2^{(1)}(t)\right|^2 = \left(\frac{eF_o 16L_z\Delta t}{9\pi\hbar}\right)^2 \frac{4\sin^2\left(\frac{3E_1^{(0)}}{2\hbar}\Delta t\right)}{\left(\left(\frac{3E_1^{(0)}}{\hbar}\Delta t\right)^2 - \pi^2\right)^2}$$

so that the probability now varies as a $\sin^2$ instead of $\cos^2$. Note, however, that this $\sin^2$ term is now quite small for this particular value of Δt, specifically ~ 0.097, compared to the ~ 0.89 for the $\cos^2$ term we had for the half cycle pulse. So, for this particular pulse length, the full cycle pulse gives a much smaller probability of making the transition.

7.1.2

(i)

We use time-dependent perturbation theory, noting that the initial state is $a_1^{(0)} = 1$ and all others are $a_i^{(0)} = 0$ since the electron is in its lowest state to start with. Hence, we have

$$\dot{a}_2^{(1)} = \frac{1}{i\hbar} \exp(i\omega_{21}t)\langle\psi_2|\hat{H}_p|\psi_1\rangle$$

where

$$\omega_{21} = \frac{E_2 - E_1}{\hbar} = \frac{3\hbar}{2m_0}\left(\frac{\pi}{L_z}\right)^2$$

and

$$\hat{H}_p = eF(t)z$$

where

$$F(t) = F_o \exp(-t/\tau)$$

for $t > 0$ (and zero otherwise). Given the known forms of $|\psi_1\rangle$ and $|\psi_2\rangle$, we have

$$\langle\psi_2|\hat{H}_p|\psi_1\rangle = \frac{2eF(t)}{L_z}\int_0^{L_z} z\sin\left(\frac{\pi z}{L_z}\right)\sin\left(\frac{2\pi z}{L_z}\right)dz$$

$$= \frac{2eF(t)}{L_z}\left(\frac{L_z}{\pi}\right)^2\int_0^{\pi}\zeta\sin\zeta\sin 2\zeta\,d\zeta$$

where

$$\zeta = \frac{\pi z}{L_z}$$

From the given formula for such integrals, we have

$$\int_0^{\pi}\zeta\sin\zeta\sin 2\zeta\,d\zeta = -\frac{4\times 2}{1^2\times 3^2} = \frac{-8}{9}$$

Hence, we have

$$\dot{a}_2^{(1)} = i\frac{16}{9\pi^2}\frac{e}{\hbar}L_z F(t)\exp i\omega_{21}(t)$$

Hence

$$a_2^{(1)}(t) = i\frac{16}{9\pi^2}\frac{e}{\hbar}L_z F_o\int_0^t \exp(-t_1/\tau)\exp(i\omega_{21}t_1)\,dt_1$$

$$I = \int_0^t \exp(-t_1/\tau)\exp(i\omega_{21}t_1)\,dt_1 = \int_0^t \exp\left[\left(i\omega_{21} - \frac{1}{\tau}\right)t_1\right]dt_1$$

$$= \frac{1}{i\omega_{21} - \frac{1}{\tau}}\left[\exp\left(i\omega_{21} - \frac{1}{\tau}\right)t_1\right]_0^t$$

In the limit of $t \gg \tau$, this result becomes

$$I = -\frac{1}{i\omega_{21} - \frac{1}{\tau}} = \frac{i\omega_{21} + \frac{1}{\tau}}{\left(\frac{1}{\tau^2} + \omega_{21}^2\right)}$$

Hence, the probability of finding the electron in the second state for times $t \gg \tau$ is

$$P_2 = \left|a_2^{(1)}(t \gg \tau)\right|^2 = \left(\frac{16}{9\pi^2}\frac{e}{\hbar}L_z F_o\right)^2 \frac{(1/\tau^2 + \omega_{21}^2)}{\left(1/\tau^2 + \omega_{21}^2\right)^2}$$

i.e.,

$$P_2 = \left(\frac{16}{9\pi^2}\frac{e}{\hbar}L_z F_o\right)^2 \frac{1}{1/\tau^2 + \omega_{21}^2}$$

(ii)

Formally now we have, substituting for F_o^2

$$P_2 \propto \frac{E_p}{\tau}\frac{1}{1/\tau^2 + \omega_{21}^2} \propto \frac{1}{1/\tau + \omega_{21}^2\tau} = \frac{\tau}{1 + \omega_{21}^2\tau^2}$$

$$\frac{dP_2}{d\tau} \propto \frac{1}{1 + \omega_{21}^2\tau^2} - \frac{\tau}{\left(1 + \omega_{21}^2\tau^2\right)^2}\times 2\omega_{21}^2\tau$$

$$= \frac{1 + \omega_{21}^2\tau^2 - 2\omega_{21}^2\tau^2}{\left(1 + \omega_{21}^2\tau^2\right)^2} = \frac{1 - \omega_{21}^2\tau^2}{\left(1 + \omega_{21}^2\tau^2\right)^2}$$

Hence

$$\frac{dP_2}{d\tau} = 0 \Leftrightarrow \omega_{21}^2\tau^2 = 1$$

i.e.,

$$\tau = \frac{1}{\omega_{21}}$$

(iii)

For the GaAs case

$$\omega_{21} = \frac{3\hbar}{2m_{eff}}\left(\frac{\pi}{L_z}\right)^2 = \frac{3\times 1.055\times 10^{-34}}{2\times 0.07\times 9.11\times 10^{-31}}\times\frac{\pi^2}{10^{-16}} = 2.45\times 10^{14}\,rads/s$$

Hence

$$P_2 = \left[\frac{16}{9\pi^2} \frac{1.602 \times 10^{-19}}{1.055 \times 10^{-34}} \times 10^{-8} \times 10^5 \right]^2 \times \frac{1}{10^{26} + (2.45)^2 \times 10^{28}}$$

$$= \left[2.74 \times 10^{11} \right]^2 \times \frac{1}{6 \times 10^{28}}$$

$$= \frac{7.48 \times 10^{22}}{6 \times 10^{28}} = 1.25 \times 10^{-6}$$

(iv)

The average number of photoelectrons per pulse is now

$$P_{TOT} = 10^{11} \times 1.25 \times 10^{-6} = 1.25 \times 10^5$$

(v)

We would choose

$$\tau = \frac{1}{\omega_{21}} = \frac{1}{2.45 \times 10^{14}} \simeq 4.08 \, \text{fs}$$

in which case, the photocurrent would be larger by

$$\frac{4.08 \times 10^{-15}}{1 + (2.45 \times 10^{14} \times 4.08 \times 10^{-15})^2} \frac{1 + (2.45 \times 10^{14} \times 10^{-13})^2}{1 \times 10^{-13}} \simeq \frac{4 \times 10^{-2}}{2} \times 600$$

$$\simeq 12 \, \text{times}$$

7.2.1

(i) We start with Fermi's Golden Rule.

$$W \propto \left| \left\langle final \left| \hat{H}_{p0} \right| initial \right\rangle \right|^2$$

For the electric dipole transitions we are considering here, we therefore have

$$W \propto \left| \left\langle final \left| z \right| initial \right\rangle \right|^2$$

We can choose our position origin at the center of the well for this discussion.[1] z is an odd function with respect to the center of the well. Since the initial (second) state is an odd state with respect to the center of the well, we can therefore only make transitions to states that are even with respect to the center of the well since otherwise $\left\langle final \left| z \right| initial \right\rangle$ evaluates to zero. Hence, we can make transitions to the first state (which would be an emission transition), and to the third state (given an appropriate choice of frequency in each case).

(ii) There is no qualitative difference. The parity arguments still hold.

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[1] It actually makes no difference where we choose the position origin, but this choice makes the mathematics simpler. If we chose it at some other point, say $z = a$, then we should have $\left\langle final \left| z - a \right| initial \right\rangle$ instead of $\left\langle final \left| z \right| initial \right\rangle$. But $\left\langle final \left| a \right| initial \right\rangle = a \left\langle final \left| initial \right\rangle = 0$ because the initial and final states are orthogonal, being energy eigenstates corresponding to different energy eigenvalues. So $\left\langle final \left| z - a \right| initial \right\rangle = \left\langle final \left| z \right| initial \right\rangle$.

7.2.2

(i) The electric field should be polarized in the z direction so that the matrix element for the transition

$$\langle \psi_2 | z | \psi_1 \rangle$$

will be non-zero. $\psi_1(z)$ is odd, $\psi_2(z)$ is even, and so, unless an odd function is inserted between them, as is given by z, the matrix element will be zero.

(ii) Now we need to calculate the shift in transition energy with field. There will be no first-order shift of either level 1 or level 2 with field because the matrix elements in the expression

$$E_m^{(1)} = \langle \psi_m | \hat{H}_p | \psi_m \rangle$$

where $\hat{H}_p = eFz$ for field F, are all zero for $\hat{H}_p \propto z$ (the integral would be the product of two functions of the same parity, which gives an even result, with an odd function).

Hence, we have to calculate the second-order corrections to find the changes in these levels with field. The second order correction to a given level's energy is

$$E_m^{(2)} = \sum_{n \neq m} \frac{\left| \langle \psi_n | \hat{H}_p | \psi_m \rangle \right|^2}{E_m - E_n}$$

In general, we have, for well thickness L_z

$$\langle \psi_n | \hat{H}_p | \psi_m \rangle = \frac{zeF}{L_z} \int_0^{L_z} \sin\left(\frac{n\pi z}{L_z} \right)(z - z_0) \sin\left(\frac{m\pi z}{L_z} \right) dz$$

where we have chosen the zero of potential to be at some point z_o. It will make no difference when we choose z_o; since all the sine functions are orthogonal, adding a constant in the middle parentheses in the integral gives zero change in the integral result anyway for $n \neq m$. For simplicity we choose $z_0 = 0$. Rewriting gives, for $n \neq m$, with the substitution $\zeta = \frac{\pi z}{L_z}$

$$\langle \psi_n | \hat{H}_p | \psi_m \rangle = 2e \frac{FL_z}{\pi^2} \int_0^\pi \zeta \sin(n\zeta) \sin(m\zeta) d\zeta$$

Now, from integral tables, such as from the known integral

$$\int_0^\pi (x - \pi/2) \sin(nx) \sin(mx) dx = \frac{-4nm}{(n-m)^2 (n+m)^2}, \quad \text{for } n+m \text{ odd}$$

$$= 0, \quad \text{for } n+m \text{ even}$$

we therefore have

$$\langle \psi_n | \hat{H}_p | \psi_m \rangle = -2e \frac{FL_z}{\pi^2} \frac{4nm}{(n-m)^2 (n+m)^2}$$

i.e.,
$$\left|\langle \psi_n | \hat{H}_p | \psi_m \rangle\right|^2 = \frac{64 e^2 F^2 L_z^2}{\pi^2} \frac{n^2 m^2}{(n-m)^4 (n+m)^4}$$

for n and m of the same parity (and zero otherwise). We also have that
$$E_n = n^2 E_1$$

where
$$E_1 = \frac{\hbar^2}{2m_0} \left(\frac{\pi}{L_z}\right)^2$$

Hence, for the first level ($m = 1$)

$$
\begin{aligned}
E_1^{(2)} &= \frac{64 e^2 F^2 L_z^2}{\pi^2 E_1} \sum_{n=2,4,6\ldots} \frac{n^2}{(n-1)^4 (n+1)^4 (n^2-1)} \\
&= \frac{64 m_0 e^2 L_z^4 F^2}{\pi^4 \hbar^2} \sum_{n=2,4,6\ldots} \frac{n^2}{(n-1)^5 (n+1)^5} \\
&= \frac{64 m_0 e^2 L_z^4 F^2}{\pi^4 \hbar^2} \left[\frac{4}{1 \times 3 \times 81} + \frac{16}{81 \times 5 \times 625}\right] \\
&= \frac{64 m_0 e^2 L_z^4 F^2}{\pi^4 \hbar^2} \left[0.016 + 0.00006 + \ldots\right] \\
&\simeq 0.016 \frac{64}{\pi^4} \frac{m_0 e^2}{\hbar^2} L_z^4 F^2
\end{aligned}
$$

Similarly, for the second level ($m = 2$)

$$
\begin{aligned}
E_2^{(2)} &= \frac{64 m_0 e^2 L_z^4 F^2}{\pi^4 \hbar^2} \sum_{n=1,3,5\ldots} \frac{4n^2}{(n-2)^4 (n+2)^4 (n^2-4)} \\
&= \frac{64 m_0 e^2 L_z^4 F^2}{\pi^4 \hbar^2} \left[\frac{4}{1 \times 81 \times (-3)} + \frac{36}{1 \times 25 \times 25 \times 5}\right] \\
&= \frac{64 m_0 e^2 L_z^4 F^2}{\pi^4 \hbar^2} \left[-0.0165 + 0.0115 + \ldots\right] \\
&\simeq -0.005 \frac{64 m_0 e^2 L_z^4 F^2}{\pi^4 \hbar^2}
\end{aligned}
$$

Hence, the separation energy changes by an amount
$$\Delta E(F) \simeq E_2^{(2)} - E_1^{(2)} = -0.02 \times \frac{64 m_0 e^2 L_z^4 F^2}{\pi^4 \hbar^2}$$

(iii) For $L_z = 3 \text{ Å}$, we have

$$\Delta E(F)_{(eV)} \simeq \frac{-0.02 \times 64 \times 9.11 \times 10^{-31} \times 1.6 \times 10^{-19} \times 81 \times 10^{-40}}{\pi^4 \times (1.055 \times 10^{-34})^2} F^2$$

$$= -\frac{0.02 \times 64 \times 9.11 \times 1.6 \times 81}{\pi^4 \times 1.055 \times 1.055} \times 10^{-31-19-40+34+34} F^2$$

$$\simeq -1.4 \times 10^{-21} F^2$$

The transition energy itself is

$$E_2 - E_1 = 3E_1 = \frac{3\hbar^2}{2m_0} \left(\frac{\pi}{L_z}\right)^2$$

$$(E_2 - E_1) = \frac{3\hbar^2}{2em_0} \left(\frac{\pi}{L_z}\right)^2 = \frac{3 \times 1.055 \times 1.055 \times \pi^2 \times 10^{-34-34+19+31+20}}{2 \times 1.6 \times 9.11 \times 9}$$

$$= 0.126 \times 10^2 \, eV \simeq 12.6 \, eV$$

Hence, for

$$\left|\frac{\Delta E}{(E_2 - E_1)}\right| = \frac{1.4 \times 10^{-21} F^2}{12.6} = 10^{-3}$$

$$F^2 = \frac{12.6 \times 10^{-3}}{1.4 \times 10^{-21}}$$

i.e., $\quad F^2 = 9 \times 10^{18} \, V^2/m^2$

$$F = 3 \times 10^9 \, V/m$$

$$= 0.3 \, V/\text{Ångstrom}$$

(iv) A simple way to make this device more sensitive is to apply a d.c. bias field to it. That way, it can be turned from a device whose response is quadratic with field (and hence is weak for small fields) into one with a response that is linear with field.

(For example, at a bias field of 1 V/Å,

$$\frac{d\left|\Delta E/(E_2 - E_1)\right|}{dF}\Bigg|_{F=10^{10} V/m} = \frac{2 \times 1.4 \times 10^{-21} \times 10^{10}}{12.6} \simeq 2.2 \times 10^{-12} \, m/V$$

and so for a 10^{-3} change, we require

$$2.2 \times 10^{-12} \Delta F = 10^{-3}$$

i.e., $\qquad \Delta F = \frac{10^{-3}}{2.2 \times 10^{-12}} = 4.5 \times 10^8 \, V/m = 45 \, mV/\text{Å} \,)$

7.2.3

First we note that the energy corresponding to a 1 THz oscillation is

$$E_{1THz} = hf = 4.138 \text{ meV}$$

This is a small energy compared to the energy separations of the states in a quantum well of width 5 nm, and so we should be able to use some approximation technique to calculate the effects of the coupling of the wells. Consequently, we will tackle this problem by using the tight-binding approach, based on the solutions of the uncoupled finite well problem.

In the tight-binding approach, we start by solving the problem for a single well.

Solution for a single finite well

For a finite potential well, with the boundary conditions of continuity of the wavefunction ψ and continuity of $(1/m)d\psi/dz$, we can show that the eigenenergy solutions are the solutions of the equations

$$\tan(\frac{\pi}{2}\sqrt{\varepsilon}) = \sqrt{\frac{m_w^*}{m_b^*}}\sqrt{\frac{v_0 - \varepsilon}{\varepsilon}}$$

$$\cot(\frac{\pi}{2}\sqrt{\varepsilon}) = -\sqrt{\frac{m_w^*}{m_b^*}}\sqrt{\frac{v_0 - \varepsilon}{\varepsilon}}$$

where $\varepsilon = E/E_1$ is the dimensionless version of the energy E, $v_o = V_o/E_1$ is the dimensionless energy height of the potential barrier of actual energy height V_o, and E_1 is the energy of the first confined state in the infinitely deep well (relative to the bottom of the potential well)

$$E_1 = \frac{-\hbar^2}{2m_w^*}\left(\frac{\pi}{L_z}\right)$$

with L_z as the width of the well, v_o as the potential barrier height, and m_w^* and m_b^* as the effective masses of the electron in the well and barrier respectively. For the parameters given in the problem, we have

$$E_1 \cong 225 \text{ meV}$$

which leads, on solving the tangent equation above, to the energy E_{f1} of the lowest state in the finite well being

$$E_{f1} \cong 74 \text{ meV}$$

The resulting normalized wavefunction is

$$\phi_{f1}(z) = 0.294\exp\left[\kappa\left(z + \frac{L_z}{2}\right)\right], \quad z < -\frac{L_z}{2}$$

$$\phi_{f1}(z) = 0.473\cos(kz), \quad -\frac{L_z}{2} \le z \le \frac{L_z}{2}$$

$$\phi_{f1}(z) = 0.294 \exp\left[-\kappa\left(z - \frac{L_z}{2}\right)\right], \quad z > \frac{L_z}{2}$$

where $k = 0.36\,\text{nm}^{-1}$ and $\kappa = 0.624$ nm^{-1}, and distances are in nanometers. The resulting wavefunction is plotted below. The dotted lines mark the edges of the well.
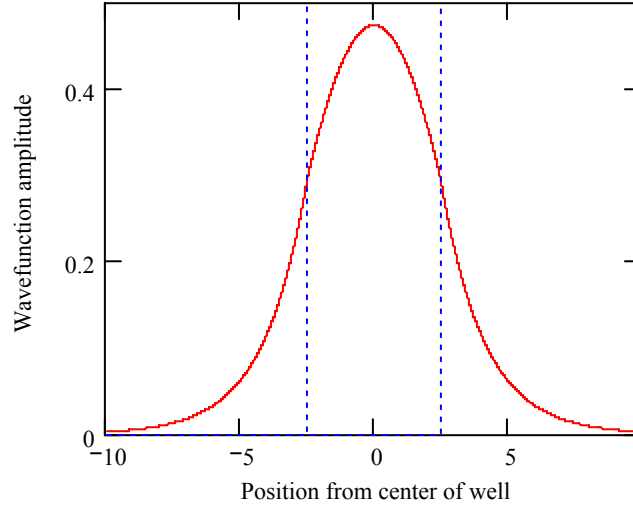
(i) Calculation of barrier thickness for desired splitting

Now, to evaluate ΔE, we note that, at any value of z, it is always true that, for the wavefunction $\phi_{f1}(z)$ that is the eigenfunction of the Hamiltonian $\hat{H} = -(\hbar^2/2m)(d^2/dz^2) + V(z)$ with eigenenergy $E_{f1} - V_o$ (i.e., the eigenenergy now referred to the zero of the potential, now at the top of the barrier),

$$\hat{H}\phi_{f1}(z) = (E_{f1} - V_o)\phi_{f1}(z)$$

and so

$$\Delta E = \int_{barrier} \phi_{leftf1}^*(z)\hat{H}\phi_{rightf1}(z)\,dz = (E_{f1} - V_o)\int_{barrier} \phi_{leftf1}^*(z)\phi_{rightf1}(z)$$

Hence, changing the origin to the middle of the barrier,

$$\Delta E = (0.294)^2 (E_{f1} - V_o)\int_{-w/2}^{w/2} \exp\left[-\kappa\left(z + \frac{w}{2}\right)\right]\exp\left[\kappa\left(z - \frac{w}{2}\right)\right]dz$$

i.e.,

$$\Delta E = (0.294)^2 (E_{f1} - V_o)w\exp(-\kappa w)$$

Hence, for a desired splitting between these levels of $\delta E = 2|\Delta E|$, we need to find w such that

$$\frac{\delta E}{2(0.294)^2 |E_{f1} - V_o|} = w\exp(-\kappa w)$$

i.e., for our specific desired separation corresponding to 500 GHz, i.e., $\delta E = 2.092$ meV, we have

$$0.074 = w\exp(-0.703w)$$

This equation has two possible solutions, one for very small w (0.078 nm), and a larger one

$$w \cong 7.37 \text{ nm}$$

This smaller solution certainly violates the assumptions of the approximation that there is little penetration of the wavefunction from one well into the other well, as can be seen from the plot of the wavefunction above, so, as suggested in the problem, we discard this small solution. Our answer is therefore a ~ 7.37 nm barrier thickness.

(ii) Calculation of splitting and relative absorption strength as a function of field

For this part of the problem, since we now know the single well wavefunctions, we can use them as a finite basis subset for calculating the splitting as a function of field. Explicitly, we have for the two wavefunctions, relative to the center of the barrier,

$$\phi_{fleft}(z) = 0.294\exp\left[\kappa\left(z + L_z + \frac{w}{2}\right)\right], \quad z < -L_z - \frac{w}{2}$$

$$\phi_{fleft}(z) = 0.473\cos\left[k\left(z + \frac{L_z + w}{2}\right)\right], \quad -L_z - \frac{w}{2} \le z \le -\frac{w}{2}$$

$$\phi_{fleft}(z) = 0.294\exp\left[-\kappa\left(z + \frac{w}{2}\right)\right], \quad z > -\frac{w}{2}$$

and

$$\phi_{fright}(z) = 0.294\exp\left[\kappa\left(z - \frac{w}{2}\right)\right], \quad z < \frac{w}{2}$$

$$\phi_{fright}(z) = 0.473\cos\left[k\left(z - \frac{L_z + w}{2}\right)\right], \quad \frac{w}{2} \le z \le L_z + \frac{w}{2}$$

$$\phi_{fright}(z) = 0.294\exp\left[-\kappa\left(z - L_z - \frac{w}{2}\right)\right], \quad z > L_z + \frac{w}{2}$$

(a) Calculation of splitting

Now our Hamiltonian, in the presence of a field F in the z-direction, becomes

$$\hat{H} = \hat{H}_0 + eFz$$

with H_0 being the double potential well Hamiltonian in the absence of fields. We now construct the matrix representation of this Hamiltonian, using $\psi_{f\,left}(z)$ as $\psi_1(z)$ and $\psi_{f\,right}(z)$ as $\psi_2(z)$. Then we have

$$\hat{H} = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix}$$

Now we formally evaluate the matrix elements

$$H_{11} = \int \psi^*_{f\,left}(z)\left(\hat{H}_0 + eF_z\right)\psi_{f\,left}(z)\,dz$$

$$= E_{f1} - V_o + eF\int z\left|\psi_{f\,left}(z)\right|^2 dz$$

Now $\psi_{f\,left}(z)$ is symmetric about the center of the well, so the result of the above integral is just the

z corresponding to the center of the well, which is $-\left(\dfrac{L_z + w}{2}\right)$. Hence

$$H_{11} = E_{f1} - V_o - eF\left(\frac{L_z + w}{2}\right) = E_{f1} - V_o - C$$

where $C = eF\left(\dfrac{L_z + w}{2}\right)$.

Similarly

$$H_{22} = E_{f1} - V_o + eF\left(\frac{L_z + w}{2}\right) = E_{f1} - V_o + C$$

Now

$$H_{12} = \int \psi^*_{f\,left}(z)\left(\hat{H}_0 + eFz\right)\psi_{f\,right}(z)\,dz$$

$$= \left(E_{f1} - V_o\right)\int \psi^*_{f\,left}(z)\psi_{f\,right}(z)\,dz + eF\int \psi^*_{f\,left}(z)\,z\psi_{f\,right}(z)\,dz$$

These two integrals are only significant in the barrier, and so we have

$$H_{12} = (0.294)^2 \left[\begin{array}{l} \left(E_{f1} - V_o\right)\displaystyle\int_{-w/2}^{w/2} \exp\left[-\kappa\left(z + \frac{w}{2}\right)\right]\exp\left[\kappa\left(z - \frac{\omega}{2}\right)\right]dz \\ +eF\displaystyle\int_{-w/2}^{w/2} z\exp\left[-\kappa\left(z + \frac{w}{2}\right)\right]\exp\left[\kappa\left(z - \frac{w}{2}\right)\right]dz \end{array} \right]$$

$$= (0.294)^2 \left[\left(E_{f1} - V_o\right)w\exp\left(-\kappa w\right) + eF\exp(-\kappa w)\int_{-w/2}^{w/2} z\,dz\right]$$

$$= (0.294)^2\, w\exp(-\kappa w)\left[E_{f1} - V_o\right] = B$$

(The integral over z vanishes by symmetry in the above algebra.) The calculation of H_{21} gives an identical result, i.e.,

$$H_{21} = H_{12}$$

(as would be required anyway by Hermiticity), and so the matrix becomes

$$\hat{H} = \begin{bmatrix} E_{f1} - V_o - C & B \\ B & E_{f1} - V_0 + C \end{bmatrix}$$

Hence, the eigen equation becomes

$$\hat{H}\psi = \begin{bmatrix} E_{f1} - V_o - C & B \\ B & E_{f1} + V_o + C \end{bmatrix}\begin{bmatrix} a_{left} \\ a_{right} \end{bmatrix} = E\begin{bmatrix} a_{left} \\ a_{right} \end{bmatrix}$$

For eigen solutions, we therefore require

$$\begin{vmatrix} E_{f1} - V_o - C - E & B \\ B & E_{f1} - V_o + C - E \end{vmatrix} = 0$$

i.e.,

$$\left(E_{f1} - V_o - E - C \right)\left(E_{f1} - V_o - E + C \right) - B^2 = 0$$

i.e., with

$$E_d = E_{f1} - V_o - E$$

$$E_d^2 - C^2 - B^2 = 0$$

i.e.,

$$E_d^2 = B^2 + C^2$$

$$E_d = \pm\sqrt{B^2 + C^2}$$

We are interested in the separation energy of the two states, which is therefore

$$E_s = 2\sqrt{B^2 + C^2}$$

and which is, explicitly

$$E_s = 2\left\{ (0.294)^4 \, w^2 \exp(-2\kappa w)\left[E_{f1} - V_o \right]^2 + e^2 F^2 \left(\frac{L_z + w}{2} \right)^2 \right\}^{1/2}$$

The resulting graph of the detected frequency as a function of field is shown below.
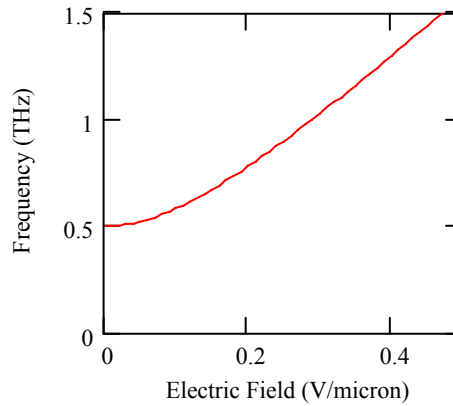
(b) Sensitivity of the detector as a function of field

To find the relative strength of the absorption we note, from Fermi's Golden Rule, that the transition rate is proportional to

$$M = \left| \langle \phi_2 | z | \phi_1 \rangle \right|^2$$

where $|\phi_1\rangle$ and $|\phi_2\rangle$ are the eigen functions of the first two solutions, since the perturbing optical Hamiltonian will be of the form

$$\hat{H}_{p\omega} = 2\hat{H}_{po\omega} \cos \omega t$$

with, in the electric dipole approximation

$$\hat{H}_{po\omega} = -eE_{opt} z$$

where E_{opt} is the optical field amplitude.

Now, $|\phi_2\rangle$ and $|\phi_1\rangle$ will be the eigen vectors of the matrix $\hat{H}$ for any given static field E, and each vector will be of the form

$$|\phi_1\rangle = a_{1\,left}|\phi_{f\,left}\rangle + a_{1\,right}|\phi_{f\,right}\rangle$$
$$|\phi_2\rangle = a_{2\,left}|\phi_{f\,left}\rangle + a_{2\,right}|\phi_{f\,right}\rangle$$

and so

$$\langle\phi_2|z|\phi_1\rangle = a^*_{2\,left}a_{1\,left}\langle\phi_{f\,left}|z|\phi_{f\,left}\rangle$$
$$+a^*_{2\,right}a_{1\,right}\langle\phi_{f\,right}|z|\phi_{f\,right}\rangle$$
$$+a^*_{2\,left}a_{1\,right}\langle\phi_{f\,left}|z|\phi_{f\,right}\rangle$$
$$+a^*_{2\,right}a_{1\,right}\langle\phi_{f\,right}|z|\phi_{f\,left}\rangle$$

For the last two terms, we can get a simple approximate analytic result for the integral if we use the "tight binding" approach of presuming that the only region for which the wavefunctions overlap enough is the barrier. Then we have

$$\langle\phi_{f\,left}|z|\phi_{f\,right}\rangle \simeq (0.294)^2\,dz\int_{-w/2}^{w/2} z\,\exp\left[-\kappa\left(z+\frac{w}{2}\right)+\kappa\left(z-\frac{w}{2}\right)\right]dz$$

$$= (0.294)^2\,\exp(-\kappa w)\int_{-w/2}^{w/2} z\,dz$$

$$= (2.94)^2\,\exp(-\kappa w)\left[\frac{z^2}{2}\right]_{-w/2}^{w/2} = 0$$

so we may discard these. Actually, even without the tight binding approach, this integral is zero, because the product $\phi_{f\,left}(z)\,\phi_{f\,right}(z)$ is even with respect to the center of the structure.

For the first term, we may write

$$\langle\phi_{f\,left}|z|\phi_{f\,left}\rangle = \int_{-\infty}^{\infty} z\,|\phi_{f\,left}(z)|^2\,dz$$

Now we may move the origin to the middle of the left well, i.e., choose a new variable

$$\zeta_L = z + \frac{L_z + w}{2}$$

and so we have

$$\left\langle \phi_{f\,left} \left| z \right| \phi_{f\,left} \right\rangle = \int_{-\infty}^{\infty} \left[\zeta_L - \left(\frac{L_z + w}{2} \right) \right] \left| \phi_{f\,left} \left(\zeta_L - \left(\frac{L_z + w}{2} \right) \right) \right|^2 d\zeta_L$$

$$= -\left(\frac{L_z + w}{2} \right) \int_{-\infty}^{\infty} \left| \phi_{f\,left} \left(\zeta - \left(\frac{L_z + w}{2} \right) \right) \right|^2 d\zeta + \int_{-\infty}^{\infty} \zeta_L \left| \phi_{f\,left} \left(\zeta_L - \frac{L_z + w}{2} \right) \right|^2 d\zeta_L$$

The first integral is just the normalization integral, and so equals 1. The second integral is zero; this is just the integral with respect to the center of the well of the single well solution squared (an even function with respect to the center of the well), multiplied by the distance from the center (an odd function).

Hence, we have

$$\left\langle \phi_{f\,left} \left| z \right| \phi_{f\,left} \right\rangle = -\left[\frac{L_z + w}{2} \right]$$

Similarly

$$\left\langle \phi_{f\,right} \left| z \right| \phi_{f\,right} \right\rangle = \frac{L_z + w}{2}$$

The reader may decide these are quite obvious results in retrospect, since they correspond to the expectation value of z in each case, which in each case is just at the center of these symmetrically-shaped wavefunctions.

Hence, we have

$$\left\langle \phi_2 \left| z \right| \phi_1 \right\rangle = \left[\frac{L_z + w}{2} \right] \left(a_{2\,right}^* a_{1\,right} - a_{2\,left}^* a_{1\,left} \right)$$

and the transition rate is proportional to

$$M = \left| \left\langle \phi_2 \left| z \right| \phi_1 \right\rangle \right|^2$$

$$= \left[\frac{L_z + w}{2} \right]^2 \left| a_{2\,right}^* a_{1\,right} - a_{2\,left}^* a_{1\,left} \right|^2$$

$$\propto \left| a_{2\,right}^* a_{1\,right} - a_{2\,left}^* a_{1\,left} \right|^2$$

Numerically, we proceed for each field to evaluate the coefficients $a_{1\,left}, a_{1\,right}$ and $a_{2\,left}, a_{2\,right}$ that are the eigen vector elements for the lower and upper eigen solutions, respectively. We must remember to normalize the eigen vectors, i.e., set

$$\left| a_{1\,left} \right|^2 + \left| a_{1\,right} \right|^2 = 1$$

$$\left| a_{2\,left} \right|^2 + \left| a_{2\,right} \right|^2 = 1$$

before calculating the relative value of M.

The resulting calculation of relative sensitivity as a function of field is shown below.

Relative Sensitivity
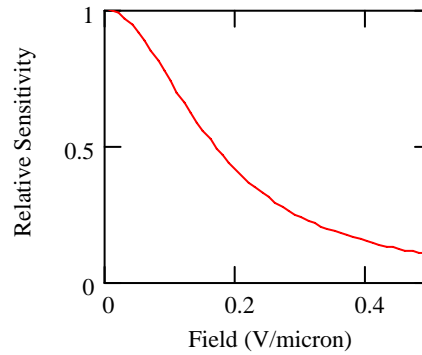
Field (V/micron)

(c) 3dB range

The field at which this sensitivity has fallen to 50% is ~ 0.167 V/micron, with a corresponding frequency of ~ 706 GHz.

Hence the response of this detector is within 3 dB of its peak from 500 GHz to 706 GHz.

See the following Mathcad worksheet for detailed calculations.

Mathcad worksheet for Problem 7.2.3

Fundamental constants

$$mo := 9.11 \cdot 10^{-31} \qquad hbar := 1.055 \cdot 10^{-34} \qquad e := 1.602 \cdot 10^{-19}$$

$ORIGIN := 1$ formally sets the indexing of matrices starting from 1 rather than zero

For a 1 THz electromagnetic oscillation, the corresponding energy (the photon energy) is, in eV

$$Ep := 2 \cdot \pi \cdot hbar \cdot \frac{10^{12}}{e} \qquad Ep = 4.138 \times 10^{-3}$$

For this AlGaAs/GaAs quantum well problem, for distances in nanometers

$$mw := 0.067 \cdot mo \quad mb := 0.092 \cdot mo \qquad Vo := 0.235 \cdot e \qquad Lz := 5$$

For an infinitely deep quantum well, the energy of the first state is, in eV

$$E1 := \frac{hbar^2 \cdot \left(\dfrac{\pi}{Lz \cdot 10^{-9}} \right)^2}{2 \cdot mw \cdot e} \qquad E1 = 0.225$$

and hence

$$vo := \frac{Vo}{e \cdot E1} \qquad vo = 1.046$$

Now we find the energy of the first state in the finite potential well. We start by formally creating the function that will be zero at the root. Starting from the known solution for a finite semiconductor potential well, we have

$$f(\varepsilon) := \tan\left(\pi \frac{\sqrt{\varepsilon}}{2} \right) - \sqrt{\frac{mw}{mb}} \cdot \sqrt{\frac{(vo - \varepsilon)}{\varepsilon}}$$

Now we formally solve for the root between 0.1 and 1 dimensionless units of energy

$$\varepsilon1 := root(f(\varepsilon), \varepsilon, 0.1, 1) \qquad \varepsilon1 = 0.329$$

That is, for the actual first energy level of the finite well, in eV, we have

$$Ef1 := \varepsilon1 \cdot E1 \qquad Ef1 = 0.074$$

Now we should construct the normalized wavefunction. In the well, the wavefunction is cosinusoidal with respect to the center of the well (i.e., of the form cos kz), with k value, in inverse nanometers

$$k := \frac{10^{-9} \sqrt{2 \cdot mw \cdot Ef1 \cdot e}}{hbar} \qquad k = 0.36$$

In the barriers on either side of the single finite well, the wavefunction is exponentially decaying (e.g., on the right hand side of the form exp(-κz)), with κ value in inverse nanometers

$$\kappa := 10^{-9} \cdot \frac{\sqrt{2mb \cdot (Vo - Ef1 \cdot e)}}{hbar} \qquad \kappa = 0.624$$

If we were arbitrarily for the moment to choose unit peak value for the function inside the well, then at the edges of the well, the function would have the value ψedgeunnorm

$$\psi edgeunnorm := \cos\left(k \cdot \frac{Lz}{2}\right) \qquad \psi edgeunnorm = 0.621$$

We can now normalize this wavefunction. Inside the well, we have, for distances in nanometers

$$Inormwell := \int_{-\frac{Lz}{2}}^{\frac{Lz}{2}} (\cos(k \cdot z))^2 \, dz \qquad Inormwell = 3.852$$

In one barrier, we have

$$Inormbarrier := \int_{0}^{\infty} \psi edgeunnorm^2 \exp(-2\kappa \cdot z) \, dz \quad Inormbarrier = 0.31$$

The entire normalization integral is therefore

$$Inorm := Inormbarrier + Inormwell + Inormbarrier \qquad Inorm = 4.471$$

To normalize the wavefunction, we must therefore multiply the wavefunction by 1/squareroot(Inorm), i.e.,

$$Normfact := \frac{1}{\sqrt{Inorm}} \qquad Normfact = 0.473$$

Hence we have, choosing z=0 in the middle of the well, for the left barrier,

$$\psi leftbarrier(z) := Normfact \cdot \psi edgeunnorm \cdot \exp\left[\kappa \cdot \left(z + \frac{Lz}{2}\right)\right]$$

in the well,

$$\psi well(z) := Normfact \cdot \cos(k \cdot z)$$

and on the right

$$\psi rightbarrier(z) := Normfact \cdot \psi edgeunnorm \cdot \exp\left[-\kappa \cdot \left(z - \frac{Lz}{2}\right)\right]$$

where we note that

$$Bamp := Normfact \cdot \psi edgeunnorm$$

Bamp = 0.294

To check that our wavefunction makes sense, we graph it. We first formally define the wavefunction as a single function. We formally use the Heaviside step function $\Phi(z)$, and also its opposite

$$\Phi i(z) := 1 - \Phi(z)$$

$$\psi total(z) := \Phi i\left(z + \frac{Lz}{2}\right)\psi leftbarrier(z) + \Phi\left(z + \frac{Lz}{2}\right)\cdot\Phi i\left(z - \frac{Lz}{2}\right)\cdot\psi well(z) + \Phi\left(z - \frac{Lz}{2}\right)\psi rightbarrier(z$$

$$zz := -10, -9.99 .. 10$$
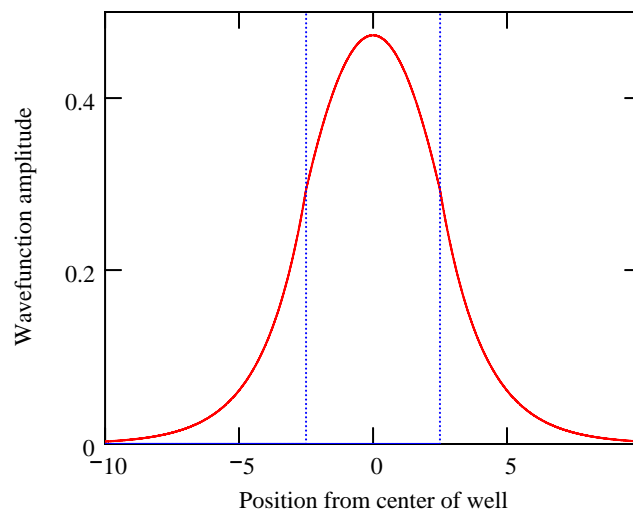
Note, incidentally, that the derivative of the wavefunction is not continuous across the boundary between well and barrier, as expected from the 1/m in the derivative boundary condition.

We can also check that this wavefunction is normalized.

$$\int_{-20}^{20} \left(\psi total(z)\right)^2 dz = 1$$

Now we can evaluate w, the barrier width.

We know our desired splitting is

$$\delta E := 2\cdot\pi\cdot hbar\cdot 500\cdot\frac{10^9}{e} \qquad \delta E = 2.069 \times 10^{-3}$$

Following the algebra in the solution, we need to evaluate the constant

$$\text{Econst} := \frac{\delta E}{2 \cdot \text{Bamp}^2 \cdot \left| \text{Ef1} - \dfrac{\text{Vo}}{e} \right|} \qquad\qquad \text{Econst} = 0.074$$

Following the algebra in the solution, we need to solve for the root of the function

$$g(w) := w \cdot \exp(-\kappa \cdot w) - \text{Econst}$$

Graphing this function show that it has two roots, one at very small w (which we will call wsmall) and one at larger w..

$$zz := 0, 0.05 .. 10$$
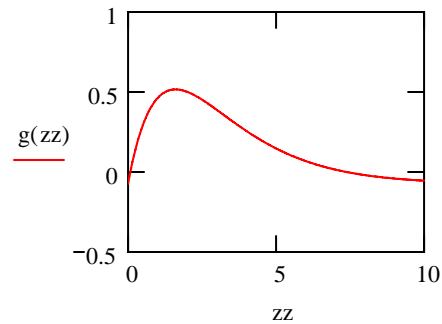
$$\text{wsmall} := \text{root}(g(ws), ws, 0, 1) \qquad\qquad \text{wsmall} = 0.078$$

We discard this smaller root because it goes beyond the validity of the approximation, leaving the larger root.

$$w := \text{root}(g(w1), w1, 2, 10) \qquad\qquad w = 7.372$$

(a) Frequency separation with field

From the algebra in the solution, we have, for fields in Volts per nanometer, and energies in electron volts

$$\text{Es}(F) := 2 \left[\text{Bamp}^4 \cdot w^2 \cdot \exp(-2 \cdot \kappa \cdot w) \cdot \left(\text{Ef1} - \frac{\text{Vo}}{e} \right)^2 + F^2 \left[\frac{(\text{Lz} + w)}{2} \right]^2 \right]^{\frac{1}{2}}$$

$$\text{FF} := 0, 10^{-5} .. 5 \cdot 10^{-4}$$
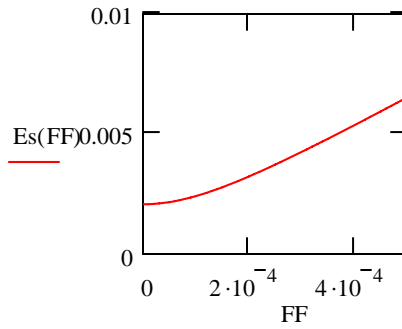
The corresponding frequency separation with field, now graphing with a field in Volts per micron to get a more convenient unit
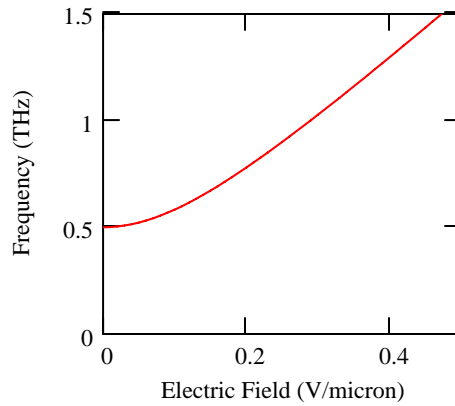
(b) Relative optical transition strength with field

From the algebra in the solution, we have deduced that a measure of the transition strength is given by

$$M2(a1left, a1right, a2left, a2right) := \left(\left|\overline{a2right}\,a1right - \overline{a2left}\,a1left\right|\right)^2$$

The arguments in this expression are the respective coefficients of the left and right single well states for the first and second levels respectively.

Now we formally construct the matrix

$$B(F) := Bamp^2 \cdot w \cdot \exp(-\kappa \cdot w) \cdot \left(Ef1 - \frac{Vo}{e}\right) \qquad\qquad C(F) := F \cdot \frac{(Lz + w)}{2}$$

so that

$$H(F) := \begin{pmatrix} Ef1 - C(F) - \dfrac{Vo}{e} & B(F) \\[2ex] B(F) & Ef1 + C(F) - \dfrac{Vo}{e} \end{pmatrix}$$

We can now use the built in functions of Mathcad to evaluate the eigenvectors. One such function returns the normalized eigenvectors as the columns in a matrix. We formally write this

matrix of normalized eigenvectors as a function of F.

$G(F) := \text{eigenvecs}(H(F))$

Formally we can now define a quantity MM representing a measure of the transition strength at field F

$$MM(F) := M2\left(G(F)_{1,1}, G(F)_{2,1}, G(F)_{1,2}, G(F)_{2,2}\right)$$

We will first of all evaluate the quantity M for zero field, so that we can relate other results to this

$MMnorm := MM(0)$ $\qquad\qquad$ $MMnorm = 1$

We find that this quantity is in fact 1 so we can henceforth ignore it in setting the relative values.

Hence now we can graph the relative transition strength as a function of field
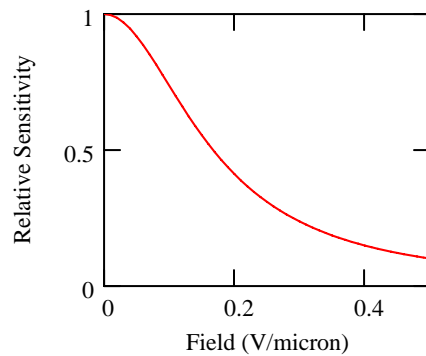
We can formally find the value of field at which MM falls off to 1/2

$Fhalf := \text{root}\left(MM(F) - 0.5, F, 0, 5 \cdot 10^{-4}\right)$ $\qquad$ $Fhalf = 1.672 \times 10^{-4}$ Volts per nm

At this field, the corresponding frequency is

$fhalf := Es(Fhalf) \cdot \dfrac{e}{2 \cdot \pi \cdot hbar \cdot 10^{12}}$ $\qquad$ $fhalf = 0.707$ $\quad$ Terahertz

For interest, we will graph the wavefunctions as a function of field. First we formally construct the potential structure as a function of field

$$Vtot(z, F) := \Phi\left(Lz + z + \frac{w}{2}\right) \cdot \Phi i\left(z + \frac{w}{2}\right) \cdot \left(\frac{-Vo}{e}\right) + \Phi\left(z - \frac{w}{2}\right) \cdot \Phi i\left(z - Lz - \frac{w}{2}\right) \cdot \left(\frac{-Vo}{e}\right) + F \cdot z$$

$$\phi1(z, F) := G(F)_{1,1} \psi total\left[z + \frac{(w + Lz)}{2}\right] + G(F)_{2,1} \psi total\left[z - \frac{(w + Lz)}{2}\right]$$

$$\phi2(z, F) := G(F)_{1,2} \psi total\left[z + \frac{(w + Lz)}{2}\right] + G(F)_{2,2} \psi total\left[z - \frac{(w + Lz)}{2}\right]$$

$$zz := -10, -9.98 .. 10$$

$$Eplot1(F) := eigenvals(H(F))_1 \qquad\qquad \phi plot1(z, F) := 0.01 \cdot \phi1(z, F) + Eplot1(F)$$

$$Eplot2(F) := eigenvals(H(F))_2 \qquad\qquad \phi plot2(z, F) := 0.01 \cdot \phi2(z, F) + Eplot2(F)$$

The following is the code to animate the wavefunctions as a function of field

$$F := FRAME \cdot 5 \times 10^{-5} + .001 \cdot 10^{-5} \quad Field := F \cdot 10^{3}$$

Vtot(zz, F)

φplot1(zz, F)

Eplot1(F)

φplot2(zz, F)

Eplot2(F)
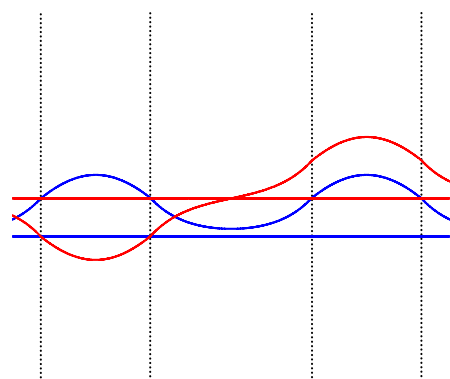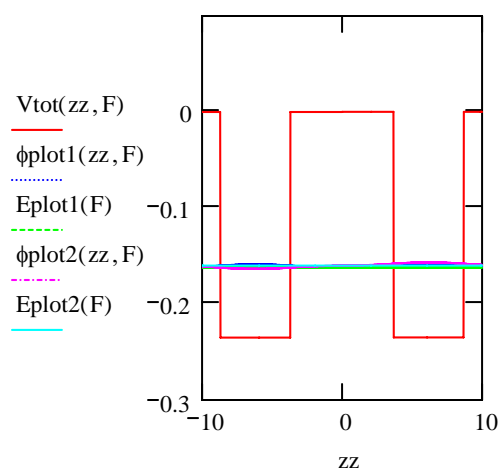
Field = 0   Volts/micron

7.4.1

(i) We know that

$$\dot{a}_i^{(1)}(t) = \frac{1}{i\hbar} \sum_n a_n^{(0)} \exp(i\,\omega_{in}\,t)\left\langle \psi_i \left| \hat{H}_p(t) \right| \psi_n \right\rangle$$

where $\left| \psi_i \right\rangle$ and $\left| \psi_n \right\rangle$ are purely spatial wavefunctions. For the steady state oscillating field, we have

$$\dot{a}_i^{(1)}(t) = \frac{e\varepsilon_0}{i\hbar} \sum_n a_n^{(0)} \exp(i\,\omega_{in}\,t)\left\langle \psi_i \left| z \right| \psi_n \right\rangle \left[\exp(i\omega t) + \exp(-i\omega t) \right]$$

We know from the problem that $a_1^{(0)} = 1$ and $a_2^{(0)} = 0$ because the system is in state 1 in the absence of any perturbation. Given that we only have two possible states in the system, the sum is greatly simplified to only being over two possible states, and since $a_2^{(0)} = 0$, the sum is particularly simple, being

$$\dot{a}_2^{(1)}(t) = \frac{e\varepsilon_0}{i\hbar}\left\langle \psi_2 \left| z \right| \psi_1 \right\rangle \left\{ \exp\left[i(\omega_{21} + \omega)t \right] + \left[\exp\left[i(\omega_{21} - \omega)t \right] \right] \right\}$$

where $\omega_{21} = E_{21}/\hbar \neq \omega$.

$$a_2^{(1)}(t) = \frac{-e\varepsilon_0}{\hbar}\left\langle \psi_2 \left| Z \right| \psi_1 \right\rangle \left[\frac{\exp\left[i(\omega_{21} + \omega)t \right]}{(\omega_{21} + \omega)} + \frac{\exp\left[i(\omega_{21} - \omega)t \right]}{(\omega_{21} - \omega)} \right]$$

We know because the states have definite parity that

$$\left\langle \psi_1 \left| z \right| \psi_1 \right\rangle = 0$$

and so in performing the similar sum for $a_1^{(1)}(t)$, we find

$$\dot{a}_1^{(1)}(t) = 0$$

To find the higher order corrections, we use the relation

$$\dot{a}_i^{(p+1)}(t) = \frac{1}{i\hbar} \sum_n a_n^{(p)} \exp(i\,\omega_{in}\,t)\left\langle \psi_i \left| \hat{H}_p \right| \psi_n \right\rangle$$

Hence, we have for the second order correction here

$$\dot{a}_i^{(2)}(t) = \frac{1}{i\hbar} a_2^{(1)} \exp(i\,\omega_{i2}\,t)\left\langle \psi_i \left| \hat{H}_p \right| \psi_2 \right\rangle$$

Hence $\quad \dot{a}_2^{(2)}(t) = \frac{1}{i\hbar} a_2^{(1)} \exp(i\,\omega_{22}\,t)\left\langle \psi_2 \left| \hat{H}_p \right| \psi_2 \right\rangle = 0$ because $\left\langle \psi_2 \left| \hat{H}_p \right| \psi_2 \right\rangle = 0$

Hence, in the steady state, $a_2^{(2)}(t) = 0$ (or at least is constant), which answers part (i).

(ii) For part (ii), we note that for any of the perturbation corrections to be finite, since $\left\langle \psi_2 \left| z \right| \psi_2 \right\rangle = \left\langle \psi_1 \left| z \right| \psi_1 \right\rangle = 0$ we need $\left\langle \psi_1 \left| z \right| \psi_2 \right\rangle$ to be nonzero, which means that $\left| \psi_1 \right\rangle$ and $\left| \psi_2 \right\rangle$ need to have opposite parity.

7.4.2

(i) We are considering an atom or molecule in which three levels are relevant for the single electron of interest

$$3 \underline{\qquad} \quad |\psi_3\rangle$$
$$2 \underline{\qquad} \quad |\psi_2\rangle$$

$$1 \underline{\qquad} \quad |\psi_1\rangle$$

with the system initially or predominantly in state 1, $|\psi_1\rangle$. For this one atom, we will consider the expectation value of the dipole moment (we are here formally taking the electric dipole approximation to the interaction of a classical electric field with the system).

$$\mu_{dip} = -ez \tag{1}$$

and so the quantum mechanical expectation value is written

$$\langle \mu_{dip} \rangle = -e\langle z \rangle \tag{2}$$

We are going to consider terms up to second order in the perturbation that will be provided by the electric field, so will need to consider a wave function with terms up to second order in the perturbation, i.e.,

$$|\psi\rangle = |\Phi^{(0)}\rangle + |\Phi^{(1)}\rangle + |\Phi^{(2)}\rangle \tag{3}$$

Here $|\Phi^{(0)}\rangle$ is the unperturbed (time-dependent) state vector and $|\Phi^{(1)}\rangle$ is the first order time-dependent correction.

$$|\Phi^{(1)}\rangle = \sum_n a_n^{(1)}(t) \exp(-i\omega_n t)|\psi_n\rangle \tag{4}$$

and $|\Phi^{(2)}\rangle$ is the second order correction.

$$|\Phi^{(2)}\rangle = \sum_n a_n^{(2)}(t) \exp(-i\omega_n t)|\psi_n\rangle \tag{5}$$

With such a state vector, (3), the expectation value of the dipole moment is

$$\langle \mu_{dip} \rangle = -e\langle z \rangle = -e\langle \Psi |z| \Psi \rangle \tag{6}$$

i.e.,

$$\begin{aligned}
\langle \mu_{dip} \rangle = -e\Big[&\langle \Phi^{(0)} |z| \Phi^{(0)} \rangle + \langle \Phi^{(0)} |z| \Phi^{(1)} \rangle + \langle \Phi^{(1)} |z| \Phi^{(0)} \rangle \\
&+ \langle \Phi^{(1)} |z| \Phi^{(1)} \rangle + \langle \Phi^{(0)} |z| \Phi^{(2)} \rangle + \langle \Phi^{(2)} |z| \Phi^{(0)} \rangle \\
&+ \langle \Phi^{(1)} |z| \Phi^{(2)} \rangle + \langle \Phi^{(2)} |z| \Phi^{(1)} \rangle \\
&+ \langle \Phi^{(2)} |z| \Phi^{(2)} \rangle \Big]
\end{aligned} \tag{7}$$

For this problem, we only want to consider the terms that are second order in the perturbation. The zeroth order term is static polarization and the first order terms are the linear polarization terms associated with linear refractive index and linear absorption (these terms are on the first line of (7)). The terms on the third and fourth lines of (7) are third and fourth order in the perturbation, respectively, and we are not interested in them here. Hence, the second order dipole moment expectation value can be written using only terms from the second line of (7) as

$$\left\langle \mu_{dip}^{(2)} \right\rangle = -e\left[\left\langle \Phi^{(1)} \left| z \right| \Phi^{(1)} \right\rangle + \left\langle \Phi^{(0)} \left| z \right| \Phi^{(2)} \right\rangle + \left\langle \Phi^{(2)} \left| z \right| \Phi^{(0)} \right\rangle \right] \tag{8}$$

We can if we wish rewrite this as

$$\left\langle \mu_{dip}^{(2)} \right\rangle = -e\left[\frac{1}{2} \left\langle \Phi^{(1)} \left| z \right| \Phi^{(1)} \right\rangle + \left\langle \Phi^{(0)} \left| z \right| \Phi^{(2)} \right\rangle \right] + c.c. \tag{9}$$

where the "c.c." means the complex conjugate. This is a typical notation in nonlinear optics, and can reduce the number of terms we must write out. (Note that $\left\langle \Phi^{(1)} \left| z \right| \Phi^{(1)} \right\rangle$ is necessarily a real number because z is a Hermitian operator, and so we can write it as $\frac{1}{2}\left\langle \Phi^{(1)} \left| z \right| \Phi^{(1)} \right\rangle + c.c.$).

Now we need to examine explicitly what the various vectors $\left| \Phi^{(0)} \right\rangle, \left| \Phi^{(1)} \right\rangle$ and $\left| \Phi^{(2)} \right\rangle$ are. By choice of the initial state of the unperturbed system, we have, writing the full-time dependent form

$$\left| \Phi^{(0)} \right\rangle = \exp\left(-i\omega_1 t\right)\left| \psi_1 \right\rangle \tag{10}$$

where $\omega_1 \equiv E_1 / \hbar$ (with E_1 being the energy of state 1). Now, we will choose a perturbation consisting of a simple oscillating electric field of one frequency, i.e.,

$$E(t) = 2E_0 \cos \omega t = E_0 \left[\exp(i\omega t) + \exp(-i\omega t) \right] \tag{11}$$

which gives a perturbing Hamiltonian, for the field being polarized in the z-direction, of

$$\hat{H}_p(t) = E(t)z = \hat{H}_{p0}\left[\exp(i\omega t) + \exp(-i\omega t) \right] \tag{12}$$

where

$$\hat{H}_{p0} = eE_0 z \tag{13}$$

In our steady state situation, therefore, we obtain, from first-order time-dependent perturbation theory

$$\dot{a}_i^{(1)}(t) = \frac{eE_0}{i\hbar} \left\langle \psi_i \left| z \right| \psi_1 \right\rangle \exp(i\omega_{i1}t)\left[\exp(i\omega t) + \exp(-i\omega t) \right] \tag{14}$$

where

$$\omega_{ij} \equiv (E_i - E_j)/\hbar \tag{15}$$

Integrating, we obtain

$$a_i^{(1)}(t) = -\frac{eE_0}{\hbar} z_{i1}\left[\frac{\exp\left[i(\omega_{i1} - \omega)t\right]}{(\omega_{i1} - \omega)} + \frac{\exp\left[i(\omega_{i1} + \omega)t\right]}{(\omega_{i1} + \omega)} \right] \tag{16}$$

where we have introduced the notation

$$z_{ij} = \langle \psi_i | z | \psi_j \rangle$$

We also know that successive higher-order coefficients can be evaluated from the preceding ones through

$$\dot{a}_i^{(p+1)}(t) = \frac{1}{i\hbar} \sum_n a_n^{(p)} \exp(i\omega_{in}t) \langle \psi_i | \hat{H}_p(t) | \psi_n \rangle \qquad (17)$$

and so, in our present case, we have

$$\dot{a}_i^{(2)}(t) = +\frac{eE_0}{i\hbar} \sum_{n(\neq 1)} a_n^{(1)}(t) \exp(i\omega_{in}t) \langle \psi_i | z | \psi_n \rangle \left[\frac{\exp[i(\omega_{i1} - w)t]}{(w_{i1} - w)} + \frac{\exp[i(\omega_1 + \omega)t]}{\omega_{i1} + \omega} \right] \qquad (18)$$

i.e.,

$$\dot{a}_i^{(2)}(t) = -\frac{1}{i} \left(\frac{eE_o}{\hbar} \right)^2 \sum_{n(\neq 1)} \left\{ z_{n1} \left[\frac{\exp[i(\omega_{n1} - \omega)t]}{\omega_{n1} - \omega} + \frac{\exp[i(\omega_{n1} + \omega)t]}{\omega_{n1} + \omega} \right] \right\}$$
$$\times \exp(i\omega_{in}t) z_{in} \left[\exp(i\omega t) + \exp(-i\omega t) \right]$$
$$= \frac{-1}{i} \left(\frac{eE_o}{\hbar} \right)^2 \sum_n z_{in} z_{n1} \qquad (19)$$
$$\times \left\{ \frac{1}{\omega_{n1} - \omega} \left[\exp(i\omega_{i1}t) + \exp[i(\omega_{i1} - 2\omega)t] \right] + \frac{1}{\omega_{n1} + \omega} \left[\exp(i\omega_{i1}t) + \exp[i(\omega_{i1} + 2\omega)t] \right] \right\}$$

Note that

$$\omega_{in} + \omega_{n1} = \omega_{i1}$$

Hence, for $i \neq 1$

$$a_i^{(2)}(t) = \left(\frac{eE_o}{\hbar} \right)^2 \sum_n z_{in} z_{n1} \left\{ \frac{\exp(i\omega_{i1}t)}{\omega_{i1}(\omega_{n1} - \omega)} + \frac{\exp[i(\omega_{i1} - 2\omega)t]}{(\omega_{i1} - 2\omega)(\omega_{n1} - \omega)} + \frac{\exp(i\omega_{i1}t)}{\omega_{i1}(\omega_{n1} + \omega)} + \frac{\exp[i(\omega_{i1} + 2\omega)t]}{(\omega_{i1} + 2\omega)(\omega_{n1} + \omega)} \right\} \quad (20)$$

and for $i = 1$

$$a_1^{(2)}(t) = \left(\frac{eE_o}{\hbar} \right)^2 \sum_n z_{1n} z_{n1} \left\{ \frac{1}{\omega_{n1} - \omega} - \frac{\exp[-2i\omega t]}{2\omega(\omega_{n1} - \omega)} + \frac{1}{\omega_{n1} + \omega} + \frac{\exp[2i\omega t]}{2\omega(\omega_{n1} - \omega)} \right\} \quad (21)$$

Now let us evaluate the terms in (9). We have

$$\langle \Phi^{(1)} | z | \Phi^{(1)} \rangle = \sum_{j,k} z_{jk} a_j^{*(1)}(t) a_k^{(1)}(t) \exp(i\omega_{jk}t)$$
$$= \left(\frac{eE_o}{\hbar} \right)^2 \sum_{j,k} z_{1j} z_{jk} z_{k1} \left[\frac{\exp[-i(\omega_{j1} - \omega)t]}{\omega_{j1} - \omega} + \frac{\exp[-i(\omega_{j1} + \omega)t]}{\omega_{j1} + \omega} \right] \quad (22)$$
$$\times \left[\frac{\exp[i(\omega_{k1} - \omega)t]}{\omega_{k1} - \omega} + \frac{\exp[i(\omega_{k1} + \omega)t]}{\omega_{k1} + \omega} \right] \exp(i\omega_{jk}t)$$

where we have noted that $z_{j1}^* = z_{1j}$. I.e.,

$$\left\langle \Phi^{(1)} \middle| z \middle| \Phi^{(1)} \right\rangle = \left(\frac{eE_o}{\hbar} \right)^2 \sum_{j,k} z_{1j} z_{jk} z_{k1}$$

$$\times \left[\frac{1}{(\omega_{j1} - \omega)(\omega_{k1} - \omega)} + \frac{\exp(2i\omega t)}{(\omega_{j1} - \omega)(\omega_{k1} + \omega)} + \frac{\exp(-2i\omega t)}{(\omega_{j1} + \omega)(\omega_{k1} - \omega)} + \frac{1}{(\omega_{j1} + \omega)(\omega_{k1} + \omega)} \right]$$

(23)

For the next term in (9), we have

$$\left\langle \Phi^{(0)} \middle| z \middle| \Phi^{(2)} \right\rangle = \sum_{j} z_{1j} a_j^{(2)} \exp(i\omega_{1j} t)$$

$$= \left(\frac{eE_o}{\hbar} \right)^2 \sum_{j \neq 1, k \neq 1} z_{1j} z_{jk} z_{k1}$$

(24)

$$\times \left[\frac{1}{\omega_{j1}(\omega_{k1} - \omega)} + \frac{\exp(-2i\omega t)}{(\omega_{j1} - 2\omega)(\omega_{k1} - \omega)} + \frac{1}{\omega_{j1}(\omega_{k1} + \omega)} + \frac{\exp(-2i\omega t)}{(\omega_{j1} + 2\omega)(\omega_{k1} + \omega)} \right]$$

Note that the terms with $j = 1$ now have disappeared. Since $z_{11} = 0$, any finite terms multiplied by z_{11} disappear. For any finite time, or for any definite integral over time with finite limits, $a_1^{(2)}(t) = 0$. Hence, we write the sum for $j \neq 1$. Of course, terms with $k = 1$ are also zero because they contain z_{11} also, so we can write the sum with $k \neq 1$ as well if we wish.

So, substituting these in (9), we have

$$\left\langle \mu_{dip}^{(2)} \right\rangle = -\frac{e^3}{\hbar^2} E_0^2 \sum_{j \neq 1, k \neq 1} z_{ij} z_{jk} z_{k1}$$

$$\times \left[\frac{1}{2(\omega_{j1} - \omega)(\omega_{k1} - \omega))} + \frac{\exp(2i\omega t)}{2(\omega_{j1} - \omega)(\omega_{k1} + \omega))} + \frac{\exp(-2i\omega t)}{2(\omega_{j1} + \omega)(\omega_{k1} - \omega))} \right.$$

(25)

$$+ \frac{1}{2(\omega_{j1} + \omega)(\omega_{k1} + \omega))} + \frac{1}{\omega_{j1}(\omega_{k1} - \omega)}$$

$$\left. + \frac{\exp(-2i\omega t)}{2(\omega_{j1} - 2\omega)(\omega_{k1} - \omega))} + \frac{1}{\omega_{j1}(\omega_{k1} + \omega)} + \frac{\exp(2i\omega t)}{(\omega_{j1} + 2\omega)(\omega_{k1} + \omega))} \right] + c.c.$$

i.e.,

$$\left\langle \mu_{dip}^{(2)} \right\rangle = -\frac{e^3}{\hbar^2} E_0^2 \sum_{j \neq 1, k \neq 1} z_{ij} z_{jk} z_{k1}$$

$$\times \left\{ \left[\frac{1}{(\omega_{j1} - \omega)(\omega_{k1} - \omega)} + \frac{1}{(\omega_{j1} + \omega)(\omega_{k1} + \omega)} + \frac{2}{\omega_{j1}(\omega_{k1} - \omega)} + \frac{2}{\omega_{j1}(\omega_{k1} + \omega)} \right] \right.$$

(26)

$$\left. + \cos(2\omega t) \left[\frac{1}{(\omega_{j1} - \omega)(\omega_{k1} + \omega)} + \frac{1}{(\omega_{j1} + \omega)(\omega_{k1} - \omega)} + \frac{2}{(\omega_{j1} - 2\omega)(\omega_{k1} - \omega)} + \frac{2}{(\omega_{j1} + 2\omega)(\omega_{k1} + \omega)} \right] \right\}$$

(ii) The term in the above equation that is not the second harmonic generation term is one that has no time variation. It corresponds to an induced static dipole, and hence gives a static electric field (hence the term "optical rectification") that is proportional to the light intensity.

(iii) If all the wave functions have definite parity, then all terms containing the matrix elements of the state with itself are zero, i.e., $z_{jj} = 0$, and so any products containing such terms are zero. We also cannot have all of z_{12}, z_{23}, and z_{31} non-zero. If states 1 and 2 have opposite parities, so that z_{12} is finite, and states 2 and 3 have opposite parities so that z_{23} is finite, then states 3 and 1 must have the same parities. So, z_{31} must be zero. Similar arguments follow for any other choice of wave function pairs with opposite parities. Hence, if all the wave functions have definite parities

$$z_{1j} z_{jk} z_{k1} = 0 \text{ for all } j \text{ and } k$$

(iv) We can write

$$E_0^2 = Z_0 I \quad \text{and} \quad E_{dip} = \frac{10^{19} \times 10^6}{\varepsilon_0} \left\langle \mu_{dip}^{(2)} \right\rangle$$

since $10^{19} \times 10^6$ is the density of dipoles per m³. If we work in electron volts for the energies

$$E_i = \frac{\hbar \omega_i}{e}$$

and if we note that all the products $z_{1j} z_{jk} z_{k1} = 10^{-30}$ for all j and $k \neq 1$, then we have, with $\frac{\hbar \omega}{e} = E_p$,

$$
\begin{aligned}
E_{dip} = -\varepsilon_{mag} \sum_{\substack{j \neq 1, \\ k \neq 1}} \Bigg\{ & \left[\frac{1}{(E_{j1} - E_p)(E_{k1} - E_p)} + \frac{1}{(E_{j1} + E_p)(E_{k1} + E_p)} + \frac{2}{E_{j1}(E_{k1} - E_p)} + \frac{2}{E_{j1}(E_{k1} + E_p)} \right] \\
& + \cos(2\omega t) \left[\frac{1}{(E_{j1} - E_p)(E_{k1} + E_p)} + \frac{1}{(E_{j1} + E_p)(E_{k1} - E_p)} \right. \\
& \left. \left. + \frac{2}{(E_{j1} - 2E_p)(E_{k1} - E_p)} + \frac{2}{(E_{j1} + 2E_p)(E_{k1} + E_p)} \right] \right\}
\end{aligned}
\tag{27}
$$

where

$$E_{mag} = 10^{25} \times 10^{-30} \frac{e Z_0 I}{2 \varepsilon_0} = \frac{10^{-5} \times 1 \cdot 6 \times 10^{-19} \times 377}{2 \times 8 \cdot 85 \times 10^{-12}} \times 10^{10} = \frac{1 \cdot 6 \times 377}{2 \times 8 \cdot 85} \times 10^{-5-19+12+10} = 0.34 \, V / m \tag{28}$$

The summation becomes, with $E_{21} = 1 eV$, $E_{31} = 1 \cdot 9 eV$, $E_p = 0 \cdot 8 eV$, and evaluating using, e.g., Mathcad, for the optical rectification term

$$E_{dip.opt.rect.} = -0.34 \times 56 \cdot 639 = -19 \cdot 26 \, V / m$$

and for the second harmonic term

$$E_{dip.scnd.harm.} = -0.34 \times (31.881) = -10.84 \, V / m$$

For $\hbar \omega = 0.98 eV$, we similarly have

$$E_{dip.opt.rect.} = -0.34 \times 2769 = -941.5 \, V / m$$

and $\qquad E_{dip.scnd.harm.} = -0.34 \times (-1721) = 585.2 \, V / m$

Hence, the nonlinear optical effects can be seen to be greatly enhanced when we approach a resonance for at least one of the level spacings (here, 0.98 eV is very close to $E_{21} = 1$ eV).

7.4.3

(i) We know that

$$\dot{a}_j^{(1)}(t) = \frac{1}{i\hbar} \sum_{n=1}^{4} a_n^{(0)} \exp(i\omega_{jn}t) \langle \psi_j | \hat{H}_p(t) | \psi_n \rangle$$

Because we assume the system starts in $|\psi_1\rangle$ and the energy origin is E_1, i.e., $a_1^{(0)} = 1$ and all other $a_n^{(0)} = 0$, we have

$$\dot{a}_j^{(1)}(t) = \frac{1}{i\hbar} \exp(i\omega_{j1}t) \langle \psi_j | \hat{H}_p(t) | \psi_1 \rangle$$

In general, we have

$$\langle \psi_j | \hat{H}_p(t) | \psi_n \rangle = H_{jn} \left[\exp(-i\omega t) + \exp(i\omega t) \right]$$

where

$$H_{jn} = e\mathcal{E}_0 \langle \psi_j | z | \psi_n \rangle$$

Hence

$$\dot{a}_j^{(1)}(t) = \frac{1}{i\hbar} H_{j1} \left\{ \exp\left[i(\omega_{j1} - \omega)t \right] + \exp\left[i(\omega_{j1} + \omega)t \right] \right\}$$

So, neglecting the constant of integration as instructed, we have

$$a_j^{(1)}(t) = -\frac{H_{j1}}{\hbar} \left\{ \frac{\exp\left[i(\omega_{j1} - \omega)t \right]}{\omega_{j1} - \omega} + \frac{\exp\left[i(\omega_{j1} + \omega)t \right]}{\omega_{j1} + \omega} \right\}$$

(ii) Now we can establish $a_m^{(2)}$ from $a_j^{(1)}$ using the relation

$$\begin{aligned}
\dot{a}_m^{(p+1)} &= \frac{1}{i\hbar} \sum_j a_j^{(p)}(t) \exp(i\omega_{mj}t) \langle \psi_m | \hat{H}_p | \psi_j \rangle \\
&= \frac{1}{i\hbar} \sum_j a_j^{(p)}(t) H_{mj} \left\{ \exp\left[i(\omega_{mj} - \omega)t \right] + \exp\left[i(\omega_{mj} + \omega)t \right] \right\}
\end{aligned} \tag{1}$$

(which we will also use below to calculate $a_q^{(3)}$ from $a_m^{(2)}$). Hence, for $\dot{a}_m^{(2)}$, we have, noting that $\omega_{mj} + \omega_{j1} = \omega_{mj}$,

$$\dot{a}_m^{(2)} = \frac{-1}{i\hbar^2} \sum_{j=1}^{4} H_{mj} H_{j1} \left\{ \frac{\exp\left[i(\omega_{m1} - 2\omega)t \right] + \exp(i\omega_{m1}t)}{(\omega_{j1} - \omega)} + \frac{\exp\left[i\omega_{m1}t \right] + \exp\left[i(\omega_{m1} + 2\omega)t \right]}{(\omega_{j1} + \omega)} \right\}$$

and so

$$a_m^{(2)}(t) = \frac{1}{\hbar^2} \sum_{j=1}^{4} H_{mj} H_{j1} \left\{ \frac{\exp\left[i(\omega_{m1} - 2\omega)t \right]}{(\omega_{j1} - \omega)(\omega_{m1} - 2\omega)} + \frac{\exp(i\omega_{m1}t)}{(\omega_{j1} - \omega)\omega_{m1}} + \frac{\exp\left[i\omega_{m1}t \right]}{(\omega_{j1} + \omega)\omega_{m1}} + \frac{\exp\left[i(\omega_{m1} + 2\omega)t \right]}{(\omega_{j1} + \omega)(\omega_{m1} + 2\omega)} \right\}$$

[This integration does have the formal problem $m = 1$, which you were instructed to ignore for simplicity. If we do deal with that problem, instead of each occurrence of $1/\omega_{m1}$ we would have $i\Delta t$ instead, where Δt is the range of integration in time].

(iii)   Proceeding similarly, we now evaluate $a_q^{(3)}$ from $a_m^{(2)}$. We have, from (1)

$$\dot{a}_q^{(3)} = \frac{1}{i\hbar} \sum_{m=1}^{4} a_m^{(2)} H_{qm} \left\{ \exp\left[i\left(\omega_{qm} - \omega\right)t\right] + \exp\left[i\left(\omega_{qm} + \omega\right)t\right] \right\}$$

$$= \frac{1}{i\hbar^3} \sum_{m=1}^{4} \sum_{j=1}^{4} H_{qm} H_{mj} H_{j1}$$

$$\times \left\{ \frac{\exp\left[i\left(\omega_{q1} - 3\omega\right)t\right]}{\left(\omega_{j1} - \omega\right)\left(\omega_{m1} - 2\omega\right)} + \frac{\exp\left[i\left(\omega_{q1} - \omega\right)t\right]}{\left(\omega_{j1} - \omega\right)\left(\omega_{m1} - 2\omega\right)} + \frac{\exp\left[i\left(\omega_{q1} - \omega\right)t\right]}{\left(\omega_{j1} - \omega\right)\omega_{m1}} + \frac{\exp\left[i\left(\omega_{q1} + \omega\right)t\right]}{\left(\omega_{j1} - \omega\right)\omega_{m1}} \right.$$

$$\left. + \frac{\exp\left[i\left(\omega_{q1} - \omega\right)t\right]}{\left(\omega_{j1} + \omega\right)\omega_{m1}} + \frac{\exp\left[i\left(\omega_{q1} + \omega\right)t\right]}{\left(\omega_{j1} + \omega\right)\omega_{m1}} + \frac{\exp\left[i\left(\omega_{q1} + \omega\right)t\right]}{\left(\omega_{j1} + \omega\right)\left(\omega_{m1} + 2\omega\right)} + \frac{\exp\left[i\left(\omega_{q1} + 3\omega\right)t\right]}{\left(\omega_{j1} + \omega\right)\left(\omega_{m1} + 2\omega\right)} \right\}$$

Hence we have

$$a_q^{(3)} = \frac{-1}{\hbar^3} \sum_{m=1}^{4} \sum_{j=1}^{4} H_{qm} H_{mj} H_{j1}$$

$$\times \left\{ \frac{\exp\left[i\left(\omega_{q1} - 3\omega\right)t\right]}{\left(\omega_{j1} - \omega\right)\left(\omega_{m1} - 2\omega\right)\left(\omega_{q1} - 3\omega\right)} + \frac{\exp\left[i\left(\omega_{q1} - \omega\right)t\right]}{\left(\omega_{j1} - \omega\right)\left(\omega_{m1} - 2\omega\right)\left(\omega_{q1} - \omega\right)} \right.$$

$$+ \frac{\exp\left[i\left(\omega_{q1} - \omega\right)t\right]}{\left(\omega_{j1} - \omega\right)\omega_{m1}\left(\omega_{q1} - \omega\right)} + \frac{\exp\left[i\left(\omega_{q1} + \omega\right)t\right]}{\left(\omega_{j1} - \omega\right)\omega_{m1}\left(\omega_{q1} + \omega\right)}$$

$$+ \frac{\exp\left[i\left(\omega_{q1} - \omega\right)t\right]}{\left(\omega_{j1} + \omega\right)\omega_{m1}\left(\omega_{q1} - \omega\right)} + \frac{\exp\left[i\left(\omega_{q1} + \omega\right)t\right]}{\left(\omega_{j1} + \omega\right)\omega_{m1}\left(\omega_{q1} + \omega\right)}$$

$$\left. + \frac{\exp\left[i\left(\omega_{q1} + \omega\right)t\right]}{\left(\omega_{j1} + \omega\right)\left(\omega_{m1} + 2\omega\right)\left(\omega_{q1} + \omega\right)} + \frac{\exp\left[i\left(\omega_{q1} + 3\omega\right)t\right]}{\left(\omega_{j1} + \omega\right)\left(\omega_{m1} + 2\omega\right)\left(\omega_{q1} + 3\omega\right)} \right\}$$

(iv)   We have two possible sources of contributions here for third-order terms, i.e.,

$$\mu_{dip} = \mu_{dip\,03} + \mu_{dip\,12}$$

where

$$\mu_{dip\,03} = e\left\langle \psi^{(0)} \left| z \right| \psi^{(3)} \right\rangle + \text{complex conjugate}$$

$$\mu_{dip\,12} = e\left\langle \psi^{(1)} \left| z \right| \psi^{(2)} \right\rangle + \text{complex conjugate}$$

For

$$\left\langle \psi^{(0)} \left| z \right| \psi^{(3)} \right\rangle$$

we have, retaining only terms in $\exp(i\omega t)$ and $\exp(-i\omega t)$, noting that $H_{ab} \equiv H_{ba}^{*}$ because the Hamiltonian is Hermitian, and using $e\left\langle \psi_p \left| z \right| \psi_q \right\rangle = H_{pq} / E_0$,

$$e\left\langle \psi^{(0)} \left| z \right| \psi^{(3)} \right\rangle = e \sum_{q=1}^{4} a_1^{(0)*}(t) \exp\left(i\omega_1 t\right) a_q^{(3)}(t) \exp\left(-i\omega_q t\right) \left\langle \psi_1 \left| z \right| \psi_q \right\rangle$$

$$= \frac{1}{E_0} \sum_{q=1}^{4} \sum_{m=1}^{4} \sum_{j=1}^{4} H_{1q} a_q^{(3)}(t) \exp(-i\omega_{q1} t)$$

$$= \frac{1}{\hbar^3 E_0} \sum_{q=1}^{4} \sum_{m=1}^{4} \sum_{j=1}^{4} H_{1q} H_{qm} H_{mj} H_{j1}$$

$$\times \left\{ \exp(-i\omega t) \left[\frac{1}{\left(\omega_{j1} - \omega\right)\left(\omega_{m1} - 2\omega\right)\left(\omega_{q1} - \omega\right)} \right.\right.$$

$$+ \frac{1}{\left(\omega_{j1} - \omega\right)\omega_{m1}\left(\omega_{q1} - \omega\right)} + \left. \frac{1}{\left(\omega_{j1} + \omega\right)\omega_{m1}\left(\omega_{q1} - \omega\right)} \right]$$

$$+ \exp(i\omega t) \left[\frac{1}{\left(\omega_{j1} - \omega\right)\omega_{m1}\left(\omega_{q1} + \omega\right)} \right.$$

$$+ \frac{1}{\left(\omega_{j1} + \omega\right)\omega_{m1}\left(\omega_{q1} + \omega\right)} + \left.\left. \frac{1}{\left(\omega_{j1} + \omega\right)\left(\omega_{m1} + 2\omega\right)\left(\omega_{q1} + \omega\right)} \right]\right\}$$

For

$$\left\langle \psi^{(1)} \left| z \right| \psi^{(2)} \right\rangle$$

we similarly have (before selecting terms in $\exp(i\omega t)$ and $\exp(-i\omega t)$), being careful to use a new summation index k for the $\psi^{(1)}$ expansion

$$e\left\langle \psi^{(1)} \left| z \right| \psi^{(2)} \right\rangle = e \sum_{k=1}^{4} \sum_{m=1}^{4} a_k^{*(1)} \exp\left(i\omega_k t\right) a_m^{(2)} \exp\left(-i\omega_m t\right) \left\langle \psi_k \left| z \right| \psi_m \right\rangle$$

$$= \frac{-1}{E_0 \hbar^3} \sum_{k=1}^{4} \sum_{m=1}^{4} \sum_{j=1}^{4} H_{k1}^* H_{km} H_{mj} H_{j1} \exp(i\omega_{km} t)$$

$$\times \left\{ \frac{\exp\left[-i\left(\omega_{k1} - \omega\right)t\right]}{\left(\omega_{k1} - \omega\right)} + \frac{\exp\left[-i\left(\omega_{k1} + \omega\right)t\right]}{\left(\omega_{k1} + \omega\right)} \right\}$$

$$\times \left\{ \frac{\exp\left[i\left(\omega_{m1} - 2\omega\right)t\right]}{\left(\omega_{j1} - \omega\right)\left(\omega_{m1} - 2\omega\right)} + \frac{\exp(i\omega_{m1} t)}{\left(\omega_{j1} - \omega\right)\omega_{m1}} + \frac{\exp\left(i\omega_{m1} t\right)}{\left(\omega_{j1} + \omega\right)\omega_{m1}} + \frac{\exp\left[i\left(\omega_{m1} + 2\omega\right)t\right]}{\left(\omega_{j1} + \omega\right)\left(\omega_{m1} + 2\omega\right)} \right\}$$

Because we are told that none of the energy level differences correspond to any integer multiple of ω, the only terms that can give us $\exp(i\omega t)$ and $\exp(-i\omega t)$ time dependence are those with $\pm\omega$ appearing in the final exponent in the product.

Hence we have, retaining only terms in $\exp(i\omega t)$ or $\exp(-i\omega t)$,

$$e\left\langle \psi^{(1)}\left|z\right|\psi^{(2)}\right\rangle = e\sum_{k=1}^{4}\sum_{m=1}^{4}\sum_{j=1}^{4} H_{ik}H_{km}H_{mj}H_{j1}$$

$$\times\left\{\exp(i\omega t)\left[\frac{1}{(\omega_{k1}-\omega)(\omega_{j1}-\omega)\omega_{m1}}\right.\right.$$

$$\left.+\frac{1}{(\omega_{k1}-\omega)(\omega_{j1}+\omega)\omega_{m1}}+\frac{1}{(\omega_{k1}+\omega)(\omega_{j1}+\omega)(\omega_{m1}+2\omega)}\right]$$

$$+\exp(-i\omega t)\left[\frac{1}{(\omega_{k1}+\omega)(\omega_{j1}-\omega)\omega_{m1}}\right.$$

$$\left.\left.+\frac{1}{(\omega_{k1}+\omega)(\omega_{j1}+\omega)\omega_{m1}}+\frac{1}{(\omega_{k1}-\omega)(\omega_{j1}-\omega)(\omega_{m1}-2\omega)}\right]\right\}$$

Putting everything together, and using q instead of k as the index in the sum for μ_{dip12}, we have

$$\mu_{dip}=-\frac{1}{\hbar^3\mathsf{E}_0}\sum_{q=1}^{4}\sum_{m=1}^{4}\sum_{j=1}^{4} H_{1q}H_{qm}H_{mj}H_{j1}$$

$$\times\left\{\exp(i\omega t)\left[\frac{1}{(\omega_{q1}+\omega)\omega_{m1}(\omega_{j1}-\omega)}+\frac{1}{(\omega_{q1}+\omega)\omega_{m1}(\omega_{j1}+\omega)}+\frac{1}{(\omega_{q1}+\omega)(\omega_{m1}+2\omega)(\omega_{j1}+\omega)}\right.\right.$$

$$\left.+\frac{1}{(\omega_{q1}-\omega)\omega_{m1}(\omega_{j1}+\omega)}+\frac{1}{(\omega_{q1}-\omega)\omega_{m1}(\omega_{j1}-\omega)}+\frac{1}{(\omega_{q1}+\omega)(\omega_{m1}+2\omega)(\omega_{j1}+\omega)}\right]$$

$$+\exp(-i\omega t)\left[\frac{1}{(\omega_{q1}-\omega)\omega_{m1}(\omega_{j1}+\omega)}+\frac{1}{(\omega_{q1}-\omega)\omega_{m1}(\omega_{j1}-\omega)}+\frac{1}{(\omega_{q1}-\omega)(\omega_{m1}-2\omega)(\omega_{j1}-\omega)}\right.$$

$$\left.\left.+\frac{1}{(\omega_{q1}+\omega)\omega_{m1}(\omega_{j1}-\omega)}+\frac{1}{(\omega_{q1}+\omega)\omega_{m1}(\omega_{j1}+\omega)}+\frac{1}{(\omega_{q1}-\omega)(\omega_{m1}-2\omega)(\omega_{j1}-\omega)}\right]\right\}$$

+ c.c.

[Note, returning to the formal problem of $m=1$, that for every term with $\exp(i\omega t)/\omega_{m1}$ in the above expression, there is an identical one with $\exp(-i\omega t)/\omega_{m1}$, so we end up with a collection of real terms proportional to $\cos(\omega t)/\omega_{m1}$. Making the substitution discussed above of $i\Delta t$ for $1/\omega_{11}$, and then adding in the complex conjugate to get the final result, all of these terms in Δt cancel one another out, and so the formal issue of dealing with ω_{11} finally disappears. Now we can rigorously change the summation over m to one over $m=2,3,4$, since we have just shown that the terms with $m=1$ all cancel. This completes the formal resolution of this difficulty.]

(v)(a) Given the restrictions on matrix elements, there are only a few products that survive, namely

$$H_{12}H_{24}H_{42}H_{21},\ \ H_{13}H_{34}H_{43}H_{31},\ \ H_{12}H_{24}H_{43}H_{31}\ \text{and}\ H_{13}H_{34}H_{42}H_{21}$$

plus the same set with 1 substituted for 4. Of these only the four explicitly listed will have terms with $(\omega_{41}-\omega)$ in the denominator. Hence, we are left with

$$\mu_{dip} = \frac{-2}{\hbar^3 E_0} \sum_{q=2,3} \sum_{j=2,3} H_{1q} H_{q4} H_{4j} H_{j1} \frac{\exp(-i\omega t)}{(\omega_{q1} - \omega)(\omega_{41} - 2\omega)(\omega_{j1} - \omega)} + \text{c.c.}$$

or equivalently

$$\mu_{dip} = \frac{-4e^4}{\hbar^3} z_0^4 E_o^3 \left[\sum_{q=2,3} \sum_{j=2,3} \frac{1}{(\omega_{q1} - \omega)(\omega_{41} - 2\omega)(\omega_{j1} - \omega)} \right] \cos \omega t$$

(b) From the above, noting that $\hbar\omega / e$ is an energy in electron volts, we have

$$\mu_{dip} = -4e z_0^4 E_o^3 \left[\sum_{q=2,3} \sum_{j=2,3} \frac{1}{(\hbar\omega_{q1} - \hbar\omega)_{eV}(\hbar\omega_{41} - 2\hbar\omega)_{eV}(\hbar\omega_{j1} - \hbar\omega)_{eV}} \right] \cos \omega t$$

We also have, for a density N, such systems per unit volume that, for the relevant contribution to the polarization P, we have

$$P = N \mu_{dip}$$

and hence (with the simplifying assumption that this is the only polarization)

$$\chi = \frac{P}{\varepsilon_0 E} = \frac{N \mu_{dip}}{\varepsilon_0 2E_o \cos \omega t}$$

so for the relevant contribution to the refractive index n

$$n = \sqrt{1 + \chi} \simeq 1 + \frac{\chi}{2}$$

on the assumption that we are only making small perturbations to χ, i.e., for the change due to the nonlinear effects

$$\Delta n \simeq \frac{\chi}{2} = \frac{N \mu_{dip}}{4\varepsilon_0 E_o \cos \omega t}$$

We actually want

$$n_2 = \frac{\Delta n}{I}$$

where

$$I = \frac{2E_0^2}{Z_0}$$

so we have

$$n_2 = \frac{N Z_0 \mu_{dip}}{8\varepsilon_0 E_0^3 \cos \omega t}$$

$$= -\frac{N e Z_0 z_0^4}{2\varepsilon_0} \sum_{q=2,3} \sum_{j=2,3} \left[\frac{1}{(\hbar\omega_{q1} - \hbar\omega)_{eV}(\hbar\omega_{41} - 2\hbar\omega)_{eV}(\hbar\omega_{j1} - \hbar\omega)_{eV}} \right]$$

Hence

$$n_2 = -\frac{10^{22} \times 10^6 \times 1.602 \times 10^{-19} \times 377 \times 10^{-40}}{2 \times 8.85 \times 10^{-12}} \sum_{q=2,3} \sum_{j=2,3} [\ldots]$$

$$= 3.4 \times 10^{-18} \sum_{q=2,3} \sum_{j=2,3} [\ldots]$$

For the numbers stated

$$\sum_{q=2,3} \sum_{j=2,3} [\ldots] = \frac{1}{0.05} \times \left[\frac{1}{0.5 \times 0.5} + \frac{1}{0.5 \times 1} + \frac{1}{1 \times 0.5} + \frac{1}{1 \times 1} \right] = 20[4+2+2+1] = 180$$

Hence

$$n_2 = 6.2 \times 10^{-16} \, m^2 / W$$

(or, in somewhat more common units

$$n_2 = 6.12 \times 10^{-12} \, cm^2 / W)$$

(c) We need to find the length ℓ such that, for wavelength λ

$$n_2 I \ell = \frac{\lambda}{2}$$

i.e.,

$$\ell = \frac{\lambda}{2 n_2 I}$$

The intensity is, for 10 mW in a $10 \times 10 \, \mu m^2$ area

$$I = \frac{10^{-2}}{10^{-5} \times 10^{-5}} = 10^8 \, W / m^2$$

Hence, for a photon energy of 2.5 eV, the corresponding wavelength is

$$\lambda = \frac{c}{f} = \frac{2\pi c}{\omega} = \frac{2\pi c \hbar}{\hbar \omega} = \frac{ch}{\hbar \omega} = \frac{ch}{e(\hbar \omega)_{eV}} \cong \frac{1.24 \times 10^{-6}}{\hbar \omega_{eV}} m$$

$$= \frac{1.24}{\hbar \omega_{eV}} \mu m = \frac{1.24}{2.5} \mu m \cong 0.5 \mu m$$

$$\ell = \frac{0.5 \times 10^{-6}}{2 \times 6.12 \times 10^{-16} \times 10^8} \cong 4 \, m$$

(d) For $\hbar \omega_{31} = 2.0 \, eV$, we have

$$\sum_{q=2,3} \sum_{j=2,3} [\ldots] = \frac{1}{0.05} \times \left[\frac{1}{0.5 \times 0.5} + \frac{1}{0.5 \times (-0.5)} + \frac{1}{(-0.5) \times 0.5} + \frac{1}{(-0.5) \times (-0.5)} \right]$$

$$= 0$$

What is happening here is that, though each of the possible processes is finite, because they have different signs, they quantum mechanically interfere, leading to no net quantum mechanical nonlinear effect from these terms.

Chapter 8 problem solutions

8.3.1

Taking the conventional choice

$$k = \frac{2\pi n}{Na} \quad n = 0, \pm 1, \pm 2, \ldots \pm N/2$$

for the representation of Bloch functions, we therefore have, for $N = 6$ and a repeat length $a = 0.5$ nm,

$$k = 0$$

$$k = \pm \frac{2\pi}{ba} = \pm \frac{\pi}{3a} = \pm 2.094 \, nm^{-1} = 2.094 \times 10^9 \, m^{-1}$$

$$k = \pm \frac{4\pi}{ba} = \pm \frac{2\pi}{3a} = \pm 4.189 \, nm^{-1} = 4.189 \times 10^9 \, m^{-1}$$

$$k = \pm \frac{b\pi}{ba} = \pm \frac{\pi}{a} = \pm 6.283 \, nm^{-1} = 6.283 \times 10^9 \, m^{-1}$$

So, the resulting Bloch wavefunctions are of the forms

$$\psi_{-3}(v) = u_{-3}(v) \exp\left[-6.283 \, iv\right]$$

$$\psi_{-2}(v) = u_{-2}(v) \exp\left[-4.189 \, iv\right]$$

$$\psi_{-1}(v) = u_{-1}(v) \exp\left[-2.094 \, iv\right]$$

$$\psi_0(v) = u_0(v)$$

$$\psi_{+1}(v) = u_{+1}(v) \exp\left[2.094 \, iv\right]$$

$$\psi_{+2}(v) = u_{+2}(v) \exp\left[4.189 \, iv\right]$$

$$\psi_{+3}(v) = u_{+3}(v) \exp\left[6.283 \, iv\right]$$

where v is being expressed in nm.

Note we have written all the unit cell functions $u(v)$ as being different functions, which in general they are.

To be strictly correct, we have one too many functions here, which is because of the error in the common way of stating the limits on k (including both edges of the Brillouin zone). How precisely one deals with this is a matter of taste. One could choose to eliminate either the "-3" or the "+3" function from the list above, or one could index from 0 to 5 inclusive, which might actually be a better approach for such a small finite structure, and would certainly be an acceptable alternative answer to this question.

8.4.1

The separation between allowed k values in a given direction is

$$\Delta k = \frac{2\pi}{Na}$$

where N is the number of unit cells in that direction, and a is the repeat length in that direction. For the present case, therefore, we have

$$\Delta k_x = \frac{2\pi}{1000 \times 0.5} = \left(\frac{\pi}{250}\right) nm^{-1} \quad (\simeq 0.0126\, nm^{-1})$$

$$\Delta k_y = \frac{2\pi}{1000 \times 0.4} = \left(\frac{\pi}{200}\right) nm^{-1} \quad (\simeq 0.0157\, nm^{-1})$$

$$\Delta k_y = \frac{\pi}{200} \simeq 0.0157 \text{ nm}^{-1}$$

$$\Delta k_x = \frac{\pi}{250} \simeq 0.0126 \text{ nm}^{-1}$$
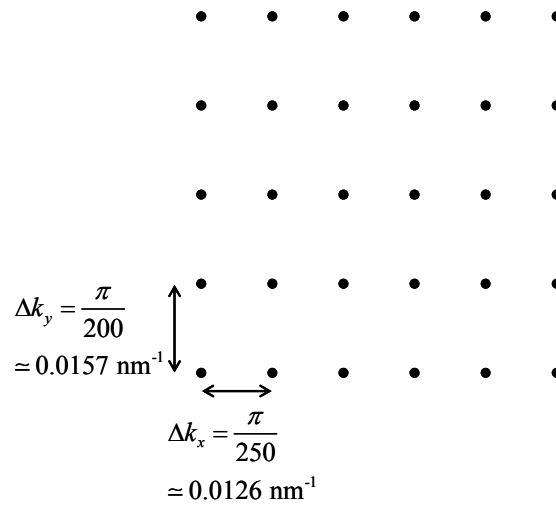
8.5.1

We take the Bloch form

$$\psi(x) = u(x)\exp(ikx)$$

where k lies within the first Brillouin zone, i.e.,

$$-\frac{\pi}{a} \le k \le \frac{\pi}{a}$$

for a one-dimensional crystal of repeat length a. Now, for any k_{new} outside the first Brillouin zone, we can write it by adding onto k an additional "reciprocal lattice vector"

$$K = \frac{2n\pi}{a}$$

for some positive or negative integer n, i.e.,

$$k_{new} = k + \frac{2n\pi}{a}$$

Then

$$\psi_{new}(x) = u(x)\exp\left[i\left(k + \frac{2n\pi}{a}\right)x\right]$$

$$= \left[u(x)\exp\left(\frac{2n\pi}{a}x\right)\right]\exp(ikx)$$

Let us write

$$v(x) = u(x)\exp\left(\frac{2n\pi x}{a}\right)$$

Then

$$v(x+a) = u(x+a)\exp\left[\frac{2n\pi(x+a)}{a}\right]$$

$$= u(x+a)\exp\left[\frac{2n\pi x}{a}\right]\exp[2n\pi]$$

$$= u(x+a)\exp\left[\frac{2n\pi x}{a}\right]$$

But, $u(x + a) = u(x)$, so $v(x + a) = v(x)$, and this function $v(x)$ is also periodic with the repeat length a. Hence, the function $\psi_{new}(x)$ can be written in the form

$$\psi_{new}(x) = v(x)\exp\left(\frac{ikx}{a}\right)$$

which is a Bloch function expressed within the first Brillouin zone.

8.6.1

We follow the derivation in the book of the effective mass Schrödinger equation, but instead of $E_{\mathbf{k}} = \dfrac{\hbar^2 k^2}{2m_{eff}} + V$, we write

$$E_{\mathbf{k}} = \frac{\hbar^2 \left|\mathbf{k} - \mathbf{k}_o\right|^2}{2m_{eff}} + V = \frac{\hbar^2 k_{new}^2}{2m_{eff}} + V$$

and also write

$$\Psi(\mathbf{r},t) = \exp(i\mathbf{k}_o \cdot \mathbf{r}) \sum_{\mathbf{k}_{new}} c_{\mathbf{k}_{new}} u_{\mathbf{k}_{new}}(\mathbf{r}) \exp(i\mathbf{k}_{new} \cdot \mathbf{r}) \exp(-iE_{\mathbf{k}_{new}} t / \hbar)$$

instead of

$$\Psi(\mathbf{r},t) = \sum_{\mathbf{k}} c_{\mathbf{k}} u_{\mathbf{k}}(\mathbf{r}) \exp(i\mathbf{k}.\mathbf{r}) \exp(-iE_{\mathbf{k}} t / \hbar)$$

Again, we approximate

$$u_{\mathbf{k}_{new}}(\mathbf{r}) \simeq u_o(\mathbf{r})$$

for the range of $\mathbf{k}$ of interest. Now we write

$$\Psi(\mathbf{r},t) = u_o(\mathbf{r}) \exp(i\mathbf{k}_o \cdot \mathbf{r}) \Psi_{envnew}(\mathbf{r},t)$$

so that

$$\Psi(\mathbf{r},t) = u_0(\mathbf{r}) \exp(i\mathbf{k}_o \cdot \mathbf{r}) \Psi_{envnew}(\mathbf{r},t)$$

as required. Then

$$\Psi_{envnew}(\mathbf{r},t) = \sum_{\mathbf{k}_{new}} c_{\mathbf{k}_{new}} \exp(i\mathbf{k}_{new} \cdot \mathbf{r}) \exp(-iE_{\mathbf{k}_{new}} t / \hbar)$$

We then follow the argument as before, obtaining

$$i\hbar \frac{\partial \Psi_{envnew}}{\partial t} = \sum_{\mathbf{k}_{new}} c_{\mathbf{k}_{new}} E_{\mathbf{k}_{new}} \exp(i\mathbf{k}_{new}.\mathbf{r}) \exp(-iE_{\mathbf{k}_{new}} t / \hbar)$$

$$= \frac{\hbar^2}{2m_{eff}} \sum_{\mathbf{k}_{new}} c_{\mathbf{k}_{new}} k_{new}^2 \exp(i\mathbf{k}_{new}.\mathbf{r}) \exp(-iE_{\mathbf{k}_{new}} t / \hbar)$$

$$+ V \sum_{\mathbf{k}_{new}} c_{\mathbf{k}_{new}} \exp(i\mathbf{k}_{new}.\mathbf{r}) \exp(-iE_{\mathbf{k}_{new}} t / \hbar)$$

$$= \frac{\hbar^2}{2m_{eff}} \sum_{\mathbf{k}_{new}} \left[-c_{\mathbf{k}_{new}} \nabla^2 \exp(i\mathbf{k}_{new}.\mathbf{r}) \right] \exp(-iE_{\mathbf{k}_{new}} t / \hbar) + V \Psi_{envnew}$$

so that, as required,

$$-\frac{\hbar^2}{2m_{eff}} \nabla^2 \Psi_{envnew}(\mathbf{r},t) + V(\mathbf{r}) \Psi_{envnew}(\mathbf{r},t) = i\hbar \frac{\partial}{\partial t} \Psi_{envnew}(\mathbf{r},t)$$

8.6.2

Using

$$E_{\mathbf{k}} = \frac{\hbar^2}{2}\left[\frac{k_x^2}{m_x} + \frac{k_y^2}{m_y} + \frac{k_z^2}{m_z}\right] + V$$

and the same assumptions as in the derivation of the original effective mass approximation, we have

$$i\hbar\frac{\partial \Psi_{env}}{\partial t} = \sum_{\mathbf{k}} c_{\mathbf{k}} E_{\mathbf{k}} \exp(i\mathbf{k}.\mathbf{r})\exp(-iE_{\mathbf{k}}t/\hbar)$$

$$= \frac{\hbar^2}{2}\sum_{\mathbf{k}} c_{\mathbf{k}}\left[\frac{k_x^2}{m_x} + \frac{k_y^2}{m_y} + \frac{k_z^2}{m_z}\right]\exp(i\mathbf{k}.\mathbf{r})\exp(-iE_{\mathbf{k}}t/\hbar) + V\sum_{\mathbf{k}} c_{\mathbf{k}} \exp(i\mathbf{k}.\mathbf{r})\exp(-iE_{\mathbf{k}}t/\hbar)$$

$$= -\frac{\hbar^2}{2}\sum_{\mathbf{k}} c_{\mathbf{k}}\left[\frac{1}{m_x}\frac{\partial^2}{\partial x^2} + \frac{1}{m_y}\frac{\partial^2}{\partial y^2} + \frac{1}{m_z}\frac{\partial^2}{\partial z^2}\right]\exp(i\mathbf{k}.\mathbf{r})\exp(-iE_{\mathbf{k}}t/\hbar) + V\Psi_{env}$$

i.e.,

$$-\frac{\hbar^2}{2}\left[\frac{1}{m_x}\frac{\partial^2}{\partial x^2} + \frac{1}{m_y}\frac{\partial^2}{\partial y^2} + \frac{1}{m_z}\frac{\partial^2}{\partial z^2}\right]\Psi_{env}(\mathbf{r},t) + V(\mathbf{r})\Psi_{env}(\mathbf{r},t) = i\hbar\frac{\partial}{\partial t}\Psi_{env}(\mathbf{r},t)$$

8.8.1

Assume the quantum wire is extremely short in the x and y directions (confined along x and y), and is long in the z direction. The confinement in x and y directions introduces subbands.

Assuming propagating waves in the z direction, for each subband,

$$E_z = \frac{\hbar^2 k_z^2}{2\,m_{eff}} \tag{1}$$

where $k_z = \dfrac{2\pi}{L_z} n$ for some integer n and L_z is the length of the wire. Now, in one dimension

$$\text{Density of states in k space} = \left\{ \frac{1}{\text{"volume" occupied by one k state in k space}} \right\} = \frac{1}{\left(\dfrac{2\pi}{L_z} \right)}$$

Hence, for a one-dimensional crystal of length L_z

$$g_{1D}(k_z) = \frac{L}{2\pi}$$

Now we convert to the density of states in energy, $g(E_z)$, for each subband. Taking into account both the forward and backward traveling waves – that is, for each (positive) k_z value, we count two states – multiplying by an additional factor of two to account for the two possible electron spins, and now evaluating this density of states per unit crystal volume (i.e., here, in this one-dimensional case, per unit crystal length), we have

$$g(E_z)\,dE_z = \frac{4 g_{1D}(k_z)\left(\dfrac{dk_z}{dE_z} \right) dE_z}{L_z}$$

Now, the magnitude of k_z, in terms of the energy E_z in a given subband is

$$k_z = \sqrt{\frac{2m_{eff}}{\hbar^2}} \sqrt{E_z} \quad \text{from (1) above}$$

so

$$dk_z = \sqrt{\frac{2m_{eff}}{\hbar^2}} \left(\frac{1}{2} \right) \frac{1}{\sqrt{E_z}} dE_z$$

Hence, for a given subband

$$g(E_z) = \frac{1}{\pi} \sqrt{\frac{2m_{eff}}{\hbar^2}} \frac{1}{\sqrt{E_z}}$$

or

$$g(E_z) = \frac{k_z}{\pi E_z}$$

8.8.2

For this case of a parabolic quantum well, the solutions for the eigenenergies for the z motion will just be the same as those of a harmonic oscillator, i.e., they will be evenly spaced by an "harmonic oscillator" quantum energy, with the first such level at half of that quantum above the bottom of the band. Associated with each such parabolic quantum well energy, there will be a sub-band, which will have the same density of states as other quantum well subbands, i.e., uniform with energy. Hence we will have a series of equally spaced steps.
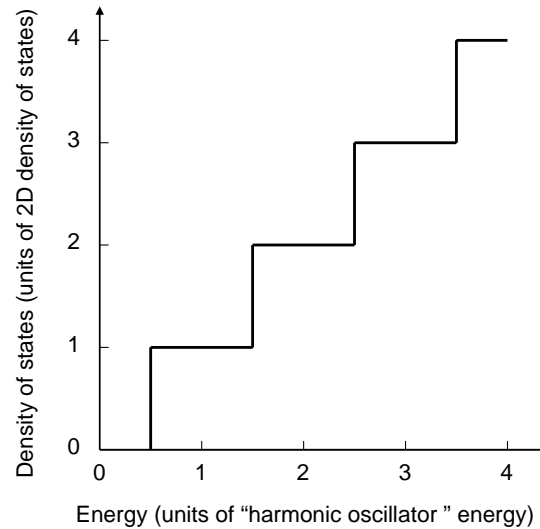
8.10.1

(i) To find the wavefunctions associated with a given k, we first find the exact energy eigenvalues in the two band model, i.e., the roots of

$$\left[E(k)\right]^2 - E_g E(k) - E_p \frac{\hbar^2 k^2}{2m_0} = 0 \tag{1}$$

With

$$b = 2\hbar k p_{12} / E_g m_0 \tag{2}$$

i.e.,

$$|b|^2 = \frac{2E_p}{E_g^2} \frac{\hbar^2 k^2}{m_0} \tag{3}$$

we can rewrite (1) as

$$\left[\varepsilon(k)\right]^2 - \varepsilon(k) - \frac{1}{4}|b|^2 = 0 \tag{4}$$

where

$$\varepsilon(k) = E(k) / E_g \tag{5}$$

Solving (4) for the eigenvalues gives

$$\varepsilon(k) = \frac{1}{2}\left[1 \pm \sqrt{1 + |b|^2}\right] \tag{6}$$

where the upper sign corresponds to the upper band, and the lower sign corresponds to the lower band.

Now we solve for the eigenvectors. We rewrite the matrix eigen equation using our new notation (and our neglect of the term $\hbar^2 k^2 / 2m_0$ in the energies, as in the Chapter), and multiplying by 2 just to simplify the algebra (this multiplication makes no difference because the right hand side is zero)

$$\begin{bmatrix} -\left[1 \pm \sqrt{1 + |b|^2}\right] & b \\ b^* & 2 - \left[1 \pm \sqrt{1 + |b|^2}\right] \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = 0$$

where we are really writing the two different eigenvector equations at once through our use of the "$\pm$" sign.

Consider, for example, the upper line of the matrix-vector multiplication. (Note: we would get the same result if we considered the bottom line). We have

$$-a_1\left[1 \pm \sqrt{1 + |b|^2}\right] + a_2 b = 0$$

i.e.,

$$a_2 = a_1 \left[\frac{1 \pm \sqrt{1+|b|^2}}{b} \right]$$

But, $|a_1|^2 + |a_2|^2 = 1$ by normalization, so

$$|a_1|^2 \left[1 + \frac{\left(1 \pm \sqrt{1+|b|^2}\right)^2}{|b|^2} \right] = 1$$

so

$$|a_1|^2 = \frac{|b|^2}{|b|^2 + \left(1 \pm \sqrt{1+|b|^2}\right)^2}$$

and

$$a_1 = \frac{1}{d_\pm}$$

where

$$d_\pm = \left(1 + \frac{1}{|b|^2}\left(1 \pm \sqrt{1+|b|^2}\right)^2 \right)^{1/2} = \left(1 + \frac{1}{|b|^2} + \frac{1}{|b|^2} + 1 \pm \frac{2\sqrt{1+|b|^2}}{|b|^2} \right)^{1/2} = \left[2\left(1 + \frac{1}{|b|^2} \pm \frac{\sqrt{1+|b|^2}}{|b|^2} \right) \right]^{1/2}$$

(at least within a complex factor of order unity, which will not make any difference to any final calculation, as can be checked "a posteriori"). So

$$a_2 = \frac{1 \pm \sqrt{1+|b|^2}}{bd_\pm}$$

Hence, now writing out the solutions explicitly for the two bands

$$a_{21k} = \frac{1}{d_+} \qquad\qquad a_{22} = \frac{1 + \sqrt{1+|b|^2}}{bd_+}$$

$$a_{11k} = \frac{1}{d_-} \qquad\qquad a_{12k} = \frac{1 - \sqrt{1+|b|^2}}{bd_-}$$

giving

$$u_{2k}(\mathbf{r}) = \frac{1}{d_+} u_{10}(\mathbf{r}) + \frac{\left(1 + \sqrt{1+|b|^2}\right)}{bd_+} u_{20}(\mathbf{r})$$

which is the required answer for part (i).

(ii) From the above, we have

$$u_{1k}(\mathbf{r}) = \frac{1}{d_-} u_{10}(\mathbf{r}) + \frac{\left(1 - \sqrt{1+|b|^2}\right)}{bd_-} u_{20}(\mathbf{r})$$

(iii) Now consider $|p_{21k}|^2$. We have

$$p_{21k} = \int\limits_{\substack{unit \\ cell}} u_{2k}^*(\mathbf{r}) p u_{rk}(\mathbf{r}) d^3\mathbf{r}$$

where

$$u_{2k}(\mathbf{r}) = a_{21k}u_{10}(\mathbf{r}) + a_{22k}u_{20}(\mathbf{r})$$
$$u_{1k}(\mathbf{r}) = a_{11k}u_{10}(\mathbf{r}) + a_{12k}u_{20}(\mathbf{r})$$

so

$$p_{21k} = a_{21k}^* a_{12k} p_{12} + a_{22k}^* a_{11k} p_{21}$$

(Note $p_{nn} = 0$, so the other possible terms disappear). I.e., noting that $p_{12}^* = p_{21}$ by Hermiticity,

$$p_{21k} = \frac{1}{d_+ d_-}\left[\left(\frac{1 - \sqrt{1+|b|^2}}{b}\right)p_{12} + \left(\frac{1 + \sqrt{1+|b|^2}}{b^*}\right)p_{12}^*\right]$$

Now

$$\frac{p_{12}}{b} = \frac{E_g m_0}{2\hbar k} = \frac{p_{12}^*}{b^*} = \frac{|p_{12}|}{|b|} = \frac{|p_{21}|}{|b|}$$

so we have

$$p_{21k} = \frac{1}{d_+ d_-}\frac{|p_{21}|}{|b|}\left[1 - \sqrt{1+|b|^2} + 1 + \sqrt{1+|b|^2}\right] = \frac{2}{d_+ d_-}\frac{|p_{21}|}{b}$$

Now

$$d_+ d_- = 2\left[\left(1 + \frac{1}{|b|^2} + \frac{1}{|b|^2}\sqrt{1+|b|^2}\right)\left(1 + \frac{1}{|b|^2} - \frac{1}{|b|^2}\sqrt{1+|b|^2}\right)\right]^{1/2} = 2\left[\left(1 + \frac{1}{|b|^2}\right)^2 - \left(\frac{\left(\sqrt{1+|b|^2}\right)}{|b|^4}\right)\right]^{1/2}$$

$$= 2\left[1 + \frac{1}{|b|^4} + \frac{2}{|b|^2} - \frac{1}{|b|^4} - \frac{1}{|b|^2}\right]^{1/2} = 2\left[1 + \frac{1}{|b|^2}\right]^{1/2} = \frac{2}{|b|}\sqrt{1+|b|^2}$$

Hence

$$p_{21k} = \frac{|p_{21}|}{\sqrt{1+|b|^2}}$$

so

$$\left|p_{21k}\right|^2 = \frac{\left|p_{21}\right|^2}{1+\left|b\right|^2} = \frac{m_0}{2} \frac{E_p}{1+\dfrac{2E_p}{E_g^2} \dfrac{\hbar^2 k^2}{m_0}}$$

(iv) First we will consider the density of the states in energy. Starting again from the expression for the eigenenergies in the two band case, we have

$$\left[E(k)\right]^2 - E_g E(k) - E_p \frac{\hbar^2 k^2}{2m_0} = 0$$

i.e., $$E(k) = \frac{E_g}{2} \pm \frac{1}{2}\sqrt{\frac{E_g^2 + 4E_p \hbar^2 k^2}{2m_0}} = \frac{E_g}{2}\left[1 \pm \sqrt{1+\frac{2E_p \hbar^2 k^2}{E_g^2 m_0}}\right]$$

i.e., $$\frac{E(k)}{E_g} = \frac{1}{2}\left[1 \pm \sqrt{1+\frac{2E_p \hbar^2 k^2}{E_g^2 m_0}}\right]$$

i.e., $$\frac{2E(k)}{E_g} = \sqrt{1+\frac{2E_p \hbar^2 k^2}{E_g^2 m_0}}$$

i.e., $$\left[\frac{2E(k)}{E_g} - 1\right]^2 = 1 + \frac{2E_p}{E_g^2}\frac{\hbar^2 k^2}{m_0}$$

i.e., $$k^2 = \frac{m_0 E_g^2}{\hbar^2 2E_p}\left\{\left[\frac{2E(k)}{E_g}-1\right]^2 - 1\right\}$$

i.e., $$k^2 = \frac{2m_0}{\hbar^2}\frac{E_g}{E_p} E\left[\frac{E}{E_g}-1\right]$$

i.e., $$k = \left(\frac{2m_0}{\hbar^2}\frac{E_g}{E_p} E\left[\frac{E}{E_g}-1\right]\right)^{1/2}$$

To evaluate *dk/dE*, we note first that

$$\frac{d}{dE} E\left[\frac{E}{E_g}-1\right] = \frac{2E}{E_g} - 1$$

so we have

$$\frac{dk}{dE} = \frac{1}{2}\left(\frac{2m_0}{\hbar^2}\frac{E_g}{E_p}\right)^{1/2} \frac{\left(\dfrac{2E}{E_g}-1\right)}{\left(E\left[\dfrac{E}{E_g}-1\right]\right)^{1/2}}$$

From expressions for densities of states in energy and *k*, we have

$$g(E)dE = 2g(k)dk = \frac{1}{\pi^2}k^2 dk$$

including the effects of spin. Hence,

$$g(E)dE = \frac{1}{\pi^2}k^2\frac{dk}{dE}dE$$

i.e.,
$$g(E) = \frac{1}{2\pi^2}\left(\frac{2m_0}{\hbar^2}\frac{E_g}{E_p}\right)^{3/2}\left(\frac{2E}{E_g}-1\right)\left(E\left[\frac{E}{E_g}-1\right]\right)^{1/2}$$

Note that the term in the square root is positive either if

$$E > E_g \text{ or } E < 0$$

as we would expect for our two bands. (To get positive densities of states, we choose the positive square root for the upper band and the negative square root for the lower band).

For an optical absorption calculation, for direct absorption, we need the joint density of states, $g_J(E_{phot})$. We are interested in an energy

$$E_{phot} = \hbar\omega = E_2(k) - E_1(k)$$

where $E_2(k)$ is the upper band energy and $E_1(k)$ is the lower. We can reason $g_J(\hbar\omega)$ directly. Because the bands are reflections of one another, a change of δE_{phot} in the photon energy corresponds to a change of $-\delta E_{phot}/2$ in the energy $E_1(k)$. Hence,

$$g_J(\hbar\omega) = \frac{1}{2}g_1\left[\left(E_g - \hbar\omega\right)/2\right]$$

where $g_1(E)$ is the density of states in band 1, so

$$g_j(\hbar\omega) = -\frac{1}{4\pi^2}\left(\frac{2m_0}{\hbar^2}\frac{E_g}{E_p}\right)^{3/2}\left(\frac{E_g-\hbar\omega}{E_g}-1\right)\left[\left(\frac{E_g-\hbar\omega}{2}\right)\left(\frac{E_g-\hbar\omega}{2E_g}-1\right)\right]^{1/2}$$

i.e.,
$$g_j(\hbar\omega) = \frac{1}{4\pi^2}\left(\frac{2m_0}{\hbar^2}\frac{E_g}{E_p}\right)^{3/2}\frac{1}{2}\frac{\hbar\omega}{E_g}\left[\left(\hbar\omega-E_g\right)\left(1+\frac{\hbar\omega}{E_g}\right)\right]^{1/2}$$

Now from the appropriate expression for the transition rate, but keeping $|p_{21k}|^2$ inside the sum

$$W_{TOT} = \frac{2\pi}{\hbar}\frac{e^2 A_0^2}{4m_0^2}\sum_k |p_{21k}|^2\,\delta\left(E_2(k) - E_1(k) - \hbar\omega\right)$$

and transitioning to an integral, we have

$$W_{TOT} = \frac{2\pi}{\hbar}\frac{e^2 A_0^2}{4m_0^2}\int |p_{21k}|^2\,g_j(\hbar\omega)\delta\left(E_j - \hbar\omega\right)dE_j$$

$$= \frac{2\pi}{\hbar}\frac{e^2 A_0^2}{4m_0^2}\frac{1}{4\pi^2}\left(\frac{2m_0}{\hbar^2}\frac{E_g}{E_p}\right)^{3/2}|p_{21k}|^2\left(1+\frac{\hbar\omega-E_g}{E_g}\right)\left[\left(\frac{\hbar\omega-E_g}{2}\right)\left(1+\left(\frac{\hbar\omega-E_g}{2E_g}\right)\right)\right]^{1/2}$$

Now moving from the transition rate to the absorption coefficient, we have

$$\alpha = \frac{2\hbar}{n_r c \varepsilon_0 \omega A_0^2} W_{TOT} = \frac{2\hbar}{n_r c \varepsilon_0 \omega A_0^2} \frac{2\pi}{\hbar} \frac{e^2 A_0^2}{4m_0^2} \frac{2\sqrt{2}}{4\pi^2} \left(\frac{m_0}{\hbar^2} \frac{E_g}{E_p}\right)^{3/2} |p_{21k}|^2 \frac{1}{2} \frac{\hbar\omega}{E_g} \left[\left(\hbar\omega - E_g\right)\left(1 + \frac{\hbar\omega}{E_g}\right)\right]^{1/2}$$

i.e.,

$$\alpha = \frac{e^2}{2\pi m_0^2 c \varepsilon_0} \frac{1}{n_r \omega} \left(\frac{m_0}{\hbar^2} \frac{E_g}{E_p}\right)^{3/2} |p_{21k}|^2 \frac{1}{\sqrt{2}} \frac{\hbar\omega}{E_g} \left[\left(\hbar\omega - E_g\right)\left(1 + \frac{\hbar\omega}{E_g}\right)\right]^{1/2}$$

(Note that
$$m_0 \frac{E_g}{E_p} = 2\mu$$

where μ is the reduced effective mass calculated in the small k limit, so this expression reduces to that calculated for the parabolic approximation for small k).

From above

$$|p_{12k}|^2 = \frac{m_0}{2} \frac{E_p}{1 + \dfrac{2E_p}{E_g^2} \dfrac{\hbar^2 k^2}{m_0}}$$

We need to rewrite this in terms of the photon energy $\hbar\omega$ rather than k^2. For a photon energy $\hbar\omega$, the corresponding energy inside band 1 is

$$E = -\left(\frac{\hbar\omega - E_g}{2}\right)$$

Substituting this in our expression for k^2 above, we have

$$\frac{2E_p \hbar^2 k^2}{E_g^2 m_0} = \left[-\left(\frac{\hbar\omega - E_g}{E_g}\right) - 1\right]^2 - 1 = \left(-\frac{\hbar\omega}{E_g} + 1 - 1\right)^2 - 1 = \left(\frac{\hbar\omega}{E_g}\right)^2 - 1$$

Hence
$$|p_{21k}|^2 = \frac{m_0}{2} \frac{E_p}{1 + \left(\dfrac{\hbar\omega}{E_g}\right)^2 - 1} = \frac{m_0 E_p E_g^2}{2(\hbar\omega)^2}$$

Hence
$$\alpha = \frac{\hbar e^2 E_g^{1/2}}{4\pi m_0 c \varepsilon_0 n_r} \left(\frac{m_0}{\hbar^2} \frac{E_g}{E_p}\right)^{3/2} \frac{E_p E_g}{(\hbar\omega)^2} \frac{1}{\sqrt{2}} \left[\left(\frac{\hbar\omega}{E_g}\right)^2 - 1\right]^{1/2}$$

i.e., with
$$f(a) = \frac{1}{\sqrt{2}} \left[a^2 - 1\right]^{1/2}$$

$$\alpha = \frac{e^2 m_0^{1/2} E_g^{1/2}}{4\pi \hbar^2 c \varepsilon_0 n_r} \frac{E_g^{5/2}}{E_p^{1/2} (\hbar\omega)^2} f\left(\frac{\hbar\omega}{E_g}\right)$$

(v) All the terms with dimensions are contained in the first quotient above. We now want to use units of eV for all energies, and reciprocal centimeters for α. Hence, we have

$$\alpha_{(cm^{-1})} = \frac{10^{-2} e^{5/2} m_0^{1/2}}{4\pi\hbar^2 c\varepsilon_0 n_r} \left(\frac{E_g^3}{E_p^{1/2}(\hbar\omega)^2} \right) f\left(\frac{\hbar\omega}{E_g} \right)$$

i.e., $\quad \alpha_{(cm^{-1})} = \frac{10^{-2} \times \left(1.60\times10^{-19}\right)^{5/2} \left(9.1\times10^{-31}\right)^{1/2}}{4\times\pi\times\left(1.055\times10^{-34}\right)^2 \times 3\times10^8 \times 8.85\times10^{-12} \times 3.5} \times \left(\frac{E_g^3}{E_p^{1/2}(\hbar\omega)^2} \right)_{eV} f\left(\frac{\hbar\omega}{E_g} \right)$

i.e., $\quad\quad\quad\quad \alpha_{(cm^{-1})} = 7.54\times10^4 \left(\frac{E_g^3}{E_p^{1/2}(\hbar\omega)^2} \right)_{eV} f\left(\frac{\hbar\omega}{E_g} \right)$

The corresponding expression for the parabolic approximation with constant $|p_{12}|^2$ can be written with the same numerical prefactor, but with different functional form

$$\alpha_{par(cm^{-1})} = 7.54\times10^4 \left(\frac{E_g^2}{E_p^{1/2}\hbar\omega} \right)_{eV} \left(\frac{\hbar\omega}{E_g} - 1 \right)^{1/2}$$
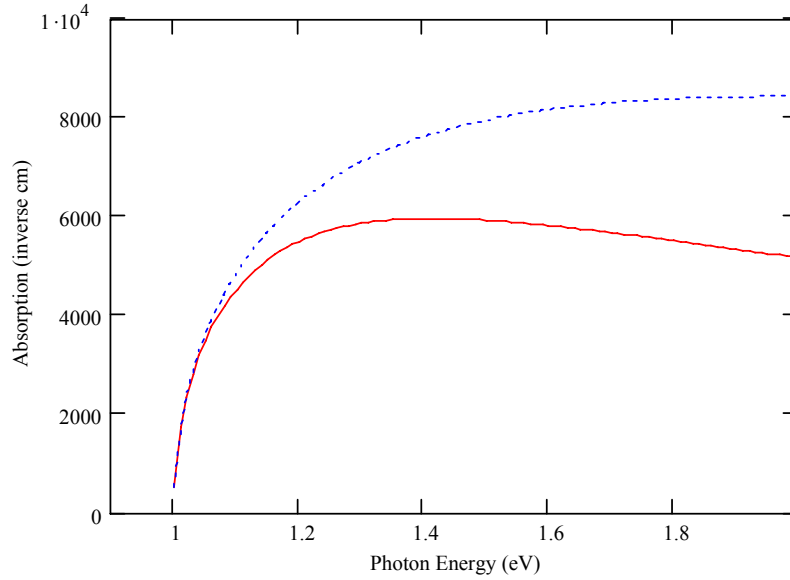
The results are shown in the figure, where the dashed line corresponds to the parabolic assumptions, and the solid line is the present model.

In the model, the density of states is somewhat larger with increasing energy than in the simple parabolic model, which tends to increase the absorption, but this is more than balanced out by the fact that the matrix element decreases with increasing transition energy because of the band mixing in the unit cell functions.

8.10.2

(i)
$$\left[\hat{H}_{e\ell},\mathbf{r}\right]=\frac{-\hbar^2}{2m_0}\nabla^2\mathbf{r}+\mathbf{r}\frac{\hbar^2}{2m_0}\nabla^2+V(\mathbf{r})\mathbf{r}-\mathbf{r}V(\mathbf{r})$$

Now for some arbitrary function $f(\mathbf{r})$

$$\nabla^2\left(\mathbf{r}\,f(\mathbf{r})\right)=\hat{\mathbf{x}}\frac{\partial^2}{\partial x^2}\left(x\,f(\mathbf{r})\right)+\hat{\mathbf{y}}\frac{\partial^2}{\partial y^2}\left(y\,f(\mathbf{r})\right)+\hat{\mathbf{z}}\frac{\partial^2}{\partial z^2}\left(z\,f(\mathbf{r})\right)$$

$$\frac{\partial^2}{\partial x^2}\left(x\,f(\mathbf{r})\right)=\frac{\partial}{\partial x}\left[f(\mathbf{r})+x\frac{\partial f(\mathbf{r})}{\partial x}\right]=2\frac{\partial f(\mathbf{r})}{\partial x}+x\frac{\partial^2 f(\mathbf{r})}{\partial x^2}$$

Hence

$$\nabla^2\left(\mathbf{r}f(\mathbf{r})\right)-\mathbf{r}\nabla^2 f(\mathbf{r})=2\nabla f(\mathbf{r})$$

Hence

$$\left[\hat{H}_{e\ell},\mathbf{r}\right]=\frac{-\hbar^2}{2m_0}2\nabla=\frac{-\hbar^2\nabla}{m_0}$$

Given that
$$\hat{\mathbf{p}}=-i\hbar\nabla$$

then
$$\frac{-i\hbar}{m_0}\hat{\mathbf{p}}=\frac{-\hbar^2}{2m_0}\nabla$$

Hence

$$\left[\hat{H}_{e\ell},\mathbf{r}\right]=\frac{-i\hbar}{m_0}\hat{\mathbf{p}}\quad Q.E.D.$$

(ii) Given that

$$\left[\hat{H}_{e\ell},\mathbf{r}\right]=\frac{-i\hbar}{m_0}\hat{\mathbf{p}}$$

with
$$\hat{H}_{e\ell}=\frac{-\hbar^2}{2m_0}\nabla^2+V(\mathbf{r})$$

Then, when $|\psi_1\rangle$ and $|\psi_2\rangle$ are eigenstates of $\hat{H}_{e\ell}$, we have

$$\langle\psi_2|\hat{\mathbf{p}}|\psi_1\rangle=\frac{im}{\hbar}\langle\psi_2|\hat{H}_{e\ell}\mathbf{r}-\mathbf{r}\hat{H}_{e\ell}|\psi_1\rangle=\frac{im}{\hbar}\langle\psi_2|E_2\mathbf{r}-\mathbf{r}E_1|\psi_1\rangle$$

$$=\frac{im}{\hbar}(E_2-E_1)\langle\psi_2|\underline{r}|\psi_1\rangle$$

i.e.,
$$\hat{\mathbf{p}}_{21}=\frac{im_0(E_2-E_1)}{\hbar}\mathbf{r}_{21}$$

(iii) Fermi's Golden Rule states that, for transitions between two states 1 and 2, the transition rate is

$$w_{12} = \frac{2\pi}{\hbar} \left| \left\langle \psi_2 \left| \hat{H}_{po} \right| \psi_1 \right\rangle \right|^2 \delta\left(E_2 - E_1 - \hbar\omega\right)$$

where the perturbing Hamiltonian $\hat{H}_p$ is of the form

$$\hat{H}_p = \hat{H}_{po} \cos \omega t$$

For the perturbing Hamiltonian

$$\hat{H}_{pA} = -\frac{e}{m} \mathbf{A}_0 \cdot \hat{\mathbf{p}} \cos \omega t$$

we therefore have

$$w_{12} = \frac{2\pi}{\hbar} \frac{e^2}{m^2} A_0^2 \left| \hat{\mathbf{e}} \cdot \mathbf{p}_{21} \right|^2 \delta\left(E_2 - E_1 - \hbar\omega\right)$$

where $\hat{\mathbf{e}}$ is the vector direction of the magnetic vector potential. For the perturbing Hamiltonian

$$\hat{H}_{pE} = -e\mathbf{E}_0 \cdot \mathbf{r} \cos \omega t$$

we similarly have

$$w_{12} = \frac{2\pi}{\hbar} e^2 E_0^2 \left| \hat{\mathbf{e}} \cdot \mathbf{r}_{21} \right|^2 \delta\left(E_2 - E_1 - \hbar\omega\right)$$

(We know we have the same polarization direction $\hat{\mathbf{e}}$ for $\mathbf{E}$ and $\mathbf{A}$ because $\mathbf{E} = -\partial \mathbf{A}/\partial t$). Now, we have

$$\mathbf{p}_{21} = \frac{im_0}{\hbar}\left(E_2 - E_1\right)\mathbf{r}_{21}$$

so we have

$$w_{12} = \frac{2\pi}{\hbar} \frac{e^2 \hbar^2 E_0^2}{m_0^2 (E_2 - E_1)^2} \left| \hat{\mathbf{e}} \cdot \mathbf{p}_{21} \right|^2 \delta\left(E_2 - E_1 - \hbar\omega\right)$$

But we are given that $\mathbf{E} = -\partial \mathbf{A}/\partial t$ and so, for the amplitude of oscillatory $\mathbf{A}$ field corresponding to $\mathbf{E}$ field of amplitude E_0 is A_0/ω, and hence

$$w_{12} = \frac{2\pi}{\hbar} \frac{e^2}{m_0^2} \frac{\hbar^2 \omega^2 A_0^2}{(E_2 - E_1)^2} \left| \hat{\mathbf{e}} \cdot \mathbf{p}_{21} \right|^2 \delta\left(E_2 - E_1 - \hbar\omega\right)$$

But the delta function ensures the only contribution occurs for $E_2 - E_1 = \hbar\omega$ and so we have also for the electric field perturbing Hamiltonian $\hat{H}_{pE}$ an identical transition rate

$$w_{12} = \frac{2\pi}{\hbar} \frac{e^2}{m_0^2} A_0^2 \left| \hat{\mathbf{e}} \cdot \mathbf{p}_{21} \right|^2 \delta\left(E_2 - E_1 - \hbar\omega\right)$$

Hence, for these conditions, the two perturbing Hamiltonians give identical transition rates.

8.10.3

(i) Consider the matrix element

$$H_{p0nm} = \left\langle \psi_n \left| \hat{H}_{p0} \right| \psi_m \right\rangle$$

We are told that the initial state $\left| \psi_m \right\rangle$ is in the valence band, band 1, so we write it as

$$\psi_m(\mathbf{r}) = \frac{1}{\sqrt{N}} u_{1\mathbf{k}_m}(\mathbf{r}) e^{i\mathbf{k}_m \cdot \mathbf{r}}$$

where $\mathbf{k}_m$ is the wavevector of this state in band 1. The intermediate state for this problem, $\left| \psi_n \right\rangle$, is in band 2 so we write it similarly as

$$\psi_n(\mathbf{r}) = \frac{1}{\sqrt{N}} u_{2\underline{k}_n}(\mathbf{r}) e^{i\mathbf{k}_n \cdot \mathbf{r}}$$

Following the argument in the chapter, we deduce

$$\left\langle \psi_n \left| \hat{H}_{p0} \right| \psi_m \right\rangle = -\frac{eA_0}{2m_0} p_{21\mathbf{k}_m}$$

with the condition

$$\mathbf{k}_m - \mathbf{k}_n + \mathbf{k}_{op} = 0$$

and, with our notation as used in preceding problems

$$u_{2k}(\mathbf{r}) = a_{21k} u_{10}(\mathbf{r}) + a_{22k} u_{20}(\mathbf{r})$$
$$u_{1k}(\mathbf{r}) = a_{11k} u_{10}(\mathbf{r}) + a_{12k} u_{20}(\mathbf{r})$$

we have

$$p_{21\underline{k}_m} = \int u_{2\mathbf{k}_m}^*(\mathbf{r}) p u_{1\mathbf{k}_m}(\mathbf{r}) d^3\mathbf{r}$$

where we neglect $\mathbf{k}_{op}$ as far as calculating this matrix element is concerned (i.e., we presume $\mathbf{k}_{op}$ is so small that $u_{2(\mathbf{k}_n - \mathbf{k}_{op})}(\mathbf{r}) \simeq u_{2\mathbf{k}_n}(\mathbf{r})$).

Hence, the sum over n reduces to only one term, which corresponds to $\mathbf{k}_n \simeq \mathbf{k}_m$.

Similarly, we examine the matrix element

$$H_{p0jn} = \left\langle \psi_j \left| \hat{H}_{p0} \right| \psi_n \right\rangle$$

which becomes

$$\left\langle \psi_j \left| \hat{H}_{p0} \right| \psi_n \right\rangle = -\frac{eA_0}{2m_0} p_{22\mathbf{k}_m}$$

with the condition

$$\mathbf{k}_n - \mathbf{k}_j + \mathbf{k}_{op} = 0$$

i.e.,
$$\mathbf{k}_m + \mathbf{k}_{op} - \mathbf{k}_j + \mathbf{k}_{op} = 0$$

i.e.,
$$\mathbf{k}_j = \mathbf{k}_m + 2\mathbf{k}_{op} \simeq \mathbf{k}_m$$

so these two photon transitions are also "vertical."

[Note here the matrix element is

$$p_{22\mathbf{k}_m} = \int u_{2\mathbf{k}_m}^*(\mathbf{r})\, p u_{2\mathbf{k}_m}(\mathbf{r})\, d^3\mathbf{r}$$

Because of the band mixing in band 2 at finite $\mathbf{k}$, this matrix element is not zero, at least away from $\mathbf{k}_m = 0$.]

We can proceed similarly for the matrix element

$$H_{p0mq} = \left\langle \psi_m \left| \hat{H}_{p0} \right| \psi_q \right\rangle$$

which will become

$$\left\langle \psi_m \left| \hat{H}_{p0} \right| \psi_q \right\rangle = -\frac{eA_0}{2m_0} p_{21\mathbf{k}_m}^* \ (\text{or}\ p_{12\mathbf{k}_m})$$

with the condition

$$\mathbf{k}_q - \mathbf{k}_m + \mathbf{k}_{0p} = 0$$

i.e.,
$$\mathbf{k}_q \simeq \mathbf{k}_m$$

so we also only have one surviving term in the sum over q. Similarly we also have

$$H_{p0qj} = \left\langle \psi_q \left| \hat{H}_{p0} \right| \psi_j \right\rangle = -\frac{eA_0}{2m_0} p_{22\mathbf{k}_m}^* \ (\text{or}\ p_{22\mathbf{k}_m})$$

with the condition

$$\mathbf{k}_j - \mathbf{k}_q + \mathbf{k}_{0p} = 0$$

i.e.,
$$\mathbf{k}_j \simeq \mathbf{k}_m$$

[Incidentally, $p_{22\mathbf{k}_m}$ is real by Hermiticity of p.]

(ii) With the above restrictions imposed by the matrix elements on the terms surviving in the sums, we have

$$\left| a_j^{(2)}(t_0) \right|^2 = \frac{t_0}{\hbar^4} \frac{e^4 A_0^4}{(2m_0)^4} \frac{\left| p_{22\mathbf{k}_m} \right|^2 \left| p_{21\mathbf{k}_m} \right|^2}{\left(\omega_{\mathbf{k}_m} - \omega \right)^2} t_0 \left[\frac{\sin\left(\omega_{\mathbf{k}_m} - 2\omega \right) t_0 / 2}{\left(\omega_{\mathbf{k}_m} - 2\omega \right) t_0 / 2} \right]^2$$

The optical intensity is

$$I = \frac{n_r c \varepsilon_0 \omega^2 A_0^2}{2}$$

i.e.,
$$A_0^2 = \frac{2I}{n_r c \varepsilon_0 \omega^2}$$

Also, because we have deduced the transitions are vertical,

$$\hbar\omega_{\mathbf{k}_m} = E_j(\mathbf{k}_m)$$

Hence, we have

$$w_{\underline{k}_m} = \frac{\left|a_j^{(2)}(t_0)\right|^2}{t_0} = \frac{e^4\hbar^2}{4m_0^4 c^2 \varepsilon_0^2} \frac{I^2}{n_r^2} \frac{1}{(\hbar\omega)^4} \frac{\left|p_{22\mathbf{k}_m}\right|^2 \left|p_{21\mathbf{k}_m}\right|^2}{\left(E_j(\mathbf{k}_m)-\hbar\omega\right)^2} t_0 \left\{ \frac{\sin\left[\left(E_j(\mathbf{k}_m)-2\hbar\omega\right)t_0/2\hbar\right]}{\left(E_j(\mathbf{k}_m)-2\hbar\omega\right)t_0/2\hbar} \right\}^2$$

(iii) Now we write

$$p_{22\mathbf{k}_m} = \int\limits_{\substack{unit\\cell}} u^*_{2\mathbf{k}_m}(\mathbf{r}) p u_{2\mathbf{k}_m}(\mathbf{r}) d^3\mathbf{r} = a^*_{21\mathbf{k}_m} a_{22\mathbf{k}_m} p_{12} + a^*_{22\mathbf{k}_m} a_{21\mathbf{k}_m} p_{21}$$

remembering that p_{11} and p_{22} are zero, i.e., noting that $d_\pm$ is real

$$p_{22k} = \frac{1}{bd_+^2}\left(1+\sqrt{1+|b|^2}\right)p_{12} + \frac{1}{b^* d_+^2}\left(1+\sqrt{1+|b|^2}\right)p_{21}$$

where we have now dropped the notation $\mathbf{k}_m$ and replaced it with k, since everything in this expression depends only on scalar quantities. Noting that, from our preceding problem,

$$\frac{p_{12}}{b} = \frac{p_{21}}{b^*} = \frac{|p_{21}|}{|b|}$$

we have

$$p_{22k} = \frac{2|p_{21}|}{|b|} \frac{\left(1+\sqrt{1+|b|^2}\right)}{d_+^2}$$

Now

$$d_+^2 = 1 + \frac{1}{|b|^2}\left(1+\sqrt{1+|b|^2}\right)^2$$

so

$$p_{22k} = 2\frac{|p_{21}|}{|b|} \frac{1+\sqrt{1+|b|^2}}{1+\frac{1}{|b|^2}\left(1+\sqrt{1+|b|^2}\right)^2}$$

and hence

$$|p_{22k}|^2 = \frac{4|p_{21}|^2}{|b|^2} \frac{\left(1+\sqrt{1+|b|^2}\right)^2}{\left[1+\frac{1}{|b|^2}\left(1+\sqrt{1+|b|^2}\right)^2\right]^2}$$

We note that $|b|^2 \propto k^2$. Now we must rewrite the function of $|b|^2$ on the right hand side to clarify the lowest order behavior.

First note that

$$1 + \frac{1}{|b|^2}\left(1 + \sqrt{1+|b|^2}\right)^2 = 1 + \frac{1}{|b|^2} + \frac{1+|b|^2}{|b|^2} + \frac{2\sqrt{1+|b|^2}}{|b|^2} = \frac{2}{|b|^2}\left[1 + |b|^2 + \sqrt{1+|b|^2}\right]$$

Hence

$$|p_{22k}|^2 \simeq |p_{21}|^2 |b|^2 \frac{\left(1 + \sqrt{1+|b|^2}\right)^2}{\left(1 + |b|^2 + \sqrt{1+|b|^2}\right)^2}$$

The two squared terms are each of the form "1+ higher order terms in powers of $|b|$", so to lowest order, we therefore have

$$|p_{22k}|^2 \simeq |p_{21}|^2 |b|^2 = \frac{4\hbar^2 k^2}{E_g^2 m_0^2}|p_{21}|^4$$

(iv) The total transition rate is

$$W_{TOT} = \frac{1}{t_0}\sum_{\mathbf{k}_m}\left|a_j^{(2)}(t_0)\right|^2$$

In working this summation out, we will want to change the sum over $\mathbf{k}_m$ to an integral over the transition energy. We already know the density of transitions per unit transition energy. That is simply $g_J(E)$, the joint density of states already worked out for the one photon case, where here $E_J = \hbar\omega_{\mathbf{k}_m}$ is the transition energy (*not* the photon energy in this case). So, we have

$$W_{TOT} = \frac{1}{t_0}\int\left|a_j^{(2)}(t_0)\right|^2 g_J(E_J)dE_J$$

Now, the form of $\left|a^{(2)}(t_0)\right|^2$ is

$$\left|a_j^{(2)}(t_0)\right|^2 = t_0 s(E_J)t_0\left[\frac{\sin(E_J - 2\hbar\omega)t_0/2\hbar}{(E_J - 2\hbar\omega)t_0/2\hbar}\right]^2$$

where

$$s(E_j) = \frac{e^4\hbar^2}{4m_0^4 c^2 \varepsilon_0^2}\frac{I^2}{n_r^2}\frac{1}{(\hbar\omega)^4}\frac{|p_{22\mathbf{k}_m}|^2 |p_{21\mathbf{k}_m}|^2}{(E_J - \hbar\omega)^2}\Bigg|_j$$

Hence

$$W_{TOT} = \int s(E_J)g_J(E_J)t_0\left[\frac{\sin(E_j - 2\hbar\omega)t_0/2\hbar}{(E_j - 2\hbar\omega)t_0/2\hbar}\right]^2 dE_J$$

As usual, t_0 can be as large as we wish,[2] making $\left[\sin(E_J - 2\hbar\omega)t_0/2\hbar\right]/\left[(E_J - 2\hbar\omega)t_0/2\hbar\right]$ as sharply peaked as we wish around the energy $E_J = 2\hbar\omega$, and so we can take the $s(E_J)g_J(E_J)$ out of the integral as $s(2\hbar\omega)g_J(2\hbar\omega)$. Hence

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[2] We might consider the finite length of the optical pulse we are going to use here, and use that for t_0. That would be strictly more correct here, though it will not make much difference to the final calculated result for the numbers here.

$$W_{TOT} = s(2\hbar\omega)g_J(2\hbar\omega)2\hbar\int\left(\frac{\sin x}{x}\right)^2 dx = 2\pi\hbar\, s(2\hbar\omega)g_J(2\hbar\omega)$$

where we have used $\int\left[\frac{\sin x}{x}\right]^2 dx = \pi$. I.e.,

$$W_{TOT} = 2\pi\hbar\frac{e^4\hbar^2}{4m_0^4 c^2\varepsilon_0^2}\frac{I^2}{n_r^2}\frac{1}{(\hbar\omega)^4}\frac{|p_{22k}|^2 |p_{21k}|^2}{(\hbar\omega)^2}g_j(2\hbar\omega)$$

Because we are interested in an answer to lowest order in k (actually k^2), we can take a parabolic band approximation to the joint density of states, $g_J(2\hbar\omega)$, i.e., we can use

$$g_J(2\hbar\omega) = \frac{1}{2\pi^2}\left(\frac{2u_{eff}}{\hbar^2}\right)^{3/2}(2\hbar\omega - E_g)^{1/2}$$

The effective masses of the individual bands in this model are both (with opposite signs) $m_{eff} = m_0 E_g / E_p$, so $\mu_{eff} = m_{eff}/2 = m_0 E_g/2E_p$, so

$$g_J(2\hbar\omega) = \frac{1}{2\pi^2}\left(\frac{m_0 E_g}{\hbar^2 E_p}\right)^{3/2}(2\hbar\omega - E_g)^{1/2}$$

We also know from our preceding problem that $|p_{21k}|^2 = \dfrac{|p_{21}|^2}{1+|b|^2}$ which, to lowest order in k,

becomes $|p_{21k}|^2 \simeq |p_{21}|^2$.

We also know in the parabolic approximation that $\dfrac{\hbar^2 k^2}{2\mu_{eff}} = E_j - E_g$, so here

$$k^2 = \frac{2u_{eff}}{\hbar^2}(2\hbar\omega - E_g) = \frac{m_0 E_g}{\hbar^2 E_p}(2\hbar\omega - E_g)$$

Putting all this together gives

$$W_{TOT} = 2\pi\hbar\frac{e^4\hbar^2}{4m_0^4 c^2\varepsilon_0^2}\frac{I^2}{n_r^2}\frac{1}{(\hbar\omega)^6}\frac{4\hbar^2}{E_g^2 m_0^2}\frac{m_0 E_g}{\hbar^2 E_p}(2\hbar\omega - E_g)|p_{21}|^6\frac{1}{2\pi^2}\left(\frac{m_0 E_g}{\hbar^2 E_p}\right)^{3/2}(2\hbar\omega - E_g)^{1/2}$$

$$= \frac{1}{\pi}\frac{e^4}{m_0^{7/2}c^2\varepsilon_0^2}\frac{I^2}{n_r^2}\frac{E_g^{1/2}}{E_p^{5/2}}\frac{1}{(\hbar\omega)^6}\frac{m_0^3 E_p^3}{8}(2\hbar\omega - E_g)^{3/2}$$

$$= \frac{1}{8\pi}\frac{e^{1/2}}{m_0^{1/2}c^2\varepsilon_0^2}\frac{I^2}{n_r^2}\left(\frac{E_g}{e}\right)^2\left(\frac{E_p}{e}\right)^{1/2}\left(\frac{e}{\hbar\omega}\right)^6\left(\frac{2\hbar\omega - E_g}{E_g}\right)^{3/2}$$

$$\simeq 2.4\times 10^9\frac{I^2}{n_r^2}\left(\frac{E_g}{e}\right)^2\left(\frac{E_p}{e}\right)^{1/2}\left(\frac{e}{\hbar\omega}\right)^6\left(\frac{2\hbar\omega - E_g}{E_g}\right)^{3/2} m^{-3}s^{-1}$$

(We have used "E/e" for the energies so that we can work with energies in electron-volts).

(v) For our problem, the power during the pulse is calculated as follows. The average power is 1 mW, with 10^8 pulses per second, so the pulse energy is

$$E_{pulse} = \frac{10^{-3}}{10^8} = 10^{-11} = 10 \; pJ$$

This pulse is 100 fs long, so the power during the pulse is

$$P_{pulse} = \frac{10^{-11}}{10^{-13}} = 100 \; W$$

This is focused in an area of $10^{-5} \times 10^{-5} m^2 = 10^{-10} m^2$, so the intensity during the pulse is

$$I = 10^2 \times 10^{10} = 10^{12} W/m^2$$

With the given parameter values, the total number of transitions per second in the volume V during the pulse is

$$W_{TOT} \times V = 2.4 \times 10^9 \times \frac{10^{24}}{3.5^2} \times \frac{1 \times \sqrt{20} \times 1 \times (0.2)^{3/2} \times 10^{-16}}{(0.6)^6} = 1.7 \times 10^{17} \; s^{-1}$$

(The total number of photons hitting the 10 × 10 μm area during the pulse, per second

$$\frac{I}{\hbar \omega} \times 10^{-10} = \frac{10^{12} \times 10^{-10}}{0.6 \times 1.602 \times 10^{-19}} \simeq 10^{21} \; photons/second$$

so the number of photon pairs absorbed is negligible compared to the incident number of photons, justifying our implicit assumption that the intensity is uniform throughout the volume.) This transition rate corresponds to a current of

$$I_C = W_{TOT} \times V \times e = 0.027 \; A$$

The "duty cycle" of this current is 100 fs/10 ns = $10^{-13}/10^{-8}=10^{-5}$ and so the time averaged current is

$$I_{Cav} \simeq 0.3 \; \mu A$$

Hence about 3×10^{-4} of the incident average power is absorbed here in this two-photon process. This is quite easy to see under laboratory conditions. If the light had been focused to an area $\sim 1 \times 1 \, \mu m^2$, multiplying the intensity by 10^2, a large fraction of the incident power would be absorbed, so large we would have to account properly for the attenuation of the beam within the sample.

Chapter 9 problem solutions

9.1.1

We have

$$\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y$$

$$\hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z$$

$$\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$$

Then we have

$$\left[\hat{L}_x, \hat{L}_y\right] = \hat{L}_x\hat{L}_y - \hat{L}_y\hat{L}_x$$
$$= \left(\hat{y}\hat{p}_z - \hat{z}\hat{p}_y\right)\left(\hat{z}\hat{p}_x - \hat{x}\hat{p}_z\right) - \left(\hat{z}\hat{p}_x - \hat{x}\hat{p}_z\right)\left(\hat{y}\hat{p}_z - \hat{z}\hat{p}_y\right)$$
$$= \hat{y}\hat{p}_z\hat{z}\hat{p}_x + \hat{z}\hat{p}_y\hat{x}\hat{p}_z - \hat{y}\hat{p}_z\hat{x}\hat{p}_z - \hat{z}\hat{p}_y\hat{z}\hat{p}_x$$
$$\quad - \hat{z}\hat{p}_x\hat{y}\hat{p}_z - \hat{x}\hat{p}_z\hat{z}\hat{p}_y + \hat{z}\hat{p}_x\hat{z}\hat{p}_y + \hat{x}\hat{p}_z\hat{y}\hat{p}_z$$

Now, momentum and position operators corresponding to different directions all commute with one another, so we can rewrite the above to obtain

$$\left[\hat{L}_x, \hat{L}_y\right] = \hat{y}\hat{p}_x\hat{p}_z\hat{z} + \hat{x}\hat{p}_y\hat{z}\hat{p}_z - \hat{y}\hat{x}\hat{p}_z^2 - \hat{p}_y\hat{p}_x\hat{z}^2 - \hat{y}\hat{p}_x\hat{z}\hat{p}_z - \hat{x}\hat{p}_y\hat{p}_z\hat{z} + \hat{p}_y\hat{p}_x\hat{z}^2 + \hat{y}\hat{x}\hat{p}_z^2$$
$$= \hat{y}\hat{p}_x\left[\hat{p}_z\hat{z}\right] - \hat{x}\hat{p}_y\left[\hat{p}_z\hat{z}\right]$$
$$= -\left[\hat{p}_z\hat{z}\right]L_z = i\hbar L_z$$

We can proceed similarly to prove the other two commutation relations

$$\left[\hat{L}_y, \hat{L}_z\right] = i\hbar\hat{L}_x$$

$$\left[\hat{L}_z, \hat{L}_x\right] = i\hbar\hat{L}_y$$

Now

$$\hat{\mathbf{L}} \times \hat{\mathbf{L}} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ \hat{L}_x & \hat{L}_y & \hat{L}_z \\ \hat{L}_x & \hat{L}_y & \hat{L}_z \end{vmatrix} = \mathbf{i}\left(\hat{L}_y\hat{L}_z - \hat{L}_z\hat{L}_y\right) + \mathbf{j}\left(\hat{L}_z\hat{L}_x - \hat{L}_x\hat{L}_y\right) + \mathbf{k}\left(\hat{L}_x\hat{L}_y - \hat{L}_y\hat{L}_x\right)$$
$$= \mathbf{i}\left[\hat{L}_y\hat{L}_z\right] + \mathbf{j}\left[\hat{L}_z\hat{L}_x\right] + \mathbf{k}\left[\hat{L}_x\hat{L}_y\right] = i\hbar\left(\mathbf{i}\hat{L}_x + \mathbf{j}\hat{L}_y + \mathbf{k}\hat{L}_z\right) = i\hbar\hat{\mathbf{L}}$$

as required (where $\mathbf{i}$, $\mathbf{j}$, and $\mathbf{k}$ are unit vectors in the x, y, and z directions, respectively).

9.1.2

The definition in Cartesian coordinates is $L_x = -i\hbar\left(y\dfrac{\partial}{\partial z} - z\dfrac{\partial}{\partial y}\right)$

Substituting for the partial derivatives, we have

$$L_x = -i\hbar\left[r\sin\theta\sin\phi\right]\left(\frac{\partial r}{\partial z}\frac{\partial}{\partial r} + \frac{\partial\theta}{\partial z}\frac{\partial}{\partial\theta} + \frac{\partial\phi}{\partial z}\frac{\partial}{\partial\phi}\right) - r\cos\theta\left(\frac{\partial r}{\partial y}\frac{\partial}{\partial r} + \frac{\partial\theta}{\partial y}\frac{\partial}{\partial\theta} + \frac{\partial\phi}{\partial y}\frac{\partial}{\partial\phi}\right)$$

where $\qquad r = \sqrt{x^2 + y^2 + z^2}\,, \qquad \theta = \sin^{-1}\left(\dfrac{\sqrt{x^2+y^2}}{\sqrt{x^2+y^2+z^2}}\right), \qquad \phi = \tan^{-1}\left(\dfrac{y}{x}\right)$

so
$$\frac{\partial r}{\partial z} = \frac{z}{r} = \cos\theta$$

$$\frac{\partial\theta}{\partial z} = \frac{-1}{\sqrt{1-\sin^2\theta}}\frac{\sqrt{x^2+y^2}\,z}{\left(x^2+y^2+z^2\right)^{3/2}} = \frac{1}{\cos\theta}\frac{\sin\theta\cos\theta}{r} = \frac{\sin\theta}{r}$$

$$\frac{\partial\phi}{\partial z} = \frac{1}{1+\dfrac{y^2}{x^2}}\times 0 = 0$$

and
$$\frac{\partial r}{\partial y} = \frac{y}{r} = \sin\theta\sin\phi$$

$$\frac{\partial\theta}{\partial y} = \frac{1}{\sqrt{1-\sin^2\theta}}\frac{\sqrt{x^2+y^2+z^2}\,\dfrac{y}{\sqrt{x^2+y^2}} - \sqrt{x^2+y^2}\,\dfrac{y}{\sqrt{x^2+y^2+z^2}}}{x^2+y^2+z^2}$$

$$= \frac{1}{\cos\theta}\frac{yz^2}{\sqrt{x^2+y^2}\left(x^2+y^2+z^2\right)^{3/2}} = \frac{\sin\phi\cos\theta}{r}$$

$$\frac{\partial\phi}{\partial y} = \frac{1}{1+\dfrac{y^2}{x^2}}\cdot\frac{1}{x} = \frac{1}{1+\tan^2\phi}\cdot\frac{1}{r\sin\theta\cos\phi} = \frac{\cos^2\phi}{\cos^2+\sin^2\phi}\cdot\frac{1}{r\sin\theta\cos\phi} = \frac{\cos\phi}{r\sin\theta}$$

Hence

$$L_x = -i\hbar\left[r\sin\theta\sin\phi\left(\cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial\theta}\right)\right]$$

$$-r\cos\theta\left[\sin\theta\sin\phi\frac{\partial}{\partial r} + \frac{\sin\phi\cos\theta}{r}\frac{\partial}{\partial\theta} + \frac{\cos\phi}{r\sin\theta}\frac{\partial}{\partial\phi}\right]$$

$$= -i\hbar\left[-\sin\phi\left(\sin^2\theta + \cos^2\theta\right)\frac{\partial}{\partial\theta} - \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right] = i\hbar\left[\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right]$$

9.2.1

$$\left[\nabla^2, \hat{L}_z\right] = -i\hbar^3\left[\nabla^2\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) - \left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\nabla^2\right]$$

$$= -i\hbar^3\left[\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) - \left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\right]$$

$$= -i\hbar^3\left[\frac{\partial}{\partial x}\left(\frac{\partial}{\partial y} + x\frac{\partial^2}{\partial x\partial y} - y\frac{\partial^2}{\partial x^2}\right) + \frac{\partial}{\partial y}\left(x\frac{\partial^2}{\partial y^2} - \frac{\partial}{\partial x} - y\frac{\partial^2}{\partial ydx}\right) + \frac{\partial^2}{\partial z^2}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\right.$$

$$\left. - x\frac{\partial}{\partial y}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + y\frac{\partial}{\partial x}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\right]$$

$$= -i\hbar^3\left[\frac{\partial^2}{\partial x\partial y} + \frac{\partial^2}{\partial x\partial y} + x\frac{\partial^3}{\partial x^2\partial y} - y\frac{\partial^3}{\partial x^3} + x\frac{\partial^3}{\partial y^3} - \frac{\partial^2}{\partial x\partial y} - \frac{\partial^2}{\partial y\partial x} - y\frac{\partial^3}{\partial y^2\partial x}\right.$$

$$\left. + x\frac{\partial^3}{\partial z^2\partial y} - y\frac{\partial^3}{\partial z^2\partial x} - x\frac{\partial^3}{\partial y\partial x^2} - x\frac{\partial^3}{\partial y^3} - x\frac{\partial^3}{\partial y\partial z^2} + y\frac{\partial^3}{\partial x^3} + y\frac{\partial^3}{\partial x\partial y^2} + y\frac{\partial^3}{\partial x\partial z^2}\right]$$

$$= 0$$

9.2.2

The associated Legendre functions, with $\cos\theta$ as the argument, become

$P_0^0(\cos\theta) = 1$ *no zeros*

$P_1^0(\cos\theta) = \cos\theta$ *zero at* $\theta = 90°$

$P_1^1(\cos\theta) = (1 - \cos^2\theta)^{1/2}\ (\equiv \sin\theta)$ *zeros at* $\theta = 0°, 180°$

$P_1^{-1}(\cos\theta) = -\dfrac{1}{2}(1 - \cos^2\theta)^{1/2}\left(\equiv -\dfrac{1}{2}\sin\theta\right)$ *zeros at* $\theta = 0°, 180°$

$P_2^0(\cos\theta) = \dfrac{1}{2}(3\cos^2\theta - 1)$

Now $(1/2)(3\cos^2\theta - 1) = 0 \Rightarrow \cos^2\theta = 1/3$, i.e., $\cos\theta = 1/\sqrt{3}$, so for the zeros of this associated Legendre function, $\theta \simeq 54.74°$ from the "north pole" and also $\theta \simeq 180° - 54.74° = 125.26°$ (or $54.74°$ up from the "south pole").

$P_2^1(\cos\theta) = 3\cos\theta(1 - \cos^2\theta)^{1/2}\left(\equiv 3\cos\theta\sin\theta \equiv \dfrac{3}{2}\sin 2\theta\right)$ *zeros at* $0°, 90°, 180°$

$P_2^{-1}(\cos\theta) = -\dfrac{1}{2}\cos\theta(1 - \cos^2\theta)^{1/2}$

$\qquad\left(\equiv -\dfrac{1}{2}\cos\theta\sin\theta = -\dfrac{1}{4}\sin 2\theta\right)$ *zeros at* $0°, 90°, 180°$

$P_2^2(\cos\theta) = 3(1 - \cos^2\theta)(\equiv 3\sin^2\theta)$ *zeros at* $0°, 180°$

$P_2^{-2}(\cos\theta) = \dfrac{1}{8}(1 - \cos^2\theta)\left(\equiv \dfrac{1}{8}\sin^2\theta\right)$ *zeros at* $0°, 180°$

Chapter 10 problem solutions

10.5.1

We are given ∇^2 in cylindrical polars, which is

$$\nabla^2 = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial z^2}$$

We consider an electron in a cylindrical shell, with inner radius r_o and thickness L_r. We therefore have a Schrödinger equation in which the potential is a function of r only

$$-\frac{\hbar^2}{2m_0}\nabla^2\psi + V(r)\psi = E\psi$$

i.e.,

$$\nabla^2\psi - \frac{2m_0}{\hbar^2}V(r)\psi = -\frac{2m_0 E}{\hbar^2}\psi$$

We propose the solution

$$\psi = R(r)\Phi(\phi)Z(z)$$

We multiply both sides by r^2, rearranging slightly

$$\Phi(\phi)Z(z)\left[r\frac{\partial}{\partial r}r\frac{\partial}{\partial r} - \frac{r^2 2m_0 V(r)}{\hbar^2}\right]R(r) + R(r)Z(z)\frac{\partial^2\Phi(\phi)}{\partial\phi^2}$$

$$+ r^2 R(r)\Phi(\phi)\frac{\partial^2 Z(z)}{\partial z^2} + \frac{2m_0 E_r^2 R(r)\Phi(\phi)Z(z)}{\hbar^2} = 0$$

We divide by ψ

$$\frac{1}{R(r)}\left[r\frac{\partial}{\partial r}r\frac{\partial}{\partial r} - \frac{r^2 2m_0 V(r)}{\hbar^2}\right]R(r) + \frac{2m_0 E_r^2}{\hbar^2} + \frac{r^2}{Z(z)}\frac{\partial^2 Z(z)}{\partial z^2} = -\frac{1}{\Phi}\frac{\partial^2\Phi(\phi)}{\partial\phi^2} = m^2$$

where m^2 is our separation constant, to be determined. Hence, we conclude that

$$\Phi(\phi) = e^{im\phi}$$

which is the solution of the ϕ part (or strictly, $\Phi(\phi) = Ae^{im\phi} + Be^{-im\phi}$, though, if we allow positive and negative m, and presume we will normalize the wavefunctions later, we can write $\psi = \exp(im\phi)$ as the (unnormalized) basis set). Continuity of the wavefunction and its derivative at $\phi = 2\pi$ requires m is an integer (positive, negative, or zero). Now we have, dividing by r^2

$$\frac{1}{R(r)}\left[\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r} - \frac{2m_0 V(r)}{\hbar^2}\right]R(r) + \frac{2mE}{\hbar^2} - \frac{m^2}{r^2} = -\frac{1}{Z(z)}\frac{\partial^2 Z(z)}{\partial z^2} = k_z^2$$

where k_z^2 is a separation constant. Hence the solution for Z is (unnormalized)

$$Z(z) = \exp(ik_z z)$$

where k_z may take any real value. Finally, the radial equation is

$$\frac{1}{R(r)}\left[\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r}-\frac{2m_0}{\hbar^2}V(r)\right]R(r)=-\frac{2mE}{\hbar^2}+\frac{m^2}{r^2}+k_z^2$$

or

$$-\frac{\hbar^2}{2m_0}\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r}R(r)+V(r)R(r)=\left[E-\frac{\hbar^2}{2m_0}\frac{m^2}{r^2}-\frac{\hbar^2}{2m_0}k_z^2\right]R(r)$$

Now, we are only interested in solving this over a very small range of r near r_o. Therefore, we can approximate r^2 in the right-hand side by r_0^2 – the error introduced in the net number will be small. Hence, we can define the quantity

$$E_r=E-\frac{\hbar^2}{2m_0}\frac{m^2}{r_0^2}-\frac{\hbar^2}{2m_0}k_z^2$$

and obtain the simple approximate equation

$$-\frac{\hbar^2}{2m_0}\frac{1}{r}\frac{\partial}{\partial r}\frac{r\partial}{\partial r}R(r)+V(r)R(r)=E_rR(r)$$

Now, with

$$R'\equiv\frac{\partial R}{\partial r}$$

we have

$$\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r}R(r)=\frac{1}{r}\frac{\partial}{\partial r}rR'=\frac{1}{r}R'+R''$$

We expect in the thin shell that the gradient R' will change by $\sim|R'|$ over the thickness of the shell as the function R goes from zero at one side of the shell to zero at the other side, i.e., we expect

$$|\overline{R''}|\sim\frac{|\overline{R'}|}{L_r}\gg\frac{|\overline{R'}|}{r_0}$$

because $r_0\gg L_r$. Hence, we can neglect the R'/r term leaving, approximately

$$-\frac{\hbar^2}{2m_0}\frac{\partial}{\partial r^2}R(r)+V(r)R(r)=E_rR(r)$$

Hence, the problem separates into

a) A 1D infinite quantum well problem for a quantum well of thickness L_r (starting at radius r_o and ending at radius r_o+L_r)

b) a propagating wave in the z direction.

c) a circular wave in the ϕ direction.

Hence, we have (neglecting normalization)

$$Z(z)=\exp(ik_zz)\ ,\ k_z\ \text{any real value}$$

$$\Phi(\phi) = \exp(im\phi) \ , \ m \ \text{any integer}$$

$$R(r) = \sin\left(\frac{n\pi(r-r_o)}{L_r}\right) \ \text{(for } r \text{ within the well), } n = 1, 2, 3, \ldots$$

with associated energies

$$E_r = \frac{\hbar^2}{2m_0}\left(\frac{n\pi}{L_r}\right)^2$$

(i) Hence multiplying the part of the wavefunction together gives the required form.

(ii) The restrictions are as above, $n = 1, 2, 3, \ldots$, m any integer, and k_z any real value.

(iii) The resulting energies adding all the parts together are

$$E_{nmk} = \frac{\hbar^2}{2m_0}\left[\left(\frac{n\pi}{L_R}\right)^2 + \left(\frac{m}{r_0}\right)^2 + k_z^2\right]$$

10.5.2

The Schrödinger equation for a particle in a spherical potential is of the form

$$-\frac{\hbar^2}{2m_0}\nabla^2\psi + V(r)\psi = E\psi$$

i.e., the potential is only a function of the radius from the center. This is true regardless of the detail of the form of the spherically-symmetric potential. This equation is therefore of the same mathematical form as the corresponding equation for the hydrogen atom and will have similar forms of solutions.

Specifically, we can write

$$\psi(\mathbf{r}) = \frac{1}{r}\chi(\mathbf{r})Y(\theta,\phi)$$

and we will have an equation

$$-\frac{\hbar}{2m_0}\frac{d^2\chi(r)}{dr^2} + \left[V(r) + \frac{\hbar^2}{2m_0}\frac{\ell(\ell+1)}{r^2}\right]\chi(r) = E\chi(r)$$

The term

$$\frac{\hbar^2}{2m_0}\frac{\ell(\ell+1)}{r^2}$$

is an effective potential energy term that increases the energy of the system as l becomes larger, so to get the lowest energy state we set $l = 0$ (its lowest allowed value, from the solution of the spherical harmonic equation), which by assumption anyway in the problem gives the lowest state. Hence, for the lowest energy state, we are looking for the lowest energy solution of the equation

$$-\frac{\hbar^2}{2m_0}\frac{d^2\chi(r)}{dr^2} + V(r)\chi(r) = E\chi(r)$$

For the "infinite" potential well, we expect a boundary condition $\chi(r_0) = 0$, and we are reminded in the problem that $\chi(0) = 0$. Hence, this problem is mathematically like a simple one-dimensional quantum well of thickness r_0 (at least for all $l = 0$ states), and so we conclude that the lowest energy is

$$E_1 = \frac{\hbar^2}{2m_0}\left(\frac{\pi}{r_0}\right)^2$$

10.5.3

The equation we are trying to solve is

$$\frac{d^2H(x)}{dx^2} - \frac{2xdH(x)}{dx} + 2nH(x) = 0$$

(We do not yet know that n is an integer).

We presume $H(x)$ is a polynomial, i.e.,

$$H(x) = \sum_{q=0}^{\infty} c_q x^q$$

Substituting in the differential equation, we obtain

$$\sum_{q=0}^{\infty} \left[c_q q(q-1) x^{q-2} - 2q c_q x^q + 2n c_q x^q \right] = 0$$

i.e.,

$$\sum_{q=0}^{\infty} \left[c_q q(q-1) x^{q-2} - 2(n-q) c_q x^q \right] = 0$$

(Note that the factor q in the first two terms eliminates their contribution for $q = 0$, and the factor $q-1$ in the first term eliminates the contribution of that term for $q = 1$. Hence, we can still perform the sum from $q = 0$ and still retain only zero or positive powers of x in the result as required, even if we write the terms in this form in the sum.)

Gathering terms in powers of x^q, we obtain

$$\sum_{q=2}^{\infty} \left[c_q q(q-1) + 2(n-q+2) c_{q-2} \right] x^{q-2} = 0$$

Presuming that this equation must hold for all x, we must have the relation hold for each power of x individually

$$c_q = \frac{2(q-n-2)}{q(q-1)} c_{q-2}, \quad q \geq 2 \quad \text{or} \quad c_{q+2} = \frac{2(q-n)}{(q+2)(q+1)} c_q, \quad q \geq 0$$

Note that this is a relation between c_q and c_{q-2} (for $q \geq 2$), and leaves us free to choose c_0 and c_1 separately. We therefore have two "interlocking" power series, one in x, x^3, x^5, ... and the other in 1, x^2, x^4, ...

For large q, the even power series has the form (if it does not terminate at finite q)

$$c_q \sim \frac{2}{q} c_{q-2}$$

i.e.,

$$c_q \sim \frac{2^q}{q(q-2)(q-4)(q-6)} ... > \frac{2^q}{q!}$$

Therefore, the power series tends to a value $\gtrsim e^{2x^2}$.

For the odd power series, it tends to a value $\tilde{>}\, xe^{2x^2}$.

Possible solutions that do not explode in this manner (which is incidentally too fast even to be controlled by the function $\sim \exp(-x^2/2)$ that occurs in the full harmonic oscillator function) require either

$$c_1 = 0 \quad n = \text{even integer} \geq 0$$

or

$$c_0 = 0 \quad n = \text{odd integer} \geq 0$$

Choosing $c_0 = 1$ and $c_1 = 1$ gives

$$n = 0; \ H_0(x) = 1 \ (\text{terminating at } q = 0)$$

$$n = 1; \ H_1(x) = x \ (\text{terminating at } q = 1)$$

$$n = 2; \ H_2(x) = 1 - 2x^2 \ (\text{terminating at } q = 2)$$

$$n = 3; \ H_3(x) = x - \frac{2 \times 2}{3 \times 2} x^3 \ (\text{terminating at } q = 3) \ = x - \frac{2}{3} x^3$$

$$n = 4; \ H_4(x) = 1 - \frac{8}{2} x^2 + \frac{8}{2} \frac{4}{4 \times 3} x^4 \ (\text{terminating at } q = 4) \ = 1 - 4x^2 + \frac{4}{3} x^4$$

Rewriting these polynomials to get them in the standard form of Hermite polynomials only requires multiplying each one by constants, i.e., obtaining

$$H_0(x) = 1 \ (\text{no change})$$

$$H_1(x) = 2x \ (\text{multiplying by 2})$$

$$H_2(x) = 4x^2 - 2 \ (\text{multiplying by -2})$$

$$H_3(x) = 8x^3 - 12x \ (\text{multiplying by -12})$$

$$H_4(x) = 16x^4 - 48x^2 + 12 \ (\text{multiplying by 12})$$

10.5.4

We start from an equation already encountered for the hydrogen atom problem, valid for the radial function for any central potential problem. In this case, we are dealing directly with the electron, so we use mass m_0, and are trying also to find eigenenergies E.

$$\frac{-\hbar^2}{2m_0}\frac{d^2\chi(r)}{dr^2} + \left[V(r) + \frac{\hbar^2}{2m_0}\frac{\ell(\ell+1)}{r^2}\right]\chi(r) = E\,\chi(r)$$

$V(r) = 0$ for $r < r_0$, $= \infty$ for $r \geq r_0$.

i.e.,
$$\frac{d^2\chi(r)}{dr^2} - \frac{\ell(\ell+1)}{r^2}\chi(r) = -\frac{2m_0}{\hbar^2}E\,\chi(r) \quad \text{for } r < r_0$$

with
$$\chi(r) = 0 \text{ at } r = 0, r = r_o.$$

The equation is, therefore, of the form

$$\frac{d^2\chi}{dr^2} + \left[a^2 - \frac{b}{r^2}\right]\chi = 0$$

where
$$a^2 = \frac{2m_0}{\hbar^2}E \qquad b = \ell(\ell+1)$$

Now the equation

$$\frac{d^2y}{dx^2} + \left[a^2 + \left(\frac{1}{4} - p^2\right)\frac{1}{x^2}\right]y = 0$$

has solutions
$$y = \sqrt{x}\left[A J_p(ax) + B Y_p(ax)\right]$$

where J_p is the usual Bessel function and Y_p is the Weber function.

The Weber function goes to ∞ at $r = 0$, and can be discounted, because $\chi(r)$ must go to zero at $r = 0$, as deduced from the asymptotic behavior argument.

So, we are left only with the J_p function. Hence

$$\chi(r) \propto \sqrt{r}J_p(ar)$$

with
$$p^2 - \frac{1}{4} = \ell(\ell+1)$$

i.e.,
$$\left(p - \frac{1}{2}\right)\left(p + \frac{1}{2}\right) = \ell(\ell+1)$$

Setting $p = \ell + \dfrac{1}{2}$ gives

$$\left(\ell + \frac{1}{2} - \frac{1}{2}\right)\left(\ell + \frac{1}{2} + \frac{1}{2}\right) = \ell(\ell+1)$$

as required. So

$$p = \ell + \frac{1}{2}$$

So we are dealing with

$$\ell = 0 \qquad J_{1/2}$$
$$\ell = 1 \qquad J_{3/2}$$
$$\ell = 2 \qquad J_{5/2}$$
$$\text{etc.}$$

Hence

$$\chi(r) \propto \sqrt{r} J_{\ell+1/2}(ar)$$

or, given that, for the spherical Bessel function

$$j_\ell(x) = \sqrt{\frac{\pi}{2x}} J_{\ell+1/2}(x)$$

$$\chi(r) \propto r j_\ell(ar)$$

or

$$R(r) = \frac{\chi(r)}{r} \propto J_\ell(ar)$$

For any given ℓ, therefore, there will be eigen solutions to this problem as long as

$$j_\ell(ar_0) = 0$$

i.e.,

$$j_\ell\left(\sqrt{\frac{2m_0}{\hbar^2}Er}\right) = 0$$

i.e.,

$$\sqrt{\frac{2\mu}{\hbar^2}E}\, r_0 = s_{n\ell}$$

where $s_{n\ell}$ is the nth (non-zero) root of the ℓth spherical Bessel function, or, equivalently,

$$\frac{2\mu E_{n\ell}}{\hbar^2} = \left[\frac{s_{n\ell}}{r_0}\right]^2 \qquad \text{or} \qquad E_{n\ell} = \frac{\hbar^2}{2\mu r_0^2}s_{n\ell}^2$$

(ii) For the parameters given,

$$\frac{\hbar^2}{2\mu r_o^2 e} = 7.626 \text{ meV}$$

and so, given the zeros of the spherical Bessel functions as obtained from mathematical tables and as stated below, we obtain the following results for each of the energy eigenvalues requested.

s	n=1	n=2	n=3	E (meV)	n=1	n=2	n=3
l=0	3.14	6.28	9.42	l=0	75.27	301.06	677.39
l=1	4.49	7.73	10.90	l=1	153.97	455.12	906.73
l=2	5.76	9.91	12.32	l=2	253.32	748.18	1158.04

10.5.5

Consider a quantum wire of circular cross-section. Then we will write the Schrödinger wave equation in cylindrical polar coordinates

$$\left[\frac{-\hbar^2}{2m_{eff}}\nabla^2_{r,\theta}\frac{-\hbar^2}{2m_{eff}}\frac{\partial^2}{\partial z^2}+V(r)\right]\Psi(r,\theta,z)=E\Psi(r,\theta,z)$$

Separating with presumed form

$$\Psi(r,\theta,z)=C(r,\theta)\psi(z)$$

gives, with the (arbitrary) choice $-E_z$ as the separation constant

$$\frac{-\hbar^2}{2m_{eff}}\frac{1}{C(r,\theta)}D^2_{r,\theta}C(r,\theta)+V(r)-E=\frac{\hbar^2}{2m_{eff}}\frac{1}{\psi(z)}\frac{\partial^2\psi(z)}{\partial z}=-E_z$$

As a result, we deduce the simple z solutions

$$\psi(z)\propto e^{ikz}$$

$$E_z=\frac{\hbar^2k^2}{2m_{eff}}$$

and we could presume that we are working with a crystalline quantum wire that is periodic in z, so that we would obtain allowed values of k spaced by $2\pi/L_z$.

For the remaining "circular" part, we note that

$$\nabla^2_{r\theta}=\frac{1}{r}\frac{\partial}{\partial r}\left(\frac{r\partial}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}$$

Hence we have

$$\left[\frac{-\hbar^2}{2m}\frac{1}{r}\frac{\partial}{\partial r}\frac{r\partial}{\partial r}-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}+V(r)\right]C(r,\theta)=E_{r\theta}C(r,\theta)$$

where

$$E_{r\theta}=E-E_z$$

We can postulate a form

$$C(r,\theta)=R(r)A(\theta)$$

which leads to

$$\frac{-\hbar^2}{2m_{eff}}\frac{A(\theta)}{r}\frac{r\partial}{\partial r}R(r)+V(r)R(r)A(\theta)\frac{-\hbar^2}{2m_{eff}}\frac{R(r)}{r^2}\frac{\partial^2A(\theta)}{\partial\theta^2}=E_{r\theta}R(r)A(\theta)$$

Dividing by

$$\frac{-\hbar^2}{2m_{eff}}\frac{R(r)A(\theta)}{r^2}$$

we have, choosing B as the separation constant

$$\frac{r}{R(r)}\frac{\partial}{\partial r}r\frac{\partial}{\partial r}R(r)-\frac{2m_{eff}}{\hbar^2}r^2V(r)+\frac{2m_{eff}}{\hbar^2}r^2E_{r\theta}=-\frac{1}{A(\theta)}\frac{\partial^2}{\partial\theta^2}=B$$

Hence we have

$$\frac{\partial^2 A}{\partial\theta^2}=-BA$$

so

$$A=e^{im\theta}\qquad\text{(or formally }Ee^{im\theta}+Fe^{-im\theta}\text{)}$$

with
$$B=m^2$$

and m is chosen as an integer so that for each complete cycle the wavefunction returns to the same value.

For the r equation, we now have

$$r\frac{\partial}{\partial r}r\frac{\partial R}{\partial r}-r^2\frac{2m_{eff}}{\hbar^2}\left[V(r)-E_{r0}\right]R=m^2R$$

Within the cylinder, $V(r)=0$, and outside $V(r)=\infty$. The "$V(r)=\infty$ at $r=r_o$" condition will force the boundary condition $R(r_0)=0$, and we then have the equation

$$r\frac{\partial}{\partial r}r\frac{\partial R}{\partial r}+\left[r^2\varepsilon-m^2\right]R=0$$

where

$$\varepsilon=\frac{2m_{eff}}{\hbar^2}E_{r\theta}$$

or equivalently

$$\frac{\partial}{\partial r}r\frac{\partial R}{\partial r}+\left[\varepsilon r-\frac{m^2}{r}\right]R=0$$

The solution of this equation is, from standard mathematical reference books

$$R(r)=DJ_m\left(\sqrt{\varepsilon}r\right)+GY_p\left(\sqrt{\varepsilon}r\right)$$

where D and G are arbitrary constants, and J_p and Y_p are, respectively, the Bessel and Weber functions of order p.

The Weber functions diverge as $r\to 0$, which would necessarily lead to a wavefunction $C(r,\theta)$ that was infinite or discontinuous through $r=0$ for a least some angles, which would be unphysical, so we discard the Weber functions. Hence we have

$$R(r)\propto J_m\left(\sqrt{\varepsilon}r\right)$$

Mathematical reference books on Bessel functions tell us, incidentally, that

$$J_{-m}(x)=(-1)^m J_m(x)$$

Since the sign of the wave function is an arbitrary choice for eigenvalue problems, we can therefore write, if we wish,

$$R(r) \propto J_{|m|}\left(\sqrt{\varepsilon}r\right)$$

For eigenfunction solutions, we have to meet the boundary condition $R(r_0) = 0$. Hence we require

$$J_{|m|}\left(\sqrt{\varepsilon}r_0\right) = 0$$

Writing the nth zero of the mth order Bessel function as s_{nm}, we therefore have

$$\sqrt{\varepsilon_{nm}}\,r_0 = s_{nm}$$

i.e.,

$$\varepsilon_{nm} = \frac{s_{nm}^2}{r_0^2}$$

or

$$E_{nm} = \frac{\hbar^2}{2m_{eff}r_0^2}s_{nm}^2$$

where m is any positive or negative integer or zero, and n is any positive integer > 0.

10.5.6

The answer for this matrix element is 39.407 pm, or $128\sqrt{2}\,/\,243$ in units of the Bohr radius.

See the following Mathcad worksheet for an example calculation of this matrix element.

Mathcad worksheet for Problem 10.5.6
Matrix Elements for Hydrogen Atom Wavefunctions

To proceed to work out matrix elements of hydrogen atom wavefunctions, we need to construct various different functions.

Associated Legendre functions

First, for the spherical harmonics, we need the associated Legendre functions. We can define these using Rodrigues' formula. (Note that we use "el" instead of "l" to avoid confusion between the number "one" and the letter "el")

$$P(x, el, m) := \left(\frac{1}{2^{el} \cdot el!}\right)\left(1 - x^2\right)^{\frac{m}{2}} \frac{d^{(el+m)}}{dx^{(el+m)}}\left[\left(x^2 - 1\right)^{el}\right]$$

We can graph these to check what they look like

$$xx := -1, -.99 .. 1$$

$$
\begin{array}{l}
P(xx, 0, 0) \\
\overline{\quad\quad\quad} \\
P(xx, 1, 0) \\
\cdots\cdots\cdots \\
P(xx, 1, 1) \\
\text{-----} \\
P(xx, 1, -1) \\
\text{-·-·-·-}
\end{array}
$$
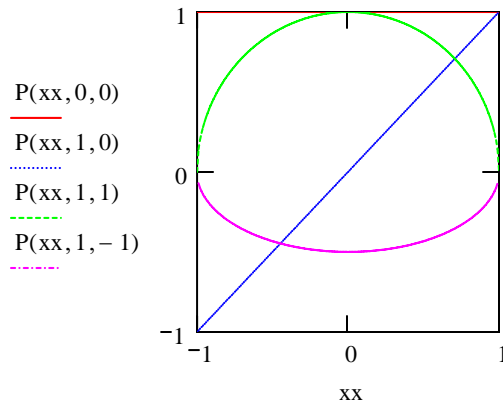
Spherical Harmonics

We will now construct the complex version of the spherical harmonics. Here we remember that θ is the angle with respect to the polar (z) axis. This angle runs from 0 to π. ϕ is the azimuthal angle in the plane, conventionally the angle with respect to the x axis, and it runs from 0 to 2π.

$$Y(\theta, \phi, el, m) := (-1)^m \cdot \sqrt{(2 \cdot el + 1) \cdot \frac{((el - m)!)}{4 \cdot \pi (el + m)!}} \cdot P(\cos(\theta), el, m) \cdot \exp(i \cdot m \cdot \phi)$$

Just as a check, we can verify that this function is normalized for a couple of different values of el and m. Note that, as usual in spherical polars, the element of solid angle is sin θ dθ dϕ.

$$NY00 := \int_0^{\pi} \left[\int_0^{2 \cdot \pi} \left(\left| Y(\theta, \phi, 0, 0) \right| \right)^2 d\phi \right] \cdot \sin(\theta) \, d\theta \qquad NY00 = 1$$

$$NY11 := \int_0^{\pi} \left[\int_0^{2 \cdot \pi} \left(\left| Y(\theta, \phi, 1, 1) \right| \right)^2 d\phi \right] \cdot \sin(\theta) \, d\theta \qquad NY11 = 1$$

Associated Laguerre polynomials

For the radial solutions, we need first to construct the associated Laguerre polynomials.

$$L(x, p, j) := \sum_{q=0}^{p} (-1)^q \frac{(p + j)! \cdot x^q}{(p - q)! \cdot (j + q)! \cdot q!}$$

Let us check the orthogonality of these polynomials.

$$I(p1, p2, j) := \int_0^{\infty} \exp(-x) \cdot x^j \cdot L(x, p1, j) \cdot L(x, p2, j) \, dx$$

$$I(0, 0, 0) = 1$$
$$I(1, 0, 0) = 8.316 \times 10^{-13}$$
$$I(1, 1, 0) = 1$$

Radial solutions

To get the scale of the radial solutions, we need the Bohr radius, which is, in picometers

$$ao := 52.9$$

The radial functions are

$$R(r, n, el) := \sqrt{\left(\frac{2}{n \cdot ao} \right)^3 \frac{(n - el - 1)!}{2 \cdot n \cdot (n + el)!}} \cdot \left(2 \cdot \frac{r}{n \cdot ao} \right)^{el} L\left(2 \cdot \frac{r}{n \cdot ao}, n - el - 1, 2 \cdot el + 1 \right) \cdot \exp\left(\frac{-r}{n \cdot ao} \right)$$

The normalization of the R functions can be checked

$$NR(n, el) := \int_0^{\infty} \left(\left| R(r, n, el) \right| \right)^2 \cdot r^2 \, dr$$

$$NR(1, 0) = 1 \quad NR(2, 0) = 1$$
$$NR(2, 1) = 1 \quad NR(3, 0) = 1$$
$$NR(3, 1) = 1 \quad NR(3, 2) = 1$$

We can plot some of these to check them.

$rr := 0, 1 .. 500$

R(rr, 1, 0)
R(rr, 2, 1)
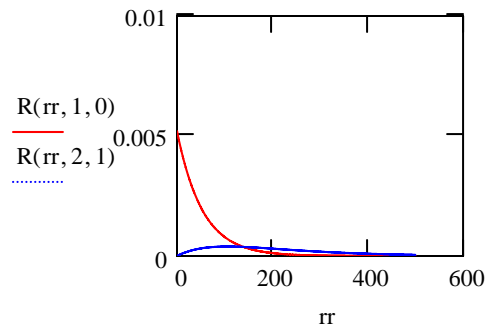
Full wave function

Now we can write the full wavefunction.

$$U(r, \theta, \phi, n, el, m) := R(r, n, el) \cdot Y(\theta, \phi, el, m)$$

We can check that this is normalized for some example values.

$$NU100 := \int_0^\infty \int_0^\pi \left[\int_0^{2\cdot\pi} \left(\left| U(r, \theta, \phi, 1, 0, 0) \right| \right)^2 d\phi \right] \cdot \sin(\theta) \, d\theta \cdot r^2 \, dr \qquad NU100 = 1$$

$$NU210 := \int_0^\infty \int_0^\pi \left[\int_0^{2\cdot\pi} \left(\left| U(r, \theta, \phi, 2, 1, 0) \right| \right)^2 d\phi \right] \cdot \sin(\theta) \, d\theta \cdot r^2 \, dr \qquad NU210 = 1$$

Example matrix element

Now we can work out a matrix element of the form <U1|z|U2>. Note that z = r cos θ. To work out integrals of complex quantities, it is necessary here to separate out the real and imaginary parts and work out each integral separately.

$$MR := \int_0^\infty \int_0^\pi \left(\int_0^{2\cdot\pi} Re\left(\overline{U(r,\theta,\phi,1,0,0)} \cdot U(r,\theta,\phi,2,1,0) \right) d\phi \right) \cdot r\cdot\cos(\theta)\cdot\sin(\theta) \, d\theta \cdot r^2 \, dr$$

$$MI := \int_0^\infty \int_0^\pi \left(\int_0^{2\cdot\pi} Im\left(\overline{U(r,\theta,\phi,1,0,0)} \cdot U(r,\theta,\phi,2,1,0) \right) d\phi \right) \cdot r\cdot\cos(\theta)\cdot\sin(\theta) \, d\theta \cdot r^2 \, dr$$

MR = 39.407   MI = 0   M := MR + i·MI

M = 39.407   picometers

10.5.7

Optical transitions between two states $\left|\psi_{starting}\right\rangle$ and $\left|\psi_{final}\right\rangle$ are possible for linearly polarized electromagnetic fields if the matrix element $\left\langle\psi_{starting}\left|z\right|\psi_{final}\right\rangle$ is non-zero. This will be the case if and only if the states have opposite parity along the z direction

(a) Transitions are possible. The $\left|1,0,0\right\rangle$ state has even parity along z, and the $\left|2,1,0\right\rangle$ has odd parity (it has a zero round the equator of the sphere).

(b) Transitions are not possible. The $\left|1,0,0\right\rangle$ state has even parity along z, but the $\left|2,1,1\right\rangle$ state also has even parity along z (it has a zero on a circle going through the poles, but not a zero round the equator).

(c) Transitions are not possible. The $\left|1,0,0\right\rangle$ state has even parity along z, and so also has the $\left|2,0,0\right\rangle$ state (it also is spherically symmetric).

(d) Transitions are possible. The $\left|1,0,0\right\rangle$ state has even parity along z, and the $\left|2,1,0\right\rangle$ has odd parity (it has a zero around the equator of the sphere), just as for (a) above. [Note for interest: this particular transition would actually be a stimulated emission transition in this theoretical model.]

10.5.8

Assume no motion is possible in the z-direction (e.g., assume infinite mass in this direction or very high, close potential barriers, though we neglect any confinement energy in this direction). We start with the Schrödinger wave equation

$$\left[-\frac{\hbar^2}{2m_e}\nabla_e^2 - \frac{\hbar^2}{2m_p}\nabla_p^2 + V\left(\left|\mathbf{r}_e - \mathbf{r}_p\right|\right) \right]\psi\left(x_e, y_e, x_p, y_p\right) = E\psi\left(x_e, y_e, x_p, y_p\right)$$

where

$$V\left(\left|\mathbf{r}_e - \mathbf{r}_p\right|\right) = \frac{-e^2}{4\pi\varepsilon_0\left|\mathbf{r}_e - \mathbf{r}_p\right|}$$

Center of Mass Coordinates

Now we change to center of mass coordinates. Define

$$x = x_e - x_p \qquad y = y_e - y_p$$

$$\mathbf{r}_{xy} = x\mathbf{i} + y\mathbf{i}$$

$$r_{xy} = \sqrt{x^2 + y^2} = \left|\mathbf{r}_e - \mathbf{r}_p\right|$$

We propose

$$\mathbf{R}_{xy} = \frac{m_e\mathbf{r}_e + m_p\mathbf{r}_p}{M}$$

$$M = m_e + m_p$$

$$\mathbf{R}_{xy} = x\mathbf{i} + Y\mathbf{j}$$

Then, e.g.,

$$X = \frac{m_e x_e + m_p x_p}{M}$$

Following through as in the 3D case, we have

$$\frac{1}{m_e}\frac{\partial^2}{\partial x_e^2} + \frac{1}{m_p}\frac{\partial^2}{\partial x_p^2} = \frac{m_e + m_h}{M^2}\frac{\partial^2}{\partial x^2} + \left(\frac{1}{m_e} + \frac{1}{m_h}\right)\frac{\partial^2}{\partial x^2} = \frac{1}{M}\frac{\partial^2}{\partial x^2} + \frac{1}{\mu}\frac{\partial^2}{\partial x^2}$$

where

$$\mu = \frac{m_e m_h}{m_e + m_h}$$

and similarly for the y direction, so we have

$$\hat{H} = -\frac{\hbar^2}{2M}\nabla_{R_{xy}}^2 - \frac{\hbar^2}{2\mu}\nabla_{r_{xy}}^2 + V(r) \tag{1}$$

Separation of Variables

Presume

$$\psi(\mathbf{R}_{xy}, \mathbf{r}_{xy}) = S(\mathbf{R}_{xy})U(\mathbf{r}_{xy})$$

hence, substituting in the Schrödinger equation with the above Hamiltonian (1) and dividing by $S(\mathbf{R}_{xy})U(\mathbf{r}_{xy})$, we have, as in the 3-D case

$$-\frac{1}{S(\mathbf{R}_{xy})}\frac{\hbar^2}{2M}\nabla^2_{\mathbf{R}_{xy}}S(\mathbf{R}_{xy}) = E + \frac{1}{U(\mathbf{r}_{xy})}\left[\frac{\hbar^2}{2\mu}\nabla^2_{\mathbf{r}_{xy}} + V(r_{xy})\right]U(\mathbf{r}_{xy})$$

Both sides must be equal to the separation constant, E_{CoM}. Hence, we have separated equations

$$-\frac{\hbar^2}{2M}\nabla^2_{\mathbf{R}_{xy}}S(\mathbf{R}_{xy}) = E_{CoM}S(\mathbf{R}_{xy})$$

and

$$\left[-\frac{\hbar^2}{2\mu}\nabla^2_{\mathbf{r}_{xy}} + V(r_{xy})\right]U(\mathbf{r}_{xy}) = E_H U(\mathbf{r}_{xy}) \tag{2}$$

where

$$E_H = E - E_{CoM}$$

Solution of Center of Mass Motion

Immediately we see

$$S(\mathbf{R}_{xy}) = \exp(i\mathbf{K}_{xy} \cdot \mathbf{R}_{xy})$$

with eigenenergies

$$E_{CoM} = \frac{\hbar^2 K^2_{xy}}{2M}$$

The two vector components of $\mathbf{K}_{xy}$ are quantum numbers that can take on any real value.

Solution of Relative Motion

Note that, in (cylindrical) polar coordinates, we have (neglecting the z motion)

$$\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \equiv \nabla^2_{\mathbf{r}_{xy}} = \frac{1}{r}\frac{\partial}{\partial r}\left(\frac{r\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial\phi^2}$$

where

$$x = r\cos\phi \qquad y = r\sin\phi$$

and, above and henceforth we use $\mathbf{r}$ instead of $\mathbf{r}_{xy}$ for simplicity of notation. Now we propose a separation

$$U(r) = R(r)W(\phi)$$

Substituting in the Schrödinger equation for the radial motion (2) we obtain

$$-\frac{\hbar^2}{2\mu}\left[W(\phi)\frac{1}{r}\frac{\partial}{\partial r}\left(\frac{r\partial}{\partial r}\right)R(r)+\frac{1}{r^2}R(r)\frac{\partial^2}{\partial\phi^2}W(\phi)\right]+V(r)R(r)W(\phi)=E_H R(r)W(\phi)$$

Dividing by $-\hbar^2 R(r)W(\phi)/2\mu r^2$ gives

$$\frac{1}{R(r)}\frac{1}{r}\frac{\partial}{\partial r}\left(\frac{r\partial}{\partial r}\right)R(r)+\frac{1}{W(\phi)}\frac{\partial^2}{\partial\phi^2}W(\phi)-\frac{2\mu}{\hbar^2}r^2V(r)=-\frac{2\mu}{\hbar^2}r^2 E_H$$

Rearranging gives

$$-\frac{1}{W(\phi)}\frac{\partial^2}{\partial\phi^2}W(\phi)=\frac{1}{R(r)}\frac{r\partial}{\partial r}\left(\frac{r\partial}{\partial r}\right)R(r)+r^2\frac{2\mu}{\hbar^2}\left(E_H-V(r)\right)=m^2$$

where m^2 is our separation constant. The angular equation

$$\frac{\partial^2}{\partial\phi^2}W(\phi)=-m^2 W(\phi)$$

has solutions

$$W(\phi)=e^{im\phi}$$

where m is an integer (positive, negative, or zero) so that $W(\phi)$ and its derivatives are continuous with the values equal for both $\phi=0$ and $\phi=2\pi$.

Hence, the separated radial equation is

$$\frac{r\partial}{\partial r}\left(\frac{r\partial}{\partial r}\right)R(r)+\left[-m^2+r^2\frac{2\mu}{\hbar^2}\left(E_H-V(r)\right)\right]R(r)=0$$

or

$$\frac{1}{r}\frac{\partial}{\partial r}\left(\frac{r\partial}{\partial r}\right)R(r)+\left[-\frac{m^2}{r^2}+\frac{2\mu}{\hbar^2}\left(E_H-V(r)\right)\right]R(r)=0 \tag{3}$$

Asymptotic Behavior $r\to\infty$

Certainly m^2/r^2 becomes negligible in (3). Also $V(r)$ becomes negligible compared to the constant term $\frac{2\mu}{\hbar^2}E_H$, so the dominant "energy" term is $\frac{2\mu}{\hbar^2}E_H R(r)$. For the derivative

$$\frac{1}{r}\frac{\partial}{\partial r}\frac{r\partial}{\partial r}R(r)=\frac{1}{r}\left[\frac{\partial}{\partial r}R(r)+\frac{r\partial^2 R(r)}{\partial r^2}\right]=\frac{\partial^2 R(r)}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}R(r)$$

We make an intelligent guess that

$$\frac{\partial^2 R(r)}{\partial r^2}\gg\frac{1}{r}\frac{\partial}{\partial r}R(r)\text{ as }r\to\infty$$

so we have

$$\frac{\partial^2 R(r)}{\partial r^2}\approx-\frac{2\mu}{\hbar^2}E_H R(r)$$

which has a solution, presuming $E_H < 0$ for a bound state

$$R(r) \propto \exp-\sqrt{-\frac{2\mu E_H}{\hbar^2}}r$$

(We neglect the exponentially growing solution as being unphysical). We choose the same variable substitution as in the 3-D problem, i.e.,

$$s = \alpha r \qquad \alpha = \frac{2}{ba_0} = 2\sqrt{-\frac{2\mu E_H}{\hbar^2}}$$

where b is a parameter to be determined, and a_o is the Bohr radius

$$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{e^2\mu}$$

Note that

$$E_H = -\frac{1}{b^2}\frac{\hbar^2}{2\mu a_0^2} = -\frac{R_y}{b^2} \tag{4}$$

where

$$R_y = \frac{\hbar^2}{2\mu a_0^2}$$

Asymptotic Behavior as $r \to 0$

We presume a power series form for $R(r)$, and need only consider the lowest term as $r \to 0$.

The m^2/r^2 term dominates in the "energy" terms, leaving

$$\frac{1}{r}\frac{\partial}{\partial r}\frac{r\partial}{\partial r}r^p - \frac{m^2}{r^2}r^p = 0$$

i.e.,

$$\frac{r\partial}{\partial r}\frac{r\partial}{\partial r}r^p - m^2 r^p = 0$$

i.e.,

$$p^2 r^p - m^2 r^p = 0$$

Hence

$$p = |m|$$

(Note the necessity of the modulus here. We know m can be positive or negative (or zero). But p must be a positive quantity for a power series expansion).

Postulated Form for Radial Function

Hence, we postulate a solution of the form

$$R\left(\frac{s}{\alpha}\right) = s^{|m|}L(s)e^{-s/2}$$

We change our equation (3) to write it in terms of $s\ (=\alpha r)$ rather than r. We have

$$\alpha^2 \frac{1}{s}\frac{\partial}{\partial s}s\frac{\partial}{\partial s}R\left(\frac{s}{\alpha}\right) + \left[-\frac{\alpha^2 m^2}{s^2} + \frac{2\mu}{\hbar^2}\left(E_H + \frac{\alpha e^2}{4\pi\varepsilon_0 S}\right)\right]R\left(\frac{s}{\alpha}\right) = 0$$

We note that

$$\frac{2\mu}{\alpha^2\hbar^2}E_H = -\frac{1}{4\left(\frac{2\mu}{\hbar^2}\right)E_H}\frac{2\mu}{\hbar^2}E_H = -\frac{1}{4}$$

and

$$\frac{1}{\alpha}\frac{2\mu}{\hbar^2}\frac{e^2}{4\pi\varepsilon_0} = \frac{1}{\alpha}\frac{2}{a_0} = \frac{ba_0}{2}\frac{2}{a_0} = b$$

Hence, we have

$$\frac{1}{s}\frac{d}{ds}s\frac{d}{ds}R\left(\frac{s}{\alpha}\right) + \left[\frac{b}{s} - \frac{m^2}{s^2} - \frac{1}{4}\right]R\left(\frac{s}{\alpha}\right) = 0 \qquad (5)$$

Now, substituting our form for $R(s/\alpha)$, we recast the equation

$$\frac{d}{ds}\left(s^{|m|}L(s)e^{-s/2}\right) = |m|s^{|m|-1}L(s)e^{-s/2} + s^{|m|}e^{-s/2}\frac{d}{ds}L(s) - \frac{1}{2}s^{|m|}L(s)e^{-s/2}$$

i.e.,

$$s\frac{d}{ds}\left(s^{|m|}L(s)e^{-s/2}\right) = \left[L(s)\left(|m|s^{|m|} - \frac{1}{2}s^{|m|+1}\right) + s^{|m|+1}\frac{dL(s)}{ds}\right]e^{-s/2}$$

i.e.

$$\frac{d}{ds}s\frac{d}{ds}\left(s^{|m|}L(s)e^{-s/2}\right) = \left\{\begin{array}{l} -\dfrac{1}{2}\left[L(s)\left(|m|s^{|m|} - \dfrac{1}{2}s^{|m|+1}\right) + s^{|m|+1}\dfrac{dL(s)}{ds}\right] \\[4mm] +\dfrac{dL}{ds}\left[|m|s^{|m|} - \dfrac{1}{2}s^{|m|+1}\right] + L(s)\left[m^2 s^{|m|-1} - \dfrac{(|m|+1)s^{|m|}}{2}\right] \\[4mm] \left(|m|+1\right)s^{|m|}\dfrac{dL}{ds} + s^{|m|+1}\dfrac{d^2L}{ds^2} \end{array}\right\}e^{-s/2}$$

so

$$\frac{1}{s}\frac{d}{ds}s\frac{d}{ds}\left(s^{|m|}L(s)e^{-s/2}\right) = s^{|m|}e^{-s/2}\left\{ \begin{array}{c} L(s)\left[\dfrac{-|m|}{2s}+\dfrac{1}{4}+\dfrac{m^2}{s^2}-\dfrac{(|m|+1)}{2s}\right] \\[4mm] \dfrac{dL}{ds}\left[\dfrac{|m|}{s}-1+\dfrac{|m|+1}{s}\right]+\dfrac{d^2L}{ds^2} \end{array} \right\}$$

$$= s^{|m|}e^{-s/2}\left\{ \begin{array}{c} L(s)\left[\dfrac{m^2}{s^2}-\dfrac{(|m|+1/2)}{s}+\dfrac{1}{4}\right] \\[4mm] +\dfrac{dL}{ds}\left[\dfrac{2(|m|+1/2)}{s}-1\right]+\dfrac{d^2L}{ds^2} \end{array} \right\}$$

Hence, Eq. (5) becomes

$$s\frac{d^2L}{ds^2}+\left[2|m|+1-s\right]\frac{dL}{ds}+\left[\frac{m^2}{s}-|m|-\frac{1}{2}+\frac{s}{4}+b-\frac{m^2}{s}-\frac{s}{4}\right]L=0$$

i.e.,

$$s\frac{d^2L}{ds^2}+\left[2|m|+1-s\right]\frac{dL}{ds}+\left[b-|m|-\frac{1}{2}\right]L=0 \tag{6}$$

Series Solution

Postulate a power series for L

$$L(s) = \sum_{q=0}^{\infty} c_q s^q$$

and substitute this in (6). First note that

$$\frac{dL}{ds} = \sum_{q=0}^{\infty}(q+1)c_{q+1}s^q$$

$$\frac{d^2L}{ds^2} = \sum_{q=0}^{\infty}(q+2)(q+1)c_{q+2}s^q$$

Hence we have, collecting terms in a specific power s^q in Eq. (6)

$$(q+1)qc_{q+1}+\left(2|m|+1\right)(q+1)c_{q+1}-qc_q+\left(b-|m|-\frac{1}{2}\right)c_q=0$$

i.e.,

$$c_{q+1} = \frac{-\left(b - |m| - q - \frac{1}{2}\right)}{(q+1)(2|m|+1+q)} c_q \tag{7}$$

For this series to stop, i.e., for $c_{q+1} = 0$ (with finite c_q)

$$b - |m| - q - \frac{1}{2} = 0$$

for some q (where $q = 0,1,2,...$), i.e.,

$$b = |m| + q + \frac{1}{2}$$

Quantum Numbers and Energies

Hence the possible values of b must be

$$b - \frac{1}{2} = 0,1,2..., \text{ i.e., } b = \frac{1}{2}, \frac{3}{2}, \frac{5}{2},...$$

or equivalently

$$b = n + \frac{1}{2}$$

with

$$n = 0,1,2...$$

(note the allowed values of n start at zero, not one). We also have the restriction

$$|m| \leq b - \frac{1}{2}$$

so that we have at least one term in the series., i.e.,

$$|m| \leq n$$

(We previously noted that m can otherwise be any positive, negative, or zero integer.) Working back from Eq. (4), we find that the allowed energies are

$$E_H = -\frac{R_y}{\left(n + \frac{1}{2}\right)^2}$$

so the energy of the lowest state is

$$E_H = -\frac{R_y}{\left(\frac{1}{2}\right)^2} = -4R_y = -4 \times 13.6 \ eV \simeq -54.4 \ eV$$

Radial Wavefunctions

Using the relation (7), which we now write as

$$c_q = -\frac{(n-|m|-q+1)}{q(2|m|+q)}c_{q-1}$$

and so the coefficients in the power series are

$$c_q = (-1)^q \frac{(n-|m|)!(2|m|)!}{(n-|m|-q)!q!(2|m|+q)!}c_0$$

(Note: $(n-|m|)(n-|m|-1)...(n-|m|-q+1) = \dfrac{(n-|m|)!}{(n-|m|-q)!}$)

The stopping condition (8) can be rewritten as $q = n-|m|$; this value of q corresponds to the last non-zero term in the series. Hence, the radial wavefunctions can be written as

$$L_{n,m}(s) = c_0 \sum_{q=0}^{n-|m|} (-1)^q \frac{(n-|m|)!(2|m|)!}{(n-|m|-q)!(2|m|+q)!}s^q$$

(Incidentally, these polynomials are also the associated Laguerre polynomials, $L_{n-|m|}^{2|m|}(s)$. The formal equivalence requires the specific choice

$$c_0 = \frac{(n+|m|)!}{(n-|m|)!(2|m|)!}$$

which leads to

$$L_{n,m}(s) \equiv L_{n-|m|}^{2|m|}(s) = \sum_{q=0}^{n-|m|} (-1)^q \frac{(n+|m|)!}{(n-|m|-q)!q!(2|m|+q)!}$$

though this formal equivalence was not required for the solution to this problem.)

Hence, the final statement of the unnormalized wavefunction is

$$\psi(\mathbf{R}_{xy},\mathbf{r}_{xy}) \propto \exp(iK_{xy},R_{xy})r_{xy}^{|m|}L_{n,m}(\alpha r_{xy})\exp(-\alpha r_{xy}/2)\exp(im\phi)$$

where

$$\alpha = \frac{2}{\left(n+\dfrac{1}{2}\right)a_0}$$

The eigenenergies are

$$E = \frac{\hbar^2 K_{xy}^2}{2M} - \frac{R_y}{\left(n+\dfrac{1}{2}\right)^2}$$

The allowed values of the discrete quantum numbers are

$$n = 0, 1, 2, \ldots$$

$$m = \text{any positive, negative, or zero integer such that } |m| \leq n.$$

The lowest energy is $\simeq -54.6 \, eV$.

This problem is discussed in M. Shinada and S. Sugano, J. Phys. Soc. Japan <u>21</u>, 1936-1946 (1966).

10.5.9

There are 4 degenerate (i.e., same energy) $n = 2$ levels in hydrogen, corresponding to the 2S state ($n = 2, l = 0, m = 0$), and the three 2P states ($n = 2, l = 0, m = -1, 0, 1$). The unperturbed energy of all of these states is $E_o = -Ry / n^2 = -Ry / 4$.

The perturbing Hamiltonian for an electron in an electric field F in the positive z direction is $\hat{H}_p = eFz$.

The problem to be solved here is a degenerate perturbation theory problem. This will involve matrix elements of the perturbing Hamiltonian $\hat{H}_p$ between the various degenerate $n = 2$ states. The method of solution of such a problem is to solve the matrix equation, as discussed in Chapter 6 (Eq. (6.67)).

$$\begin{bmatrix} H_{pm1m1} & H_{pm1m2} & \cdots & H_{pm1mr} \\ H_{pm2m1} & H_{pm2m2} & \cdots & H_{pm2mr} \\ \vdots & \vdots & \ddots & \vdots \\ H_{pmrm1} & H_{pmrm2} & \cdots & H_{pmrmr} \end{bmatrix} \begin{bmatrix} a_{m1} \\ a_{m2} \\ \vdots \\ a_{mr} \end{bmatrix} = E^{(1)} \begin{bmatrix} a_{m1} \\ a_{m2} \\ \vdots \\ a_{mr} \end{bmatrix}$$

where the H_{pmimj} are the matrix elements of the perturbation between the various degenerate wavefunctions of the r-fold degenerate level m of the unperturbed problem (m here is not the magnetic quantum number), and the a_{mi} are the amplitudes of the various basis functions in the resulting solution of the perturbed problem. In our current problem, we have a degeneracy of 4, and will therefore have a 4 x 4 matrix.

We can therefore write a matrix with the wavefunctions in the vector being written in the order from top to bottom of ($l = 0$, $m = 0$), ($l = 1$, $m = +1$), ($l = 1$, $m = 0$), ($l = 1$, $m = -1$). The only non-zero elements are the element corresponding to ($l = 0$, $m = 0$) to ($l = 1$, $m = 0$) and the identical element corresponding to ($l = 1$, $m = 0$) to ($l = 0$, $m = 0$). We could deduce this result either by direct calculation, or by noting that the only one of the 2P states that is antisymmetric along the z direction is the one with $m = 0$ (it has a nodal circle around the equator). Since the perturbing Hamiltonian is odd in the z direction, this particular matrix element between the 2S state (which is even in all directions) and this 2P orbital (which is odd in only the z direction) is non-zero. The other matrix elements between different 2P states are all zero by related parity arguments. Hence the Hamiltonian matrix can be written

$$\hat{H}_p = \begin{bmatrix} 0 & 0 & h_{01} & 0 \\ 0 & 0 & 0 & 0 \\ h_{01} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

where

$$h_{01} = eF \langle n = 2, l = 0, m = 0 | z | n = 2, l = 1, m = 0 \rangle$$

and we can numerically evaluate

$$\langle n=2, l=0, m=0 | z | n=2, l=1, m=0 \rangle \simeq 159 \text{ pm}$$

(Note that $h_{01} = h_{10}$ here because the Hamiltonian is Hermitian h_{01} is real.) We can simplify the matrix we need to deal with to a 2x2 matrix, with functions ($l = 0$, $m = 0$) and ($l = 1$, $m = 0$) from top to bottom in the corresponding 2 element vector. Solving the resulting matrix eigenvalue and eigenvector problem gives the results

$$|\psi_+\rangle = \frac{1}{\sqrt{2}}\left(|n=2, l=0, m=0\rangle - |n=2, l=1, m=0\rangle\right) \text{ with eigenenergy } 1.59 \times 10^{-10} F \text{ eV}$$

$(1.59 \times 10^{-5} \text{ eV at } 10^5 \text{ V/m})$

$$|\psi_-\rangle = \frac{1}{\sqrt{2}}\left(|n=2, l=0, m=0\rangle + |n=2, l=1, m=0\rangle\right) \text{ with eigenenergy } -1.59 \times 10^{-10} F \text{ eV}$$

$(-1.59 \times 10^{-5} \text{ eV at } 10^5 \text{ V/m})$

where the field F is in V/m, and the energies are expressed relative to the energy $E_o = -Ry/n^2 = -Ry/4$. The other two states are unaffected by the field (the degeneracy of these other two states is not lifted). Those other two states can be described by any orthogonal pair of linear combinations of the states $|n=2, l=1, m=+1\rangle$ and $|n=2, l=1, m=-1\rangle$.

The change of spectral lines of hydrogen was first observed by Johannes Stark in 1913, and was a clear example of a physical effect that could not be explained classically. A linear shift of spectral lines with field is unusual in atomic spectra, and is a consequence of the exact degeneracy of the 2S and 2P levels in hydrogen; such a shift is called a linear Stark effect. More common is the quadratic Stark effect, a shift proportional to the square of the field, and understandable as primarily the shift in energy in a field caused by creating a dipole whose magnitude is itself proportional to the field.

Stark shifts are also observable with so-called excitons (electron-hole pairs) in semiconductor quantum wells, in which case the resulting very large shifts possible are called the quantum-confined Stark effect, and are used to make optical modulators for telecommunications and other applications.

See the following Mathcad worksheet for example calculations.

Problem 10.5.9 Solution Mathcad worksheet
Stark Shift of n=2 Levels in Hydrogen

These solutions are presented as a Mathcad worksheet, though the description should be readable even for those not using this software.

Preparing constants and wavefunction formulae

We start this solution by defining some physical constants we will require.

$$Ry := 13.6 \qquad q := 1.602 \cdot 10^{-19} \qquad ao := 5.292 \cdot 10^{-11}$$

(Note that we have stated the Rydberg Ry in electron-volts. We will use these energy units throughout the problem.)

Next, since we will need the wavefunctions for calculation of the matrix elements, we formally construct them mathematically here. First, the associated Laguerre polynomials are, from Chapter 10,

$$L_p^j(s) = \sum_{q=0}^{p} (-1)^q \frac{(p+j)!}{(p-q)!(j+q)!q!} s^q \qquad \text{Eq. 10.65}$$

which we can write in Mathcad notation as

$$L(j,p,s) := \sum_{q=0}^{p} (-1)^q \cdot \left(\frac{(p+j)!}{(p-q)! \cdot (j+q)! \, q!} \right) \cdot s^q$$

From the Chapter, we have the radial function for the hydrogen atom as

$$R(r) = \left[\frac{(n-l-1)!}{2n(n+l)!} \left(\frac{2}{na_o} \right)^3 \right]^{1/2} \left(\frac{2r}{na_o} \right)^l L_{n-l-1}^{2l+1} \left(\frac{2r}{na_o} \right) \exp\left(-\frac{r}{na_o} \right) \qquad \text{Eq. 10.72}$$

In Mathcad notation, we write this as

$$R(r,n,l) := \left[\left(\frac{(n-1-1)!}{2 \cdot n \cdot (n+1)!} \right) \left(\frac{2}{n \cdot ao} \right)^3 \right]^{\frac{1}{2}} \cdot \left(2 \cdot \frac{r}{n \cdot ao} \right)^1 L\left(2l+1, n-1-1, 2 \cdot \frac{r}{n \cdot ao} \right) \cdot \exp\left(\frac{-r}{n \cdot ao} \right)$$

For the spherical harmonics, we first define the associated Legendre functions. We can use Rodrigues' formula

$$P_l^m(x) = \frac{1}{2^l l!} (1-x^2)^{m/2} \frac{d^{l+m}}{dx^{l+m}} (x^2-1)^l \qquad \text{Eq. 9.31}$$

In Mathcad notation this becomes

$$P(x,l,m) := \left(\frac{1}{2^l l!} \right) \left(1 - x^2 \right)^{\frac{m}{2}} \cdot \frac{d^{l+m}}{dx^{l+m}} \left[\left(x^2 - 1 \right)^l \right]$$

From the Chapter, we have for the definition of the spherical harmonics

$$Y_{lm}(\theta, \phi) = (-1)^m \sqrt{\frac{2l + 1}{4\pi} \frac{(l - m)!}{(l + m)!}} P_l^m(\cos\theta) \exp(im\phi)$$ Eq. 9.34

which becomes in Mathcad notation

$$YS(\theta, \phi, l, m) := (-1)^m \cdot \sqrt{\frac{[(2 \cdot l + 1) \cdot (l - m)!]}{4 \cdot \pi \cdot (l + m)!}} P(\cos(\theta), l, m) \cdot \exp(i \cdot m \cdot \phi)$$

Actually in the problem, it will be more instructive, though not strictly necessary, to break this function into a product of a θ function.

$$YStheta(\theta, l, m) := (-1)^m \cdot \sqrt{\frac{[(2 \cdot l + 1) \cdot (l - m)!]}{4 \cdot \pi \cdot (l + m)!}} \cdot P(\cos(\theta), l, m)$$

and a ϕ function

$$YSphi(\phi, m) := \exp(i \cdot m \cdot \phi)$$

The final statement of the hydrogen wavefunction then becomes

$$U(r, \theta, \phi, n, l, m) := R(r, n, l) \cdot YS(\theta, \phi, l, m)$$

or equivalently

$$Us(r, \theta, \phi, n, l, m) := R(r, n, l) \, YStheta(\theta, l, m) \, YSphi(\phi, m)$$

Set up of problem proper

There are 4 degenerate (i.e., same energy) n=2 levels in hydrogen, corresponding to the 2S state (n=2, l=0, m=0), and the three 2P states (n=2, l=1, m= -1, 0, +1). The unperturbed energy of all of these states is Eo= - Ry/n^2 = - Ry/4

$$Eo := \frac{-Ry}{4} \qquad Eo = -3.4$$

The perturbing Hamiltonian for an electron in an electric field F in the positive z direction is Hp=qFz. We will drop the q in this formula because we are going to express the resulting energies in electron volts, and for the purposes of the integration, we will formally express z in terms of r and θ

$$z(r, \theta) := r \cdot \cos(\theta)$$

The problem to be solved here is a degenerate perturbation theory problem. This will involve matrix elements of the perturbing Hamiltonian H_p between the various degenerate n=2 states. The method of solution of such a problem is to solve the matrix equation, as discussed in Chapter 6

$$
\begin{bmatrix}
H_{pm1m1} & H_{pm1m2} & \cdots & H_{pm1mr} \\
H_{pm2m1} & H_{pm2m2} & \cdots & H_{pm2mr} \\
\vdots & \vdots & \ddots & \vdots \\
H_{pmrm1} & H_{pmrm2} & \cdots & H_{pmrmr}
\end{bmatrix}
\begin{bmatrix}
a_{m1} \\ a_{m2} \\ \vdots \\ a_{mr}
\end{bmatrix}
= E^{(1)}
\begin{bmatrix}
a_{m1} \\ a_{m2} \\ \vdots \\ a_{mr}
\end{bmatrix}
\qquad \text{Eq. 6.67}
$$

where the H_{pmimj} are the matrix elements of the perturbation between the various degenerate wavefunctions of the r-fold degenerate level m of the unperturbed problem, and the a_{mi} are the amplitudes of the various basis functions in the resulting solution of the perturbed problem. In our current problem, we have a degeneracy of 4, and will eventually have a 4 x 4 matrix.

In our problem, a matrix element can be written, using the indices l and m to label the unperturbed basis states

$$
\text{Hp(la, ma, lb, mb, F)} := \int_0^\infty \int_0^\pi \int_0^{2\cdot\pi} \overline{U(r,\theta,\phi,2,\text{la},\text{ma})} \cdot F \cdot z(r,\theta) \cdot U(r,\theta,\phi,2,\text{lb},\text{mb}) \cdot r^2 \cdot \sin(\theta)\, d\theta\, d\phi\, dr
$$

It will, however, be more instructive to separate this into several successive parts. In fact, we can rewrite the integral as the product of three integrals, one (Ir) over r, one (Iθ) over θ, and one (Iϕ) over ϕ, and take the field outside as a multiplying factor, i.e., Hp = F Ir Iθ Iϕ. The only one with any complex part to it is Iϕ, which we may deal with first, i.e.,

$$
\text{I}\phi(\text{ma}, \text{mb}) := \int_0^{2\pi} \overline{\text{YSphi}(\phi, \text{ma})} \cdot \text{YSphi}(\phi, \text{mb})\, d\phi
$$

or equivalently, writing out the explicit expression for YSphi

$$
\text{I}\phi(\text{ma}, \text{mb}) := \int_0^{2\cdot\pi} \exp\left[i\cdot\left[(\text{mb} - \text{ma})\cdot\phi\right]\right] d\phi
$$

The analytic answer to this integral is 2π if ma and mb are equal and is zero otherwise (for integer ma and mb). Hence we know the matrix elements are zero unless the magnetic quantum number is identical. (I.e., the electric field does not mix the wavefunctions of different m values.)

The θ integral is

$$
\text{I}\theta(\text{la}, \text{ma}, \text{lb}, \text{mb}) := \int_0^\pi \left(\text{YStheta}(\theta, \text{la}, \text{ma})\cos(\theta)\, \text{YStheta}(\theta, \text{lb}, \text{mb})\right)\sin(\theta)\, d\theta
$$

We know immediately that, for la=lb, ma=mb, the answer to the integral is zero because we are multiplying an even function (YStheta*YStheta) by an odd one (cosθ).

We also know, from the discussion of the ϕ integral, that we need only consider ma=mb=m equal, and, because n=2, we only need to consider l=0 (in which case m=0) and l=1. Hence the only possibly non-zero integrals involve la not equal to lb, and ma = mb =m. Hence the only possible non-zero matrix elements are those involving the following choices

$$
\text{la} := 0 \qquad \text{lb} := 1 \qquad \text{ma} := 0 \qquad \text{mb} := 0 \qquad \text{I}\theta(\text{la}, \text{ma}, \text{lb}, \text{mb}) = 0.092
$$

$$la := 1 \qquad lb := 0 \qquad ma := 0 \qquad mb := 0 \qquad I\theta(la, ma, lb, mb) = 0.092$$

The only remaining integral to be performed is the r integral. We have

$$Ir(la, lb) := \int_0^{2\times 10^{-9}} r \cdot r^2 R(r, 2, la) \cdot R(r, 2, lb) \, dr$$

[Note: to evaluate this integral successfully using numerical techniques, it was necessary to force Mathcad to use a numerical integration, which can be done by right-clicking the integral, and selecting, e.g., Romberg. To get the integral not to give a zero answer, a finite upper limit also had to be chosen. Choosing too large a limit means that the integration misses the region of actual interest, which is for r within a few angstroms of zero. This limit was chosen large enough to capture all the range where the integrand is significant, but not so large that the integral value started to change again.]

We only have to consider the cases of different la and lb, i.e., the cases

$$la := 0 \qquad lb := 1 \qquad Ir(la, lb) = -2.75 \times 10^{-10}$$

and the physically identical case

$$la := 1 \qquad lb := 0 \qquad Ir(la, lb) = -2.75 \times 10^{-10}$$

We can therefore write a matrix with the wavefunctions in the vector being written in the order from top to bottom of (l=0,m=0), (l=1,m=+1), (l=1,m=0), (l=1,m=-1). The only non-zero elements are

the element corresponding to (l=0,m=0) to (l=1,m=0), i.e.,

$$h01 := 2 \cdot \pi \, I\theta(0, 0, 1, 0) \cdot Ir(0, 1) \qquad\qquad h01 = -1.59 \times 10^{-10}$$

and the identical element corresponding to (l=1,m=0) to (l=0,m=0)

Hence the matrix, leaving out the electric field magnitude F for the moment, would be

$$h := \begin{pmatrix} 0 & 0 & h01 & 0 \\ 0 & 0 & 0 & 0 \\ h01 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Clearly this perturbation correction matrix does nothing to the (l=1,m=+1) and (l=1,m=-1) states, so we conclude that they are unperturbed by this field. Remember that, for degenerate states, any orthogonal linear combination of them is also a valid choice of eigenfunctions. The fact that this matrix has nothing to say about the (l=1,m=+1) and (l=1,m=-1) states means we are, as before, free to choose any linear combination of them as eigenfunctions also of this perturbed problem.

However, the (l=0,m=0) and (l=1,m=0) states are clearly mixed. We construct therefore a simpler matrix for them alone, i.e., using only those two basis states to construct the matrix, we have

$$hnew := \begin{pmatrix} 0 & h01 \\ h01 & 0 \end{pmatrix}$$

We can formally evaluate the eigenvalues and eigenvectors of this matrix.

$$\text{eigenvals(hnew)} = \begin{pmatrix} 1.59 \times 10^{-10} \\ -1.59 \times 10^{-10} \end{pmatrix}$$

$$\text{eigenvec}\left(\text{hnew}, 1.59 \times 10^{-10}\right) = \begin{pmatrix} -0.707 \\ 0.707 \end{pmatrix}$$

$$\text{eigenvec}\left(\text{hnew}, -1.59 \times 10^{-10}\right) = \begin{pmatrix} 0.707 \\ 0.707 \end{pmatrix}$$

Hence we conclude that the perturbed states have energies, relative to the original unperturbed energy of -Ry/4, of (in electron volts)

$$\text{Eplus(F)} := 1.59 \times 10^{-10} \cdot F$$

and

$$\text{Eminus(F)} := -1.59 \times 10^{-10} \cdot F$$

with associated wavefunctions

$$\left| \psi_+ \right\rangle = \frac{1}{\sqrt{2}} \left(\left| n=2, l=0, m=0 \right\rangle - \left| n=2, l=1, m=0 \right\rangle \right)$$

and

$$\left| \psi_- \right\rangle = \frac{1}{\sqrt{2}} \left(\left| n=2, l=0, m=0 \right\rangle + \left| n=2, l=1, m=0 \right\rangle \right)$$

where the ket notation refers to the unperturbed hydrogen atom wavefunctions with these quantum numbers. The two states that are perturbed by the field have energies that depart linearly with field from the unperturbed energy level.

There are also two degenerate solutions with the same energy as the original unperturbed n=2 solutions, i.e., these two degenerate solutions are unperturbed by the field. Their wavefunctions are orthogonal linear combinations of the (n=2,l=1,m=-1) and (n=2,l=1,m=+1) hydrogen states. Hence the electric field partly lifts the degeneracy of the 4 n=2 hydrogen states, splitting off two in opposite directions linear with field, and leaving two degenerate ones.

Specifically, for a field of 10^5 V/m (a field easily achieved in the laboratory), we would find one state shifted down by 0.016 meV, one shifted up by 0.016 meV and two degenerate states unaffected by the field.

Chapter 11 problem solutions

11.1.1

Consider an electron wave of electron (kinetic) energy E incident on a barrier of width L and of height V, where $V > E$. On the left of the barrier we have

$$\psi(z) = A \exp(ikz) + B \exp(-ikz)$$

where

$$k = \sqrt{\frac{2m_0 E}{\hbar^2}}$$

(We are taking the energy origin at the energy of the "bottom" of the barrier).

Inside the barrier, we have

$$\psi(z) = C \exp(-\kappa z) + D \exp(\kappa z)$$

where

$$\kappa = \sqrt{\frac{2m_0(V - E)}{\hbar^2}}$$

where we will choose $z = 0$ at the "left" side of the barrier (the side on which the electrons are incident).

On the right of the barrier, we have

$$\psi(z) = F \exp(ikz)$$

Starting with the "exit" face on the right (i.e., $z = L$), from the continuity of ψ we have

$$F = CG + \frac{D}{G} \tag{1}$$

where $G = \exp(-\kappa L)$, and from continuity of $d\psi / dz$

$$ikF = -\kappa CG + \kappa \frac{D}{G}$$

i.e.,

$$-\frac{ikF}{\kappa} = CG - \frac{D}{G} \tag{2}$$

Adding (1) and (2) gives

$$2CG = F\left(1 - \frac{ik}{\kappa}\right)$$

so

$$CG = \frac{F}{2}\left(1 - \frac{ik}{\kappa}\right) \tag{3}$$

and

$$C = \frac{F}{2G}\left(1 - \frac{ik}{\kappa}\right) = -\frac{ik}{\kappa}\frac{F}{2G}\left(1 + \frac{i\kappa}{k}\right) \tag{4}$$

From (1) and (3), we have

$$F = \frac{F}{2}\left(1 - \frac{ik}{\kappa}\right) + \frac{D}{G}$$

i.e.,

$$D = \frac{GF}{2}\left(1 + \frac{ik}{\kappa}\right) = \frac{GF}{2}\frac{ik}{\kappa}\left(1 - \frac{i\kappa}{k}\right)$$

Now we presume that the barrier is thick so that G is a very small number. Hence

$$|D| = \frac{G|F|}{2}\frac{k}{\kappa}\left[1 + \left(\frac{\kappa}{k}\right)^2\right]^{1/2} << |C| = \frac{1}{G}\frac{|F|}{2}\frac{k}{\kappa}\left[1 + \left(\frac{\kappa}{k}\right)^2\right]^{1/2}$$

Hence the boundary condition for continuity of ψ at $z = 0$ becomes

$$A + B = C + D \simeq C$$

and for continuity of $d\psi / dz$ at $z = 0$ becomes

$$ik(A - B) = -\kappa(C - D) \simeq -\kappa C$$

i.e.,

$$A - B = \frac{i\kappa}{k}C$$

So

$$A = \frac{1}{2}\left(1 + \frac{i\kappa}{k}\right)C$$

so, using C from (4),

$$A = \frac{1}{2}\left(1 + \frac{i\kappa}{k}\right)\frac{F}{2G}\left(1 - \frac{ik}{\kappa}\right) = \frac{F}{4G}\left(1 + \frac{i\kappa}{k}\right)\left(1 - \frac{ik}{\kappa}\right)$$

So,

$$\eta = \frac{16G^2}{\left|\left(1 + \frac{i\kappa}{k}\right)\left(1 - \frac{ik}{\kappa}\right)\right|^2} = \frac{16G^2}{\left[1 + \left(\frac{\kappa}{k}\right)^2\right]\left[1 - \left(\frac{k}{\kappa}\right)^2\right]} = \frac{16G^2}{1 + 1 + \left(\frac{\kappa}{k}\right)^2 + \left(\frac{k}{\kappa}\right)^2}$$

$$= \frac{16G^2}{2 + \frac{\kappa^4 + k^4}{k^2\kappa^2}} = \frac{16G^2 k^2\kappa^2}{k^4 + \kappa^4 + 2k^2\kappa^2} = \frac{16G^2 k^2\kappa^2}{\left(k^2 + \kappa^2\right)^2}$$
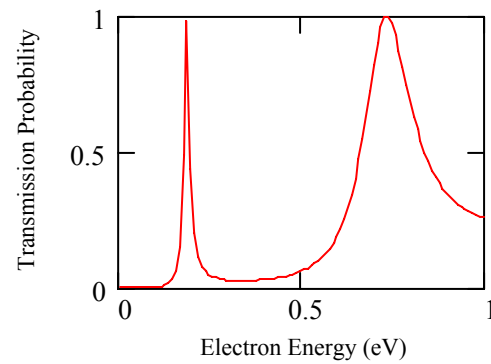
i.e.,

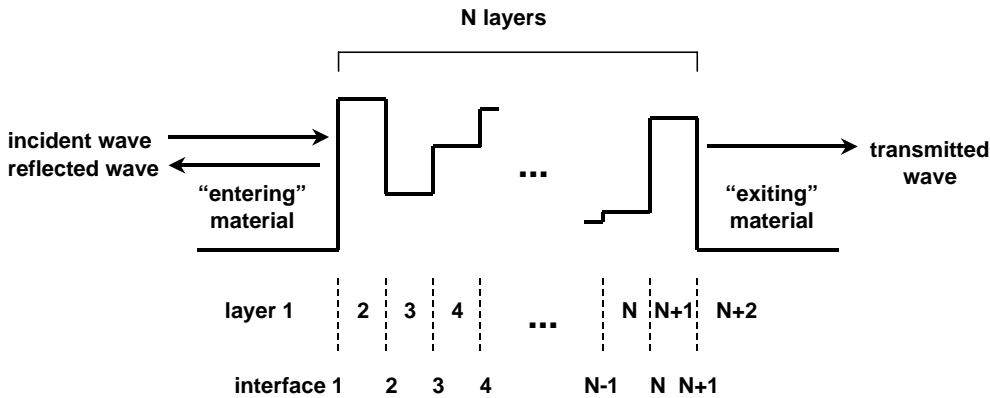$$\eta = \frac{16k^2\kappa^2 \exp(-2\kappa L)}{\left(k^2 + \kappa^2\right)^2}$$

11.2.1

For this problem, one needs to set up an appropriate computer program for the transfer matrix method, using the formulae in the book. For example computer code, see the following Mathcad worksheet.

The calculated transmission resulting from this model is as shown in the figure.

Problem 11.2.1 Solution Mathcad worksheet

This solutions is given here as a Mathcad worksheet, though it should be relatively obvious how the problem is being solved. (In Mathcad, the symbol ":=" means "is defined to be equal to". The equals sign itself ("=") is used to give the current value of whatever variable is on the left of the equals sign.) Formally, we wish to calculate the transfer matrix for a structure with a series of steps of potential as shown in the figure.

For future formal mathematical use, we formally choose the origin of all matrices and vectors at an index of 1 (rather than zero).

$$\text{ORIGIN} := 1$$

Formal construction of matrices

We first define the necessary fundamental constants.

$$\text{hbar} := 1.055 \cdot 10^{-34} \qquad \text{mo} := 9.1095 \cdot 10^{-31} \qquad q := 1.602 \cdot 10^{-19}$$

For a given layer m of potential energy V_m, mass m_{fm}, and thickness d_m, we can define the necessary quantities required by the algebra. To allow the use of mass units of the free electron mass m_o, thickness units of nanometers, and energy units of electron volts for inputting the parameter - namely the wavevector k, which may be real or imaginary - we define a units scaling parameter s by

$$s := \frac{2q \cdot mo \cdot 10^{-18}}{\text{hbar}^2} \qquad \text{which gives} \qquad s = 26.22299$$

Using this scaling parameter, we can write the formula for the wavevector as a function of the appropriate

$$k(E, Vm, mfm) := \sqrt{s \cdot mfm \cdot (E - Vm)}$$

and the quantity

$$\Delta(E, Vm, mfm, Vm1, mfm1) := k(E, Vm1, mfm1) \cdot \frac{mfm}{k(E, Vm, mfm) \cdot mfm1}$$

where by mfm we mean m_{fm} and by mfm1 we mean m_{fm+1}, i.e., the quantity in the layer $m+1$, and similarly for Vm and $Vm1$.

This leads to a boundary condition matrix

$$D(E, Vm, mfm, Vm1, mfm1) := \frac{\begin{pmatrix} 1 + \Delta(E, Vm, mfm, Vm1, mfm1) & 1 - \Delta(E, Vm, mfm, Vm1, mfm1) \\ 1 - \Delta(E, Vm, mfm, Vm1, mfm1) & 1 + \Delta(E, Vm, mfm, Vm1, mfm1) \end{pmatrix}}{2}$$

relating the forward and backward amplitudes just inside the right side of layer m to those just inside the layer $m+1$, and a propagation matrix in layer m

$$P(E, Vm, mfm, dm) := \begin{pmatrix} \exp(-i \cdot k(E, Vm, mfm) \cdot dm) & 0 \\ 0 & \exp(i \cdot k(E, Vm, mfm) \cdot dm) \end{pmatrix}$$

For a given structure, we have to choose these parameters V_m, the mass will be m_{fm}, and the thickness will be d_m. We will use mass units of the free electron mass m_o, thickness units of nanometers, and energy units of electron volts for inputting the parameters.

Choice of parameters

Now we choose the number N of layers in the structure (not including the "entering" and "exiting" layers)

$N := 3$

Now we explicitly input the values of the parameters.

$mf_1 := 1 \qquad Vm_1 := 0$

$mf_2 := 1 \qquad Vm_2 := 1 \qquad dm_2 := 0.3$

$mf_3 := 1 \qquad Vm_3 := 0 \qquad dm_3 := 1$

$mf_4 := 1 \qquad Vm_4 := 1 \qquad dm_4 := 0.3$

$mf_5 := 1 \qquad Vm_5 := 0$

Now we can formally construct the overall transfer matrix by multiplying the various constituent matrices. (Note: Be careful in your program that the multiplication of the matrices is done in the correct order. The following does give the correct order for Mathcad's conventions.)

$$T(E) := D\left(E, Vm_1, mf_1, Vm_2, mf_2\right) \cdot \prod_{q=2}^{N+1} P\left(E, Vm_q, mf_q, dm_q\right) \cdot D\left(E, Vm_q, mf_q, Vm_{q+1}, mf_{q+1}\right)$$

and we can define the transmission fraction by

$$\eta(E) := 1 - \frac{\left(\left|T(E)_{2,1}\right|\right)^2}{\left(\left|T(E)_{1,1}\right|\right)^2}$$

So that we can plot the results, we define a range variable. The following variable takes on the values 0.005, 0.015, 0.025, and so on, all the way to 0.995.

$$EE := .005, .015 .. 0.995$$

EE is used as the horizontal ordinate in the following graph, and $\eta(EE)$ is used as the vertical value plotted, hence giving the following graph.
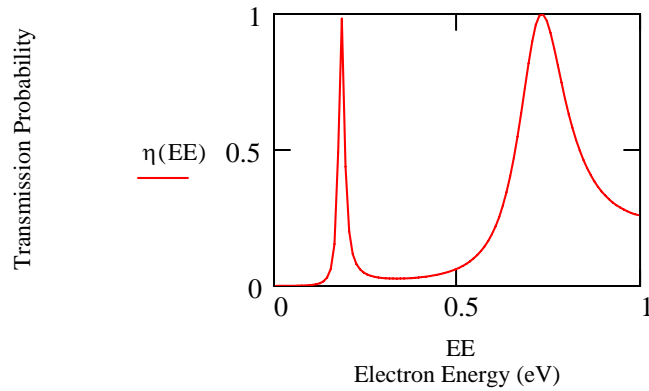
11.2.2

A typical calculated transmission is as shown in the figure, for the case of 4 nm barriers.
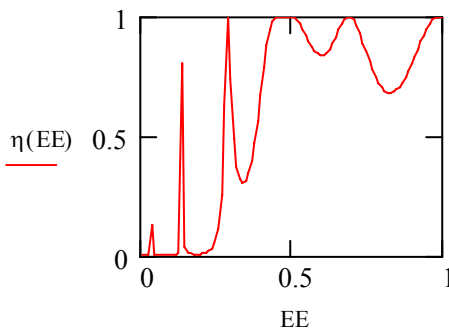
The peak transmissions in this case are all actually unity, though to see that, we need finer resolution on this figure. (Lossless structures with equal front and back reflectivities generally have unity transmission on resonance.)

(i) 0.0347 eV

(ii) 0.0348 eV

(iii) 0.0348 eV

The convergence of these answers illustrates that, as the resonance becomes very sharp, the state converges to a specific energy, which is also a good approximation to the eigenenergy if we make the barriers arbitrarily thick (see Problem 11.2.3).

For example computer code, see the code after Problem 11.2.3.

11.2.3

The graph illustrates the magnitude of the T_{11} matrix element for this problem as a function of energy (here plotted as a variable Emm). Numerically, the position of the minimum of the magnitude of the T_{11} matrix element occurs at 0.0348 eV, which is therefore (within 0.1 meV) the energy of this particular eigensolution.

Note that this result is the same as the converging answer for Problem 11.2.2, confirming that the position of the "tunneling resonance" gives a good approximation for the eigenenergy of a structure with infinite barriers.
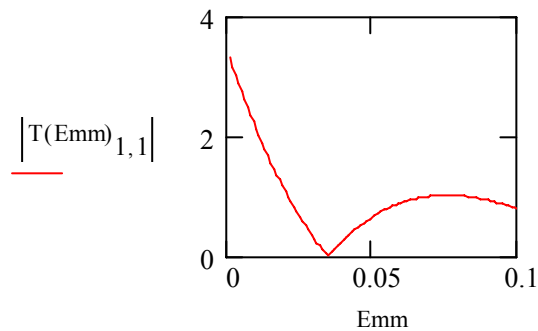
For example computer code, see the following code.

Problems 11.2.1, 11.2.2 and 11.2.3 Solutions Mathcad worksheet

This set of solutions is given here as a Mathcad worksheet, though it should be relatively obvious how th problem is being solved. First we set up the formalism for all three problems.

Formally, we wish to calculate the transfer matrix for a structure with a series of steps of potential as shown in the figure.

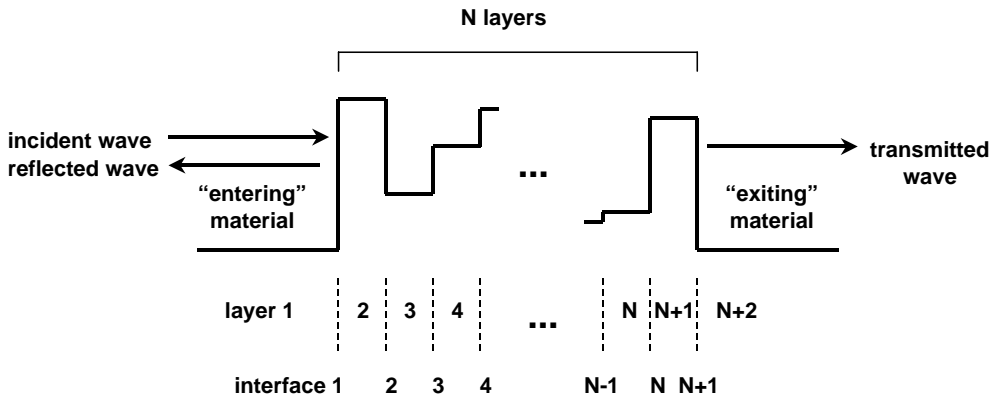For future formal mathematical use, we formally choose the origin of all matrices and vectors at an index of 1 (rather than zero).

$$\text{ORIGIN} := 1$$

Formal construction of matrices

We first define the necessary fundamental constants.

$$\text{hbar} := 1.055 \cdot 10^{-34} \qquad \text{mo} := 9.1095 \cdot 10^{-31} \qquad q := 1.602 \cdot 10^{-19}$$

For a given layer *m* of potential energy V_m, mass m_{fm}, and thickness d_m, we can define the necessary quantities required by the algebra. To allow the use of mass units of the free electron mass m_o, thickness units of nanometers, and energy units of electron volts for inputting the parameternamely the wavevector *k*, which may be real or imaginary, we define a units scaling parameter *s* by

$$s := \frac{2q \cdot mo \cdot 10^{-18}}{\text{hbar}^2} \qquad \text{which gives} \qquad s = 26.22299$$

$$k(E, Vm, mfm) := \sqrt{s \cdot mfm \cdot (E - Vm)}$$

and the quantity

$$\Delta(E, Vm, mfm, Vm1, mfm1) := k(E, Vm1, mfm1) \cdot \frac{mfm}{k(E, Vm, mfm) \cdot mfm1}$$

where by mfm we mean m_{fm} and by mfm1 we mean m_{fm+1}, i.e., the quantity in the layer *m+1*, and similarly for *Vm* and *Vm1*.

This leads to a boundary condition matrix

$$D(E, Vm, mfm, Vm1, mfm1) := \frac{\begin{pmatrix} 1 + \Delta(E, Vm, mfm, Vm1, mfm1) & 1 - \Delta(E, Vm, mfm, Vm1, mfm1) \\ 1 - \Delta(E, Vm, mfm, Vm1, mfm1) & 1 + \Delta(E, Vm, mfm, Vm1, mfm1) \end{pmatrix}}{2}$$

relating the forward and backward amplitudes just inside the right side of layer *m* to those just inside the layer *m+1*, and a propagation matrix in layer *m*

$$P(E, Vm, mfm, dm) := \begin{pmatrix} \exp(-i \cdot k(E, Vm, mfm) \cdot dm) & 0 \\ 0 & \exp(i \cdot k(E, Vm, mfm) \cdot dm) \end{pmatrix}$$

For a given structure, we have to choose these parameters V_m, the mass will be m_{fm}, and the thickness will be d_m. We will use mass units of the free electron mass m_o, thickness units of nanometers, and energy units of electron volts for inputting the parameters.

We will also set up the parameters for the potentials and masses in AlGaAs alloys for the conduction band, as a function of x, the fraction of aluminum in the alloy (with the fraction of GaAs being 1-x).

$$VAlGaAs(x) := 0.77 \cdot x \qquad meffAlGaAs(x) := 0.067 + 0.083 \cdot x$$

Choice of parameters for the first structure (Problem 11.2.1)

Now we choose the number *N* of layers in the structure (not including the "entering" and "exiting" layers)

$$N := 3$$

Now we explicitly input the values of the parameters.

$$mf_1 := 1 \qquad Vm_1 := 0$$
$$mf_2 := 1 \qquad Vm_2 := 1 \qquad dm_2 := 0.3$$
$$mf_3 := 1 \qquad Vm_3 := 0 \qquad dm_3 := 1$$
$$mf_4 := 1 \qquad Vm_4 := 1 \qquad dm_4 := 0.3$$
$$mf_5 := 1 \qquad Vm_5 := 0$$

Now we can formally construct the overall tranfer matrix by multiplying the various constituent matrices.

$$T(E) := D\left(E, Vm_1, mf_1, Vm_2, mf_2\right) \cdot \prod_{q=2}^{N+1} P\left(E, Vm_q, mf_q, dm_q\right) \cdot D\left(E, Vm_q, mf_q, Vm_{q+1}, mf_{q+1}\right)$$

and we can define the transmission fraction by

$$\eta(E) := 1 - \frac{\left(\left| T(E)_{2,1} \right|\right)^2}{\left(\left| T(E)_{1,1} \right|\right)^2}$$

EE := .005, .015 .. 0.995

Transmission Probability

$\eta(EE)$ 0.5

EE
Electron Energy (eV)

Graphing the probability density (this is not required for the Problem)

For completeness, we show here how the probability density can be graphed. We first choose the energy for which we wish to graph the probability density.

$$EG := 0.2 + FRAME \cdot 0.0125$$

(The FRAME variable above is a formal internal variable in Mathcad that can be incremented in units of 1 for each successive frame in an animation.)

We next evaluate the forward amplitude in layer 1 (the "entering" layer) on the assumption of unit forward amplitude (and no backward amplitude) in the exiting layer.

$$FB1 := T(EG) \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad FB1 = \begin{pmatrix} -0.77825 - 1.70034i \\ 1.58014i \end{pmatrix} \quad rm := FB1_1 \quad Renorm = -0.77825 - 1.70034i$$

We will use this to normalize all other results to a unit forward amplitude in layer 1. For future use, we start by constructing a normalized version of this first amplitude itself.

$$FB1norm := \frac{FB1}{Renorm} \qquad FB1norm = \begin{pmatrix} 1 \\ -0.76834 - 0.35167i \end{pmatrix}$$

Now we construct a function that gives us the forward and backward amplitudes on the left of any layer with index greater than 1.

$$FB(p) := \frac{\left[\left(\displaystyle\prod_{q=p}^{N+1} P\left(EG, Vm_q, mf_q, dm_q\right) \cdot D\left(EG, Vm_q, mf_q, Vm_{q+1}, mf_{q+1}\right) \right) \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right]}{Renorm}$$

Now we construct a vector that gives us the distance from the left of the structure (i.e., from the position of the first interface on the left) at the left of any layer of the structure. For reasons of mathematical convenience in this formula, we first define dm1=0, though we do not in fact restrict this layer to zero thickness.

$$dm_1 := 0$$

$$dp(p) := \sum_{q=1}^{p-1} dm_q$$

Now we construct a function that tells us, for any given position z what layer of the structure we are in.

$$pp(z) := \begin{vmatrix} 1 & \text{if } z < 0 \\ \text{otherwise} \\ \quad \begin{vmatrix} (N+2) & \text{if } z \geq dp(N+2) \\ \text{otherwise} \\ \quad \begin{vmatrix} qq \leftarrow 2 \\ \text{while } dp(qq) < z \\ \quad qq \leftarrow qq + 1 \\ qq - 1 \end{vmatrix} \end{vmatrix} \end{vmatrix}$$

Now we construct a function that gives us the wavefunction at any point z in the structure. Note that, at any given point, the wavefunction is the sum of the forward and backward propagating parts.

$$\psi(z) := \begin{vmatrix} FB1norm_1 \cdot \exp\left(i \cdot k\left(EG, Vm_1, mf_1\right) \cdot z\right) + FB1norm_2 \cdot \exp\left[-i \cdot \left(k\left(EG, Vm_1, mf_1\right) \cdot z\right)\right] & \text{if } z < 0 \\ \text{otherwise} \\ \quad \begin{vmatrix} \left(\dfrac{1}{Renorm}\right) \cdot \exp\left[i \cdot k\left(EG, Vm_{N+2}, mf_{N+2}\right) \cdot \left(z - dp(N+2)\right)\right] & \text{if } z > dp(N+2) \\ \text{otherwise} \\ \quad \begin{vmatrix} jj \leftarrow pp(z) \\ kz \leftarrow k\left(EG, Vm_{jj}, mf_{jj}\right) \cdot (z - dp(jj)) \\ FB(jj)_1 \cdot \exp(i \cdot kz) + FB(jj)_2 \cdot \exp(-i \cdot kz) \end{vmatrix} \end{vmatrix} \end{vmatrix}$$

Hence we have for the probability density

$$Pr(z) := \overline{\psi(z)} \cdot \psi(z)$$

Now we can graph the probability density. We define minimum and maximum values of position z for plotting, and an appropriate range variable.

$$zmin := -2 \qquad zmax := 2$$

$$zz := zmin, zmin + 0.01 .. zmax$$

We also prepare mathematical vectors containing the potential values and the positions of the interfaces in a form suitable for plotting the structure itself.

$$Vp(kk) := \begin{vmatrix} Vm_1 & \text{if } kk < 1 \\ \text{otherwise} \\ \quad \begin{vmatrix} Vm_{N+2} & \text{if } kk > 2 \cdot N + 2 \\ Vm_{\text{ceil}\left(\frac{kk}{2}\right)} & \text{otherwise} \end{vmatrix} \end{vmatrix} \qquad Ddp(kk) := \begin{vmatrix} zmin & \text{if } kk < 2 \\ \text{otherwise} \\ \quad \begin{vmatrix} zmax & \text{if } kk > 2 \cdot N + 3 \\ dp\left(\text{ceil}\left(\dfrac{kk+1}{2}\right)\right) & \text{otherwise} \end{vmatrix} \end{vmatrix}$$

$$kk := 1 .. 2N + 4$$
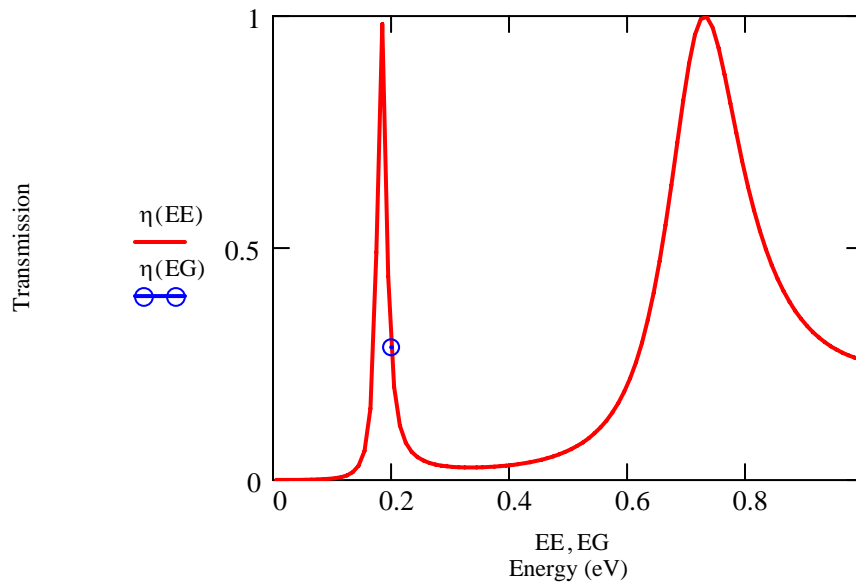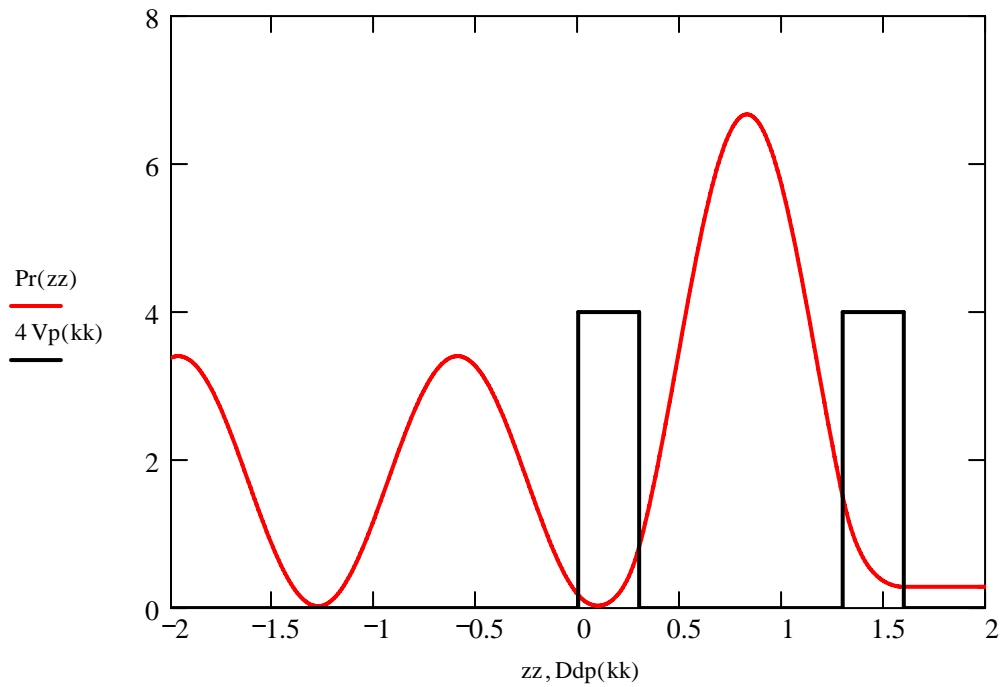
Choice of parameters for the semiconductor structure (Problem 11.2.2)

We first choose the aluminum fraction we will use for our barrier layers

$x := 0.3$

and hence calculate the potentials and masses that we will use in the various layers

VGaAs := 0	VAlGaAsx := VAlGaAs(x)	VAlGaAsx = 0.231
mGaAs := meffAlGaAs(0)	mAlGaAs := meffAlGaAs(x)	mAlGaAs = 0.0919

Problem 11.2.2, Part (i) (4 nm barriers)

Now we choose the number N of layers in the structure (not including the "entering" and "exiting" layers)

$N := 3$

Now we explicitly input the values of the parameters.

$mf_1 := mGaAs$ $Vm_1 := VGaAs$

$mf_2 := mAlGaAs$ $Vm_2 := VAlGaAsx$ $dm_2 := 4$

$mf_3 := mGaAs$ $Vm_3 := VGaAs$ $dm_3 := 9$

$mf_4 := mAlGaAs$ $Vm_4 := VAlGaAsx$ $dm_4 := 4$

$mf_5 := mGaAs$ $Vm_5 := VGaAs$

Now we can formally construct the overall tranfer matrix by multiplying the various constituent matrices.

$$T(E) := D\left(E, Vm_1, mf_1, Vm_2, mf_2\right) \cdot \prod_{q=2}^{N+1} P\left(E, Vm_q, mf_q, dm_q\right) \cdot D\left(E, Vm_q, mf_q, Vm_{q+1}, mf_{q+1}\right)$$

and we can define the transmission fraction by

$$\eta(E) := 1 - \frac{\left(\left|T(E)_{2,1}\right|\right)^2}{\left(\left|T(E)_{1,1}\right|\right)^2}$$

$EE := .001, .0011 .. 0.2$
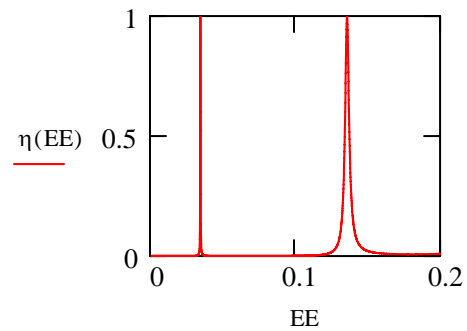
To find the energy corresponding to maximum transmission within 0.1 meV, we simply make a table of results for the transmission (progressively narrowing our range round the resonance).

$ii := 1, 2 .. 10$

$$Em_{ii} := 0.0345 + \frac{(ii - 1) \cdot .0005}{10}$$

$Results_{ii, 1} := Em_{ii}$ $Results_{ii, 2} := \eta(Em_{ii})$

$Results =$

	1	2
1	0.0345	0.22606
2	0.03455	0.33749
3	0.0346	0.52366
4	0.03465	0.79471
5	0.0347	0.99584
6	0.03475	0.87546
7	0.0348	0.59963
8	0.03485	0.38825
9	0.0349	0.25898
10	0.03495	0.18116

Hence the answer here for the position of this resonance within 0.1 meV is **0.0347 eV**.

Problem 11.2.2, Part (ii) (6 nm barriers)

We define new parameters

$$dm_2 := 6$$

$$dm_4 := 6$$

Now we can formally reconstruct the overall tranfer matrix by multiplying the various constituent matrices.

$$T(E) := D\left(E, Vm_1, mf_1, Vm_2, mf_2\right) \cdot \prod_{q=2}^{N+1} P\left(E, Vm_q, mf_q, dm_q\right) \cdot D\left(E, Vm_q, mf_q, Vm_{q+1}, mf_{q+1}\right)$$

and we can define the transmission fraction by

$$\eta(E) := 1 - \frac{\left(\left|T(E)_{2,1}\right|\right)^2}{\left(\left|T(E)_{1,1}\right|\right)^2}$$

$EE := .0347, .03471 .. 0.0349$
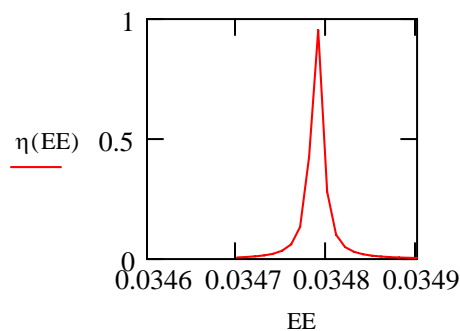
To find the energy corresponding to maximum transmission within 0.1 meV, we simply make a table of results for the transmission (progressively narrowing our range round the resonance).

$ii := 1, 2 .. 10$

$$Em_{ii} := 0.03475 + \frac{(ii - 1) \cdot .0001}{10}$$

$Results_{ii, 1} := Em_{ii}$

$Results_{ii, 2} := \eta\left(Em_{ii}\right)$

$Results =$

	1	2
1	0.03475	0.03411
2	0.03476	0.06069
3	0.03477	0.13346
4	0.03478	0.42485
5	0.03479	0.95397
6	0.0348	0.28052
7	0.03481	0.10109
8	0.03482	0.04995
9	0.03483	0.02947
10	0.03484	0.01937

Hence the answer here for the position of this resonance within 0.1 meV is **0.0348 eV**.

Problem 11.2.2, Part (iii) (8 nm barriers)

We define new parameters

$$dm_2 := 8 \qquad dm_4 := 8$$

Now we can formally reconstruct the overall tranfer matrix by multiplying the various constituent matrices.

$$T(E) := D\left(E, Vm_1, mf_1, Vm_2, mf_2\right) \cdot \prod_{q=2}^{N+1} P\left(E, Vm_q, mf_q, dm_q\right) \cdot D\left(E, Vm_q, mf_q, Vm_{q+1}, mf_{q+1}\right)$$

and we can define the transmission fraction by

$$\eta(E) := 1 - \frac{\left(\left|T(E)_{2,1}\right|\right)^2}{\left(\left|T(E)_{1,1}\right|\right)^2}$$

$EE := .03475, .034755 .. 0.03485$
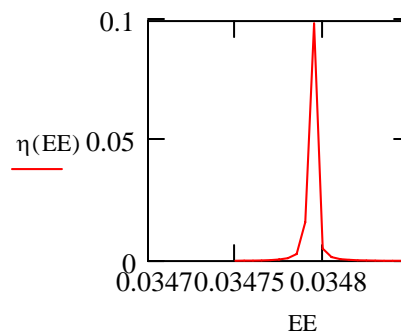
To find the energy corresponding to maximum transmission within 0.1 meV, we simply make a table of results for the transmission (progressively narrowing our range round the resonance).

$ii := 1, 2 .. 10$

$$Em_{ii} := 0.03479 + \frac{(ii - 1) \cdot .000005}{10}$$

	1	2
1	0.03479	0.016162
2	0.0347905	0.0216652
3	0.034791	0.030503
4	0.0347915	0.0459704
5	0.034792	0.0765397
6	0.0347925	0.1488287
7	0.034793	0.3683471
8	0.0347935	0.9507412
9	0.034794	0.5781407
10	0.0347945	0.2106125

$$Results_{ii, 1} := Em_{ii} \qquad Results_{ii, 2} := \eta\left(Em_{ii}\right)$$

$$Results =$$

Hence the answer here for the position of this resonance within 0.1 meV is **0.0348 eV**.

Bound eigenstate of the problem with infinitely thick barriers (Problem 11.2.3)

We consider the problem of one well with two barriers of finite height and infinite thickness on either side. In the notation of the present approach, we therefore have an entering layer, and exiting layer, and one layer in between, so

$$N := 1$$

For the GaAs well between the AlGaAs barriers, we therefore have a set of layer parameters

$$mf_1 := mAlGaAs \qquad Vm_1 := VAlGaAsx$$
$$mf_2 := mGaAs \qquad Vm_2 := VGaAs \qquad dm_2 := 9$$
$$mf_3 := mAlGaAs \qquad Vm_3 := VAlGaAsx$$

Now we can formally construct the overall tranfer matrix by multiplying the various constituent matrices.

$$T(E) := D\left(E, Vm_1, mf_1, Vm_2, mf_2\right) \cdot \prod_{q = 2}^{N+1} P\left(E, Vm_q, mf_q, dm_q\right) \cdot D\left(E, Vm_q, mf_q, Vm_{q+1}, mf_{q+1}\right)$$

Now we graph and tabulate results for the T_{11} matrix element

$$Emm := 0.001, 0.002 .. 0.1$$

$$ii := 1, 2 .. 10$$

$$Em_{ii} := 0.0347 + \frac{(ii - 1) \cdot .0002}{10}$$

$$Results_{ii, 1} := Em_{ii} \qquad Results_{ii, 2} := \left| T\left(Em_{ii}\right)1, 1 \right|$$

$\left| T(Emm)_{1,1} \right|$
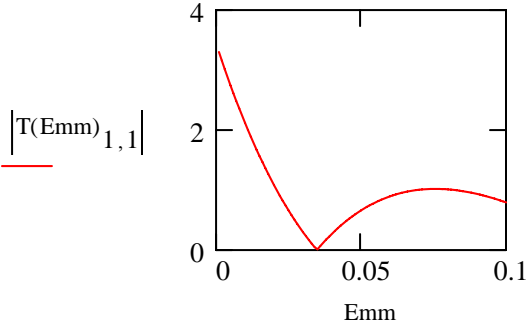
Hence the answer here for the position of this energy leve within 0.1 meV is **0.0348 eV**.

Note that the energy of the transmission resonance in the case with finite barriers corresponds closely to the bound state energy in the case with infinitely thick barriers. As the finite barriers are made thicker, the transmission resonance becomes progressively narrower, and its center position corresponds progressively more closely to the bound state energy of the infinitely thick barrier case.

$Results =$

	1	2
1	0.0347	5.38538·10 -3
2	0.03472	4.2376·10 -3
3	0.03474	3.09061·10 -3
4	0.03476	1.94441·10 -3
5	0.03478	7.99008·10 -4
6	0.0348	3.45601·10 -4
7	0.03482	1.48942·10 -3
8	0.03484	2.63244·10 -3
9	0.03486	3.77467·10 -3
10	0.03488	4.9161·10 -3

11.2.4

(i) We use the transfer matrix method to calculate the amplitudes $A_m(E)$ of the forward propagating wave and the amplitudes $B_m(E)$ of the backward propagating wave at each interface for every electron energy E of interest.

The transmission probability is then given by

$$\eta(E) = \frac{\left|A_1(E)\right|^2 - \left|B_1(E)\right|^2}{\left|A_1(E)\right|^2}$$
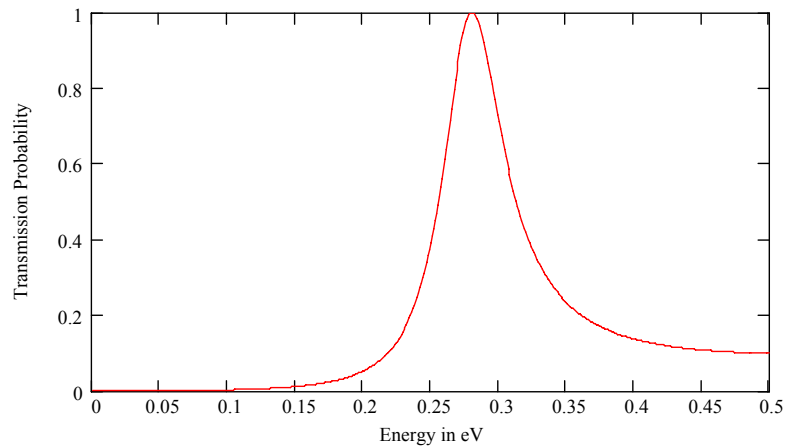
There is one resonance with an energy of 0.2804 eV.

The probability density is calculated using

$$\left|\psi(z,E)\right|^2 = \left|A_m(E)\exp\left[i\,k_m(E)(z-z_m)\right] + B_m(E)\exp\left[-i\,k_m(E)(z-z_m)\right]\right|^2$$
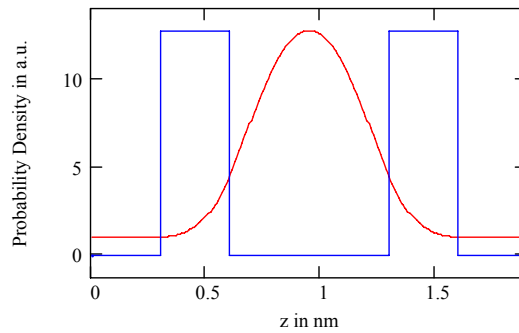
(ii) There are two resonances with energies of 0.2385 eV and 0.3334 eV.
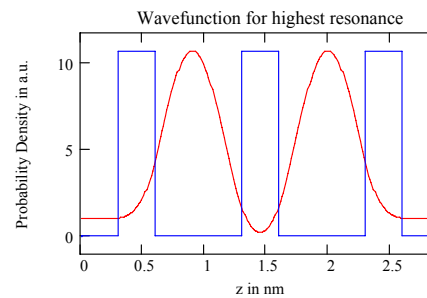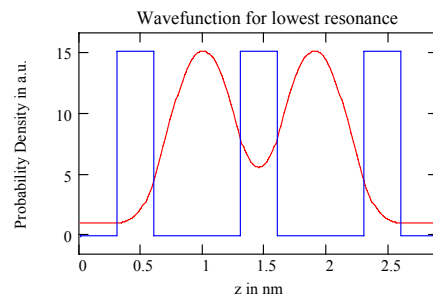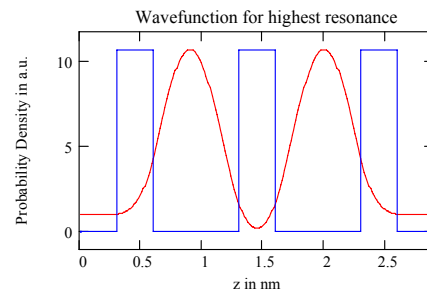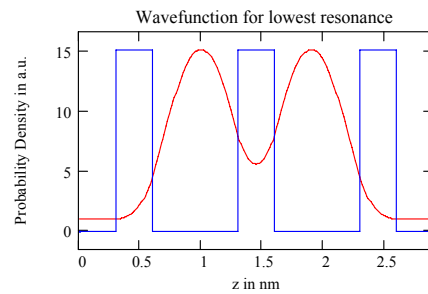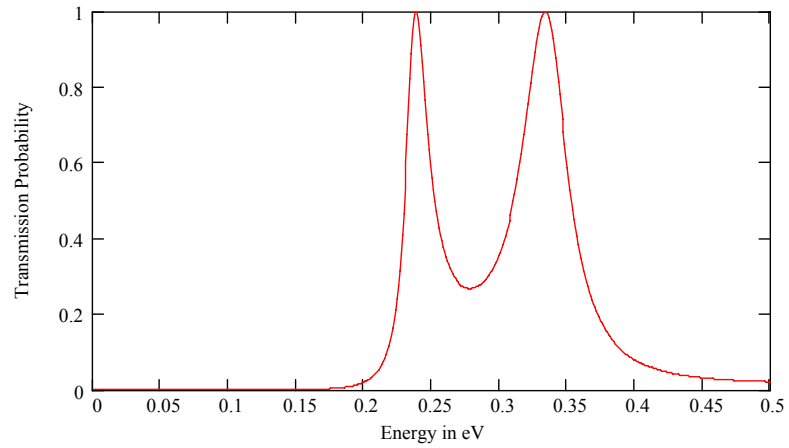
(iii) There are four resonances. The lowest one has an energy of 0.2161 eV and the highest is at 0.3762 eV.
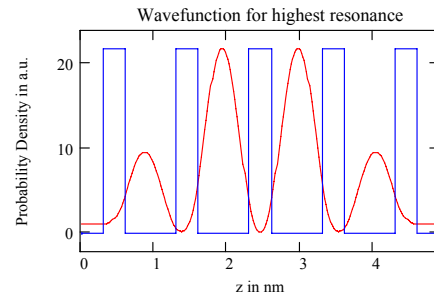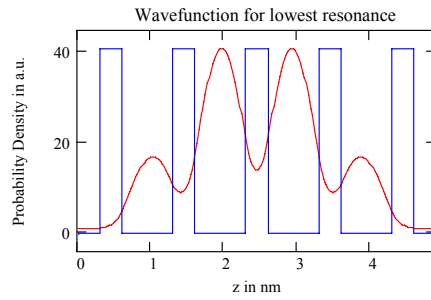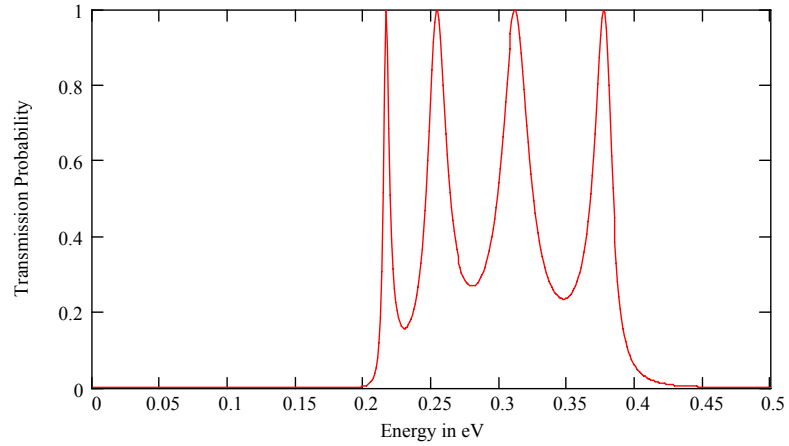
(iv) There are eight resonances. The lowest one has an energy of 0.2073 eV and the highest is at 0.3985 eV.
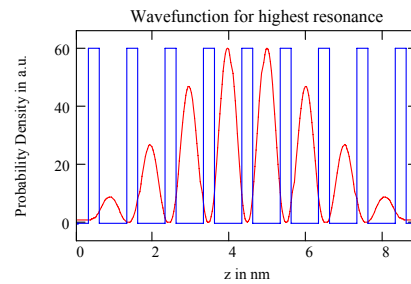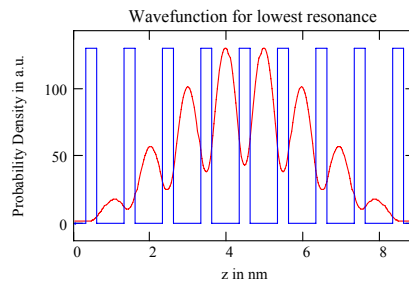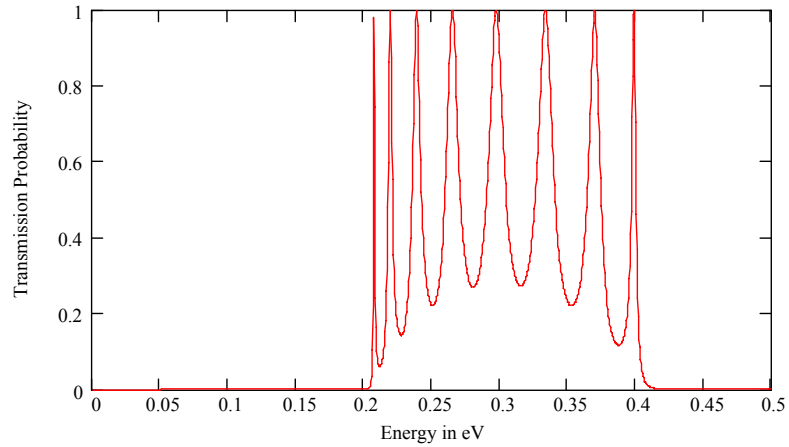
11.4.1

In the plot below, the dashed line represents the Maxwell-Boltzmann distribution, and the solid line is the approximate tunneling formula as given in the problem statement (η).
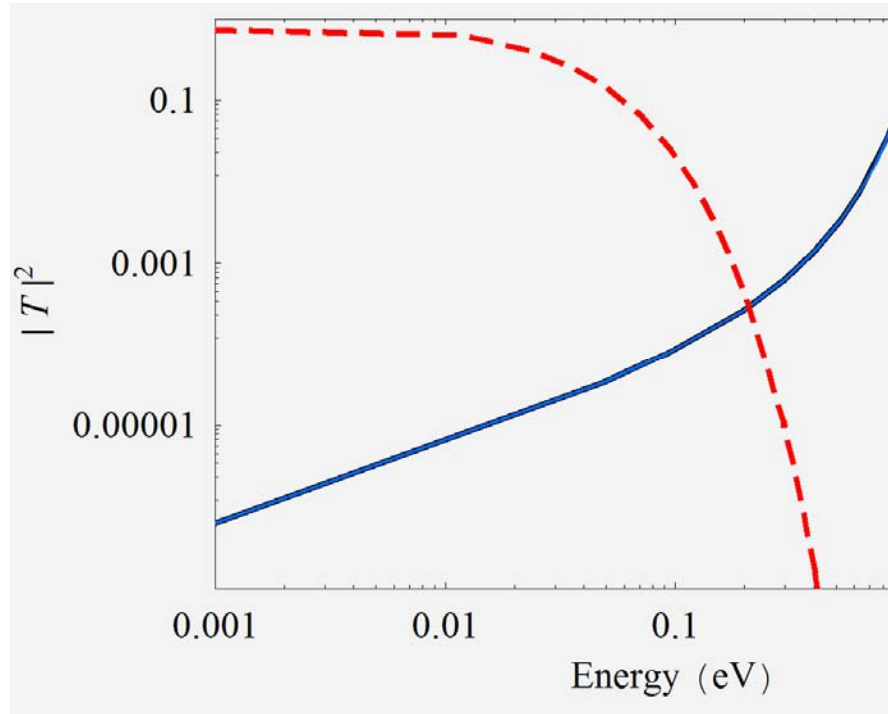
In order to calculate the tunneling current, we numerically integrate the equation

$$J = \frac{e m_f k_B T}{2\pi^2 \hbar^3} \exp\left(\frac{E_F}{k_B T}\right) \int_{E_z=0}^{\infty} \eta(E_z) \exp\left(-\frac{E_z}{k_B T}\right) dE_z$$

Note that the approximate tunneling formula is valid only for electron energies much less than the barrier potential, but it is also evident from the plot above that the Maxwell-Boltzmann probability has fallen to be extremely small even for energies well below the barrier height, so this approximate tunneling expression is expected to be valid here. Therefore, we do the numerical integration through the interval E_z from 0 to 1 eV, which gives 4.17 Amps/cm^2.

11.4.2

(i) The calculated transmission probability for an electron incident on the barrier from the left is shown in the following graph.
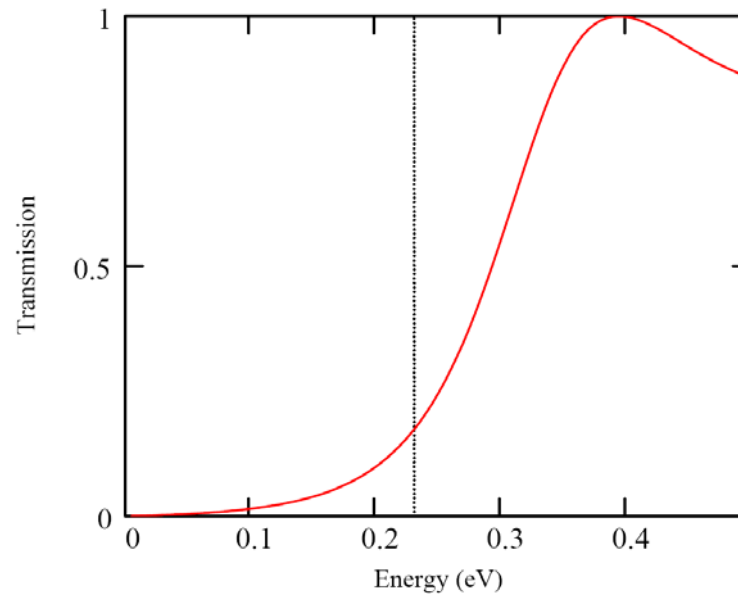
(ii) The emission current density from the classical Richardson-Dushman equation is 95.4 A/cm^2.

(iii) The current density using the quantum mechanical calculation is 1.83 kA/cm^2. Note this is significantly larger than the simple thermionic emission, and in this case this is essentially because we can get significant tunneling through the barrier below the top of the barrier

(iv) The transmission probability as a function of incident energy for this double barrier structure is as follows.
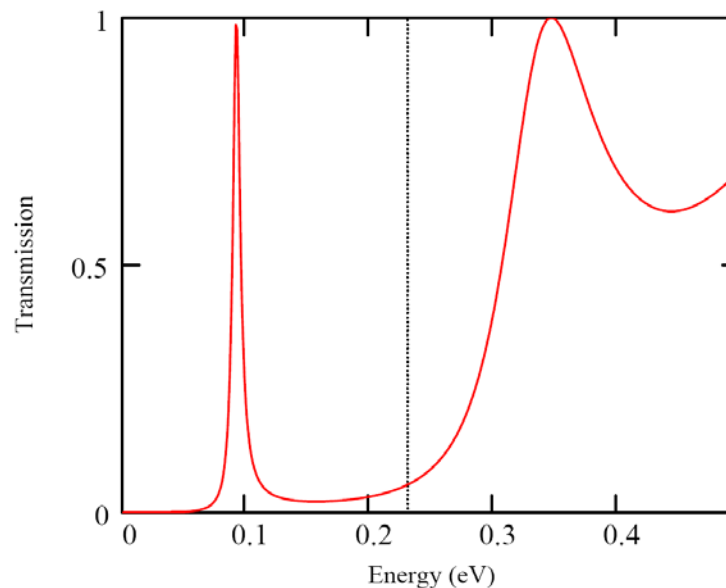
(v) The quantum mechanical calculation gives 8.66 kA/cm^2 for this double barrier structure.

See the following Mathcad worksheet for calculation details.

Problem 11.4.2 Solution Mathcad worksheet

We formally set up the transfer matrix for a structure with a series of steps of potential as shown in the figure.

For future formal mathematical use, we formally choose the origin of all matrices and vectors at an index of 1 (rather than zero).

$$\text{ORIGIN} := 1$$

Formal construction of matrices

We first define the necessary fundamental constants.

$$\text{hbar} := 1.0545887 \cdot 10^{-34} \qquad \text{mo} := 9.109534 \cdot 10^{-31} \qquad q := 1.6021892 \cdot 10^{-19} \qquad \text{kB} := 1.380662 \cdot 10^{-23}$$

From these, we can calculate the Richardson constant (in Amps per square centimeter per degree Kelvin squared).

$$\text{Ao} := 10^{-4} q \cdot \text{mo} \cdot \frac{\text{kB}^2}{\left(2 \cdot \pi^2 \text{hbar}^3\right)} \qquad\qquad \text{Ao} = 120.17265$$

For a given layer *m* of potential energy V_m, mass m_{fm}, and thickness d_m, we can define the necessary quantities required by the algebra. To allow the use of mass units of the free electron mass m_o, thickness units of nanometers, and energy units of electron volts for inputting the parameters and calculating the wavevector *k*, which may be real or imaginary, we define a units scaling parameter *s* by

$$s := \frac{2q \cdot \text{mo} \cdot 10^{-18}}{\text{hbar}^2} \qquad\qquad s = 26.24664$$

$$k(E, Vm, mfm) := \sqrt{s \cdot mfm \cdot (E - Vm)}$$

and the quantity

$$\Delta(E, Vm, mfm, Vm1, mfm1) := k(E, Vm1, mfm1) \cdot \frac{mfm}{k(E, Vm, mfm) \cdot mfm1}$$

where by mfm we mean m_{fm} and by mfm1 we mean m_{fm+1}, i.e., the quantity in the layer $m+1$, and similarly for Vm and $Vm1$.

This leads to a boundary condition matrix

$$D(E, Vm, mfm, Vm1, mfm1) := \frac{\begin{pmatrix} 1 + \Delta(E, Vm, mfm, Vm1, mfm1) & 1 - \Delta(E, Vm, mfm, Vm1, mfm1) \\ 1 - \Delta(E, Vm, mfm, Vm1, mfm1) & 1 + \Delta(E, Vm, mfm, Vm1, mfm1) \end{pmatrix}}{2}$$

relating the forward and backward amplitudes just inside the right side of layer m to those just inside the layer $m+1$, and a propagation matrix in layer m

$$P(E, Vm, mfm, dm) := \begin{pmatrix} \exp(-i \cdot k(E, Vm, mfm) \cdot dm) & 0 \\ 0 & \exp(i \cdot k(E, Vm, mfm) \cdot dm) \end{pmatrix}$$

For a given structure, we have to choose these parameters V_m, the mass will be m_{fm}, and the thickness will be d_m. We will use mass units of the free electron mass m_o, thickness units of nanometers, and energy units of electron volts for inputting the parameters.

We will also set up the parameters for the potentials and masses in AlGaAs alloys for the conduction band, as a function of x, the fraction of aluminum in the alloy (with the fraction of GaAs being 1-x).

$$VAlGaAs(x) := 0.77 \cdot x \qquad meffAlGaAs(x) := 0.067 + 0.083 \cdot x \qquad meffAlGaAs(0) = 0.067$$

Choice of parameters for structure

Now we explicitly input the values of the parameters for the material structure.

We first choose the aluminum fraction we will use for our barrier layers

$$x := 0.3$$

and hence calculate the potentials and masses that we will use in the various layers

$$VGaAs := 0 \qquad\qquad VAlGaAsx := VAlGaAs(x) \qquad VAlGaAsx = 0.231$$

$$mGaAs := meffAlGaAs(0) \qquad mAlGaAs := meffAlGaAs(x) \qquad mAlGaAs = 0.0919$$

Single barrier case

We formally choose only one layer (N=1) in the structure, excluding the entering and exiting layers from this counting.

$$N := 1$$

In setting up the thicknesses of these layers, we first set the thickness of the single barrier, d_{m2}, in nanometers

$$dm_2 := 5 \qquad\qquad dm_1 := 0 \quad dm_{N+2} := 0$$

Now we construct a vector that gives us the distance from the left of the structure (i.e., from the position of the first interface on the left) at the left of any layer of the structure.

$$dp(p) := \left(\sum_{q=1}^{p} dm_q \right) - dm_p$$

$dp(1) = 0$

$dp(2) = 0$

$dp(3) = 5$

Now we formally set up the masses and potentials in the layers

$mf_1 := mGaAs$ $\qquad Vs_1 := VGaAs$

$mf_2 := mAlGaAs$ $\qquad Vs_2 := VAlGaAsx$

$mf_3 := mGaAs$ $\qquad Vs_3 := VGaAs$

$$mf = \begin{pmatrix} 0.067 \\ 0.0919 \\ 0.067 \end{pmatrix} \qquad Vs = \begin{pmatrix} 0 \\ 0.231 \\ 0 \end{pmatrix}$$

Now we can formally construct the overall tranfer matrix by multiplying the various constituent matrices.

$$S(E) := \prod_{q=2}^{N+1} P\left(E, Vs_q, mf_q, dm_q\right) \cdot D\left(E, Vs_q, mf_q, Vs_{q+1}, mf_{q+1}\right)$$

$$T(E) := D\left(E, Vs_1, mf_1, Vs_2, mf_2\right) \cdot S(E)$$

and we can define the transmission fraction by

$$\eta(E) := 1 - \frac{\left(\left|T(E)_{2,1}\right|\right)^2}{\left(\left|T(E)_{1,1}\right|\right)^2}$$

$EE := .00, .005 .. 0.5$ $\qquad Tvbarrier_1 := 0$ $\quad Tvbarrier_2 := 1$ $\quad kkv_1 := VAlGaAsx \quad kkv_2 := VAlGaAsx$

(i) Hence we have the answer to part (i)
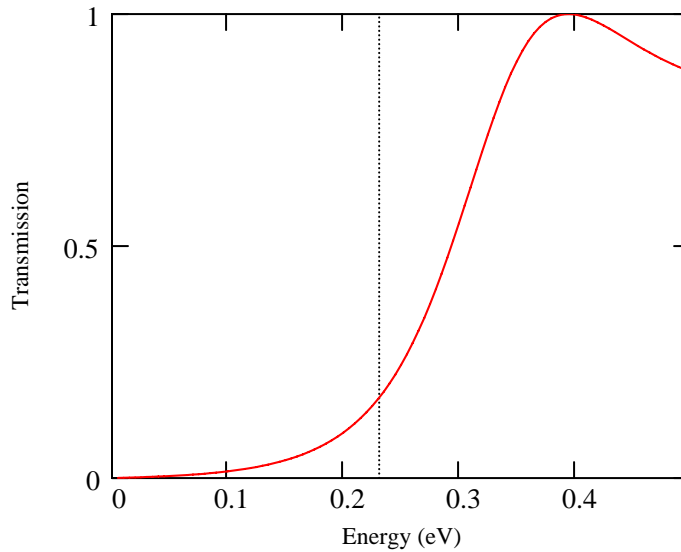
Calculation of emission current

From the approach based on a Maxwell-Boltzmann approximation for the thermal distribution of carriers involved in tunneling or thermionic emission, we have, for the emitted current density, the expression. We choose a finite upper limit for our integral since the program does not properly handle numerical integrations with infinite limits. We will discuss the validity of our particular choice below. The numerical integration becomes unstable for upper limits above 30 or so.

$$J(EF, Temp) := mGaAs \cdot Ao \cdot Temp^2 \cdot exp\left(q \cdot \frac{EF}{kB \cdot Temp}\right) \cdot \int_0^{20} \eta\left(kB \cdot Temp \cdot \frac{vint}{q}\right) exp(-vint) \, dvint$$

where E_F is the Fermi energy (in electron-Volts).

The purely thermionic result is the Richardson-Dushman equation, which, for a barrier height of EB is

$$Jtherm(EF, Temp, EB) := mGaAs \cdot Ao \cdot Temp^2 \, exp\left[\frac{q \cdot (EF - EB)}{kB \cdot Temp}\right]$$

Now we choose our Fermi energy and our temperature

$$EF := 0 \qquad Temp := 300$$

The barrier height for thermionic emission is, in electron-Volts, VAlGaAsx.

(ii) Hence the thermionic emission current would be calculated to be, using the Richardson-Dushman equation,

$$\text{Jtherm}(EF, \text{Temp}, \text{VAlGaAsx}) = 95.38934 \qquad \text{Amps per cm squared}$$

(iii) Hence the quantum mechanical calculation gives

$$J(EF, \text{Temp}) = 1.8296 \times 10^{3} \qquad \text{Amps per cm squared}$$

Note this is significantly larger than the simple thermionic emission, and in this case this is essentially because we can get significant tunneling through the barrier below the top of the barrier.

[Now let us return to the limit we have chosen in the integral above as a check. Physically, there is very little additional contribution to the current from extending the integration. beyond 20. An upper estimate of the neglected current would be the thermionic current for energies corresponding to 20 dimensionless units and above (i.e., taking the transmission to be unity), which therefore corresponds to a current

$$\text{Jtherm}\left(EF, \text{Temp}, 20 \cdot kB \cdot \frac{\text{Temp}}{q}\right) = 1.4936 \times 10^{-3} \qquad \text{Amps per cm squared}$$

Hence the current we are neglecting by our choice of upper limit in the integral is indeed negligible.]

Double barrier case

Now we have three layers

$N := 3$

We set up the thicknesses in nanometers.

$$dm_2 := 3 \qquad\qquad dm_1 := 0 \quad dm_{N+2} := 0$$

$$dm_3 := 4 \qquad\qquad dm_4 := 3$$

We can use the dp(p) function defined before for the positions of the interfaces.

Now we construct a vector that gives us the distance from the left of the structure (i.e., from the position of the first interface on the left) at the left of any layer of the structure.

Now we formally set up the masses and potentials in the layers

$$mf_1 := mGaAs \qquad\qquad Vs_1 := VGaAs$$

$$mf_2 := mAlGaAs \qquad\qquad Vs_2 := VAlGaAsx$$

$$mf_3 := mGaAs \qquad\qquad Vs_3 := VGaAs$$

$$mf_4 := mAlGaAs \qquad\qquad Vs_4 := VAlGaAsx$$

$$mf_5 := mGaAs \qquad\qquad Vs_5 := VGaAs$$

$$mf = \begin{pmatrix} 0.067 \\ 0.0919 \\ 0.067 \end{pmatrix} \qquad Vs = \begin{pmatrix} 0 \\ 0.231 \\ 0 \end{pmatrix}$$

Now we can formally construct the overall tranfer matrix by multiplying the various constituent matrices, with the new value of N.

$$S(E) := \prod_{q=2}^{N+1} P\left(E, Vs_q, mf_q, dm_q\right) \cdot D\left(E, Vs_q, mf_q, Vs_{q+1}, mf_{q+1}\right)$$

$$T(E) := D\left(E, Vs_1, mf_1, Vs_2, mf_2\right) \cdot S(E)$$

and we can define the transmission fraction by

$$\eta(E) := 1 - \frac{\left(\left|T(E)_{2,1}\right|\right)^2}{\left(\left|T(E)_{1,1}\right|\right)^2}$$

$EE := .001, .002 .. 0.495$ $Tvbarrier_1 := 0$ $Tvbarrier_2 := 1$ $kkv_1 := VAlGaAsx$ $kkv_2 := VAlGaAsx$

(iv) Hence we have the answer to part (iv)
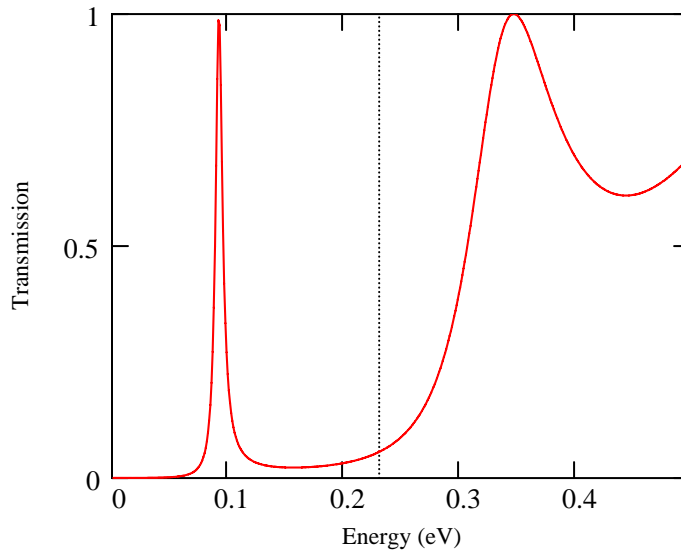
Note now we get resonant tunneling through this structure, which will lead to substantially larger total current as we will see below

Calculation of emission current

As before

$$J(EF, Temp) := mGaAs \cdot Ao \cdot Temp^2 \cdot \exp\left(q \cdot \frac{EF}{kB \cdot Temp}\right) \cdot \int_0^{20} \eta\left(kB \cdot Temp \cdot \frac{vint}{q}\right) \exp(-vint) \, dvint$$

As before, we choose the Fermi energy and temperature

EF := 0   Temp := 300

(v) Hence we have the answer to part (v)

The quantum mechanical calculation gives

$$J(EF, Temp) = 8.6628 \times 10^3 \quad \text{Amps per cm squared}$$

11.4.3

(i) The calculated thermionic emission current density based on the Richardson-Dushman equation is 95.4 A/cm^2.

(ii) The calculated emission current density using the quantum mechanical transmission coefficient at zero field is 46.3 A/cm^2. This is smaller than the result from the simple thermionic model because of quantum mechanical reflection. In particular, immediately above the barrier, where the strongest contribution to thermionic emission occurs, there is strong quantum mechanical reflection, reducing the transmission coefficient.

(iii) The quantum mechanical calculation at a field of 20 V/micron gives an emitted current density of 1.41 kA/cm^2.
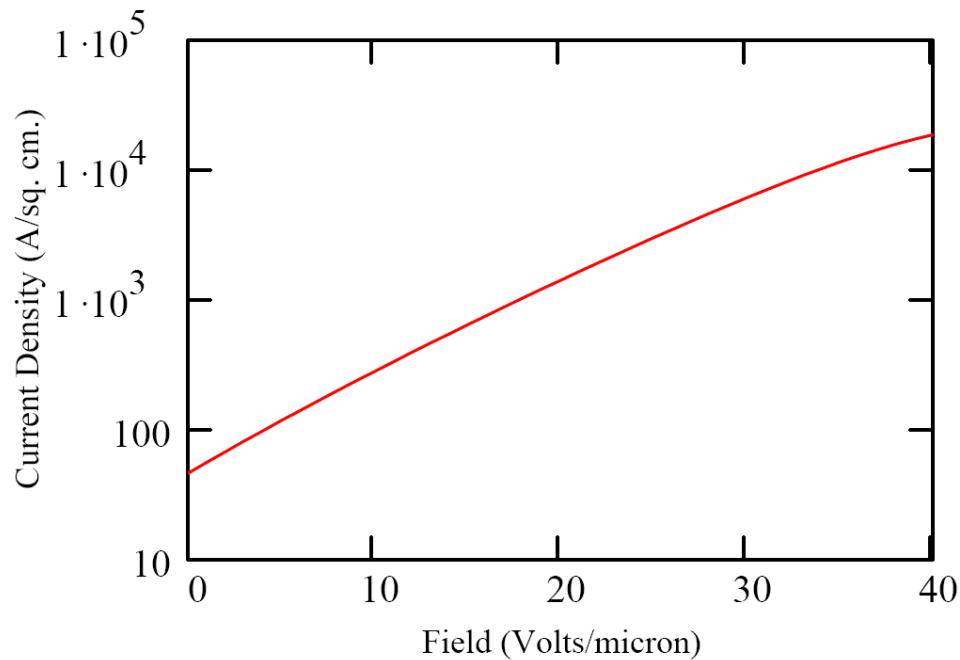
See the following Mathcad worksheet for calculation details.

Problem 11.4.3 Solution Mathcad worksheet

We formally set up the transfer matrix for a structure with a series of steps of potential as shown in the figure.

For future formal mathematical use, we formally choose the origin of all matrices and vectors at an index of 1 (rather than zero).

$$\text{ORIGIN} := 1$$

Formal construction of matrices

We first define the necessary fundamental constants.

$$\text{hbar} := 1.0545887 \cdot 10^{-34} \quad \text{mo} := 9.109534 \cdot 10^{-31} \quad q := 1.6021892 \cdot 10^{-19} \quad kB := 1.380662 \cdot 10^{-23}$$

From these, we can calculate the Richardson constant (in Amps per square centimeter per degree Kelvin squared).

$$\text{Ao} := 10^{-4} q \cdot mo \cdot \frac{kB^2}{\left(2 \cdot \pi^2 \, \text{hbar}^3\right)} \qquad \qquad \text{Ao} = 120.17265$$

For a given layer *m* of potential energy V_m, mass m_{fm}, and thickness d_m, we can define the necessary quantities required by the algebra. To allow the use of mass units of the free electron mass m_o, thickness units of nanometers, and energy units of electron volts for inputting the parameters and calculating the wavevector *k*, which may be real or imaginary, we define a units scaling parameter *s* by

$$s := \frac{2q \cdot mo \cdot 10^{-18}}{\text{hbar}^2} \qquad \qquad s = 26.24664$$

$$k(E, Vm, mfm) := \sqrt{s \cdot mfm \cdot (E - Vm)}$$

and the quantity

$$\Delta(E, Vm, mfm, Vm1, mfm1) := k(E, Vm1, mfm1) \cdot \frac{mfm}{k(E, Vm, mfm) \cdot mfm1}$$

where by mfm we mean m_{fm} and by mfm1 we mean m_{fm+1}, i.e., the quantity in the layer $m+1$, and similarly for *Vm* and *Vm1*.

This leads to a boundary condition matrix

$$D(E, Vm, mfm, Vm1, mfm1) := \frac{\begin{pmatrix} 1 + \Delta(E, Vm, mfm, Vm1, mfm1) & 1 - \Delta(E, Vm, mfm, Vm1, mfm1) \\ 1 - \Delta(E, Vm, mfm, Vm1, mfm1) & 1 + \Delta(E, Vm, mfm, Vm1, mfm1) \end{pmatrix}}{2}$$

relating the forward and backward amplitudes just inside the right side of layer m to those just inside the layer $m+1$, and a propagation matrix in layer m

$$P(E, Vm, mfm, dm) := \begin{pmatrix} \exp(-i \cdot k(E, Vm, mfm) \cdot dm) & 0 \\ 0 & \exp(i \cdot k(E, Vm, mfm) \cdot dm) \end{pmatrix}$$

For a given structure, we have to choose these parameters V_m, the mass will be m_{fm}, and the thickness will be d_m. We will use mass units of the free electron mass m_o, thickness units of nanometers, and energy units of electron volts for inputting the parameters.

We will also set up the parameters for the potentials and masses in AlGaAs alloys for the conduction band, as a function of x, the fraction of aluminum in the alloy (with the fraction of GaAs being 1-x).

$$VAlGaAs(x) := 0.77 \cdot x \qquad meffAlGaAs(x) := 0.067 + 0.083 \cdot x$$

Choice of parameters for structure

Now we explicitly input the values of the parameters for the material structure itself in the absence of any applied electric field.

We first choose the aluminum fraction we will use for our barrier layers

$$x := 0.3$$

and hence calculate the potentials and masses that we will use in the various layers

$$VGaAs := 0 \qquad\qquad VAlGaAsx := VAlGaAs(x) \qquad VAlGaAsx = 0.231$$

$$mGaAs := meffAlGaAs(0) \qquad mAlGaAs := meffAlGaAs(x) \qquad mAlGaAs = 0.0919$$

In setting up the thicknesses of these layers, we first choose the overall thickness of the barrier, d_{TOT}, in nanometers

$$dTOT := 10$$

Now we choose the number N of layers in the structure (not including the "entering" and "exiting" layers)

$$N := 11$$

Here we will choose the first and last layers within the structure (not the entering and exiting layers) to be half the thickness of all the others. This will mean that the first layer inside the structure will always have the original potential in the way that we will set up the effect of electric field, and hence will get the maximum potential barrier for the thermionic emission the same for all fields, as it should be. The thickness of all other layers within the structure will be d_{layer}. For reasons of mathematical convenience, we formally choose the thicknesses of the entering and exiting layers as zero, and we also define the thickness of a ficticious layer N+3 to be zero to keep a subsequent formula simple.

$$\text{dlayer} := \frac{\text{dTOT}}{N-1}$$

$$\text{dm}_2 := \frac{\text{dlayer}}{2} \qquad \text{dm}_{N+1} := \frac{\text{dlayer}}{2} \qquad \text{dm}_1 := 0 \quad \text{dm}_{N+2} := 0 \quad \text{dm}_{N+3} := 0$$

$$\text{jjj} := 3 .. N$$

$$\text{dm}_{jjj} := \text{dlayer}$$

$$\text{dm} =$$

	1
1	0
2	0.5
3	1
4	1
5	1
6	1
7	1
8	1
9	1
10	1
11	1
12	0.5
13	0
14	0

Now we construct a vector that gives us the distance from the left of the structure (i.e., from the position of the first interface on the left) at the left of any layer of the structure.

$$\text{dp}(p) := \left(\sum_{q=1}^{p} \text{dm}_q \right) - \text{dm}_p \qquad \text{dp}(1) = 0 \qquad \text{lll} := 1 .. N + 2 \qquad \text{dp}(\text{lll}) =$$

0
0
0.5
1.5
2.5
3.5
4.5
5.5
6.5
7.5
8.5
9.5
10

Now we formally set up the masses in the layers

$mf_1 := mGaAs$ $Vs_1 := VGaAs$

$kkk := 2 .. N + 1$

$mf_{kkk} := mAlGaAs$ $Vs_{kkk} := VAlGaAsx$

$mf_{N+2} := mGaAs$ $Vs_{N+2} := VGaAs$

$mf =$

	1
1	0.067
2	0.0919
3	0.0919
4	0.0919
5	0.0919
6	0.0919
7	0.0919
8	0.0919
9	0.0919
10	0.0919
11	0.0919
12	0.0919
13	0.067

$Vs =$

	1
1	0
2	0.231
3	0.231
4	0.231
5	0.231
6	0.231
7	0.231
8	0.231
9	0.231
10	0.231
11	0.231
12	0.231
13	0

Now we allow for an electric field, *F*, to be applied to the layers in the structure. This field will mean that the potential in a given layer *p* will be chosen to be the potential corresponding to the structure's potential in the absence of field, plus the potential energy *-Fd(p),* where d(p) is the distance to the middle of a layer (except for the first and last half-thickness layers), where we are measuring potential energy in electron volts, and the field is in Volts per nanometer. We are presuming that positive field here reduces the potential to the "right" in the structure.

$$Vm(F, mmm) := Vs_{mmm} - F \cdot \frac{\left(dp(mmm) + dp\left(mmm + 1\right)\right)}{2}$$

Now we can formally construct the overall tranfer matrix by multiplying the various constituent matrices.

$$S(E, F) := \prod_{q = 2}^{N+1} P\left(E, Vm(F, q), mf_q, dm_q\right) \cdot D\left(E, Vm(F, q), mf_q, Vm\left(F, q + 1\right), mf_{q+1}\right)$$

$$T(E, F) := D\left(E, Vm\left(F, 1\right), mf_1, Vm\left(F, 2\right), mf_2\right) \cdot S(E, F)$$

and we can define the transmission fraction by

$$\eta(E, F) := 1 - \frac{\left(\left|T(E, F)_{2, 1}\right|\right)^2}{\left(\left|T(E, F)_{1, 1}\right|\right)^2}$$

$EE := .0049, .0109 .. 0.495$ $Tvbarrier_1 := 0$ $Tvbarrier_2 := 1$ $kkv_1 := VAlGaAsx$ $kkv_2 := VAlGaAsx$
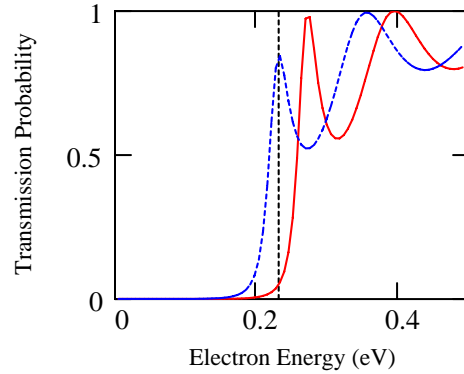
Calculation of emission current

From the approach based on a Maxwell-Boltzmann approximation for the thermal distribution of carriers involved in tunneling or thermionic emission, we have, for the emitted current density, the expression. We choose a finite upper limit for our integral since the program does not properly handle numerical integrations with infinite limits. We will discuss the validity of our particular choice below. The numerical integration becomes unstable for upper limits above 30 or so.

$$J(EF, Temp, F) := mGaAs \cdot Ao \cdot Temp^2 \cdot exp\left(q \cdot \frac{EF}{kB \cdot Temp}\right) \cdot \int_0^{20} \eta\left(kB \cdot Temp \cdot \frac{vint}{q}, F\right) exp(-vint) \, dvint$$

where E_F is the Fermi energy (in electron-Volts).

The purely thermionic result is the Richardson-Dushman equation, which, for a barrier height of EB is

$$Jtherm(EF, Temp, EB) := mGaAs \cdot Ao \cdot Temp^2 \, exp\left[\frac{q \cdot (EF - EB)}{kB \cdot Temp}\right]$$

Now we choose our Fermi energy and our temperature

$$EF := 0 \qquad Temp := 300 \qquad F := 0$$

The barrier height for thermionic emission is, in electron-Volts, VAlGaAsx. Hence the thermionic emission current would be calculated to be, using the Richardson-Dushman equation,

$$Jtherm(EF, Temp, VAlGaAsx) = 95.38934$$

The quantum mechanical calculation at zero field gives

$$J(EF, Temp, F) = 46.30539$$

which is somewhat smaller than the simple thermionic model because the transmission coefficient is always less than or equal to unity above the barrier because of quantum mechanical reflection. In particular, immediately above the barrier, where the strongest contribution to thermionic emission occurs, there is strong quantum mechanical reflection, reducing the transmission

coefficient.

The quantum mechanical calculation at a field of 20 V/micron gives

$$J(EF, Temp, 0.02) = 1.41455 \times 10^3$$

Now let us return to the limit we have chosen in the integral above. Physically, there is very little additional contribution to the current from extending the integration. beyond 20. An upper estimate of the neglected current would be the thermionic current for energies corresponding to 20 dimensionless units and above (i.e., taking the transmission to be unity), which therefore corresponds to a current

$$Jtherm\left(EF, Temp, 20 \cdot kB \cdot \frac{Temp}{q}\right) = 1.4936 \times 10^{-3}$$

Hence the current we are neglecting by our choice of upper limit in the integral is indeed negligible.

Now we can plot the emitted current density as a function of field.

$$Field := 0, 1 .. 40$$
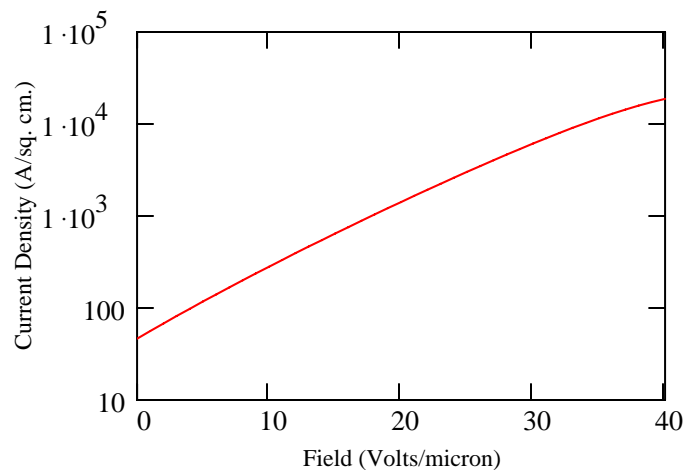
Chapter 12 problem solutions

12.4.1

For $|s\rangle = \cos(\theta/2)|\uparrow\rangle + \exp(i\phi)\sin(\theta/2)|\downarrow\rangle$

$$\langle s|\hat{\sigma}_x|s\rangle = \begin{bmatrix} \cos(\theta/2) & \exp(-i\phi)\sin(\theta/2) \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \cos(\theta/2) \\ \exp(i\phi)\sin(\theta/2) \end{bmatrix}$$

$$= \begin{bmatrix} \cos(\theta/2) & \exp(-i\phi)\sin(\theta/2) \end{bmatrix} \begin{bmatrix} \exp(i\phi)\sin(\theta/2) \\ \cos(\theta/2) \end{bmatrix}$$

$$= \cos(\theta/2)\sin(\theta/2)\{\exp(i\phi) + \exp(-i\phi)\}$$

$$= \frac{1}{2}\sin\theta \, 2\cos\phi$$

$$= \sin\theta\cos\phi$$

$$\langle s|\hat{\sigma}_y|s\rangle = \begin{bmatrix} \cos(\theta/2) & \exp(-i\phi)\sin(\theta/2) \end{bmatrix} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \begin{bmatrix} \cos(\theta/2) \\ \exp(i\phi)\sin(\theta/2) \end{bmatrix}$$

$$= \begin{bmatrix} \cos(\theta/2) & \exp(-i\phi)\sin(\theta/2) \end{bmatrix} \begin{bmatrix} -i\exp(i\phi)\sin(\theta/2) \\ i\cos(\theta/2) \end{bmatrix}$$

$$= i\cos(\theta/2)\sin(\theta/2)\{\exp(-i\phi) - \exp(i\phi)\}$$

$$= \frac{-i}{2}\sin\theta \, 2i\sin\phi = \sin\theta\sin\phi$$

$$\langle s|\hat{\sigma}_z|s\rangle = \begin{bmatrix} \cos(\theta/2) & \exp(-i\phi)\sin(\theta/2) \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} \cos(\theta/2) \\ \exp(i\phi)\sin(\theta/2) \end{bmatrix}$$

$$= \begin{bmatrix} \cos(\theta/2) & \exp(-i\phi)\sin(\theta/2) \end{bmatrix} \begin{bmatrix} \cos(\theta/2) \\ -\exp(i\phi)\sin(\theta/2) \end{bmatrix}$$

$$= \cos^2(\theta/2) - \sin^2(\theta/2)$$

$$= \cos\theta$$

Hence

$$\mathbf{P}_s = \langle s|\hat{\boldsymbol{\sigma}}|s\rangle = \mathbf{i}\sin\theta\cos\phi + \mathbf{j}\sin\theta\sin\phi + \mathbf{k}\cos\theta$$

12.4.2

We have

$$|s\rangle = \frac{1}{\sqrt{2}}|\uparrow\rangle + \frac{i}{\sqrt{2}}|\downarrow\rangle$$

and

$$\hat{\mu}_e = g\mu_B\hat{\sigma}$$

so

$$\langle\mu_e\rangle = g\mu_B\langle s|\hat{\sigma}|s\rangle$$

$$= \frac{1}{2}g\mu_B\left(\langle\uparrow| - i\langle\downarrow|\right)\hat{\sigma}\left(\langle\uparrow| + i\langle\uparrow|\right)$$

$$= \frac{1}{2}g\mu_B\left([1 \quad 0] - i[0 \quad 1]\right)\hat{\sigma}\left(\begin{bmatrix}1\\0\end{bmatrix} + i\begin{bmatrix}0\\1\end{bmatrix}\right)$$

$$= \frac{1}{2}g\mu_B[1 \quad -i]\left(\mathbf{i}\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}\right) + \mathbf{j}\begin{bmatrix}0 & -i\\i & 0\end{bmatrix} + \mathbf{k}\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}\begin{bmatrix}1\\i\end{bmatrix}$$

$$= \frac{1}{2}g\mu_B\left(\mathbf{i}[1 \quad -i]\begin{bmatrix}i\\1\end{bmatrix} + \mathbf{j}[1 \quad -i]\begin{bmatrix}1\\i\end{bmatrix} + \mathbf{k}[1 \quad -i]\begin{bmatrix}1\\-i\end{bmatrix}\right)$$

$$= \frac{1}{2}g\mu_B\left(0\mathbf{i} + 2\mathbf{j} + 0\mathbf{k}\right)$$

$$= g\mu_B\,\mathbf{j}$$

In other words, the magnetic moment has magnitude $g\mu_B$ and is pointing in the y direction.

12.4.3

$$\sigma_z \left| s \right\rangle = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} \cos\dfrac{\theta}{2} \\ \exp(i\phi)\sin\dfrac{\theta}{2} \end{bmatrix} = \begin{bmatrix} \cos\dfrac{\theta}{2} \\ -\exp(i\phi)\sin\dfrac{\theta}{2} \end{bmatrix}$$

$$= \begin{bmatrix} \cos\dfrac{\theta}{2} \\ \exp(i[\phi+\pi])\sin\dfrac{\theta}{2} \end{bmatrix}$$

Hence the effect of operating with the σ_z Pauli matrix on a general spin state is to rotate the spin by π radians (180 degrees) about the z axis on the Bloch sphere.

Chapter 13 problem solutions

13.1.1

Given that

$$\psi_{abefore}(\mathbf{r}_1)\psi_{bbefore}(\mathbf{r}_2) \rightarrow s_{straight}\psi_{aafter}(\mathbf{r}_1)\psi_{bafter}(\mathbf{r}_2) + s_{swap}\psi_{bafter}(\mathbf{r}_1)\psi_{aafter}(\mathbf{r}_2)$$

then

$$\psi_{abefore}(\mathbf{r}_1)\psi_{bbefore}(\mathbf{r}_2) \pm \psi_{abefore}(\mathbf{r}_2)\psi_{bbefore}(\mathbf{r}_1) \rightarrow$$
$$s_{straight}\left[\psi_{aafter}(\mathbf{r}_1)\psi_{bafter}(\mathbf{r}_2) \pm \psi_{aafter}(\mathbf{r}_2)\psi_{bafter}(\mathbf{r}_1)\right]$$
$$+s_{swap}\left[\psi_{bafter}(\mathbf{r}_1)\psi_{aafter}(\mathbf{r}_2) \pm \psi_{bafter}(\mathbf{r}_2)\psi_{aafter}(\mathbf{r}_1)\right]$$
$$= \psi_{aafter}(\mathbf{r}_1)\psi_{bafter}(\mathbf{r}_2)\left[s_{straight} \pm s_{swap}\right] + \psi_{bafter}(\mathbf{r}_1)\psi_{aafter}(\mathbf{r}_2)\left[s_{swap} \pm s_{straight}\right]$$

Now

$$\left[s_{swap} \pm s_{straight}\right] = \pm\left[s_{straight} \pm s_{swap}\right]$$

Hence

$$\psi_{abefore}(\mathbf{r}_1)\psi_{bbefore}(\mathbf{r}_2) \pm \psi_{abefore}(\mathbf{r}_2)\psi_{bbefore}(\mathbf{r}_1) \rightarrow$$
$$\left[s_{straight} \pm s_{swap}\right]\left[\psi_{aafter}(\mathbf{r}_1)\psi_{bafter}(\mathbf{r}_2) \pm \psi_{bafter}(\mathbf{r}_1)\psi_{aafter}(\mathbf{r}_2)\right]$$

So, the effect of this scattering is to leave the resulting wavefunction still in the right form required for identical particles. Note that this is true for both fermions and bosons, and holds regardless of the relative magnitudes of $s_{straight}$ and s_{swap}.

13.4.1

The approach here is exactly the same as taken for the case of two electrons, except we have to symmetrize the wavefunctions using the fermion form rather than the boson form. Hence the symmetrized wavefunction is

$$\psi_{tp}\left(\mathbf{r}_1,\mathbf{r}_2\right)=\frac{1}{\sqrt{2}}\left[\psi_a\left(\mathbf{r}_1\right)\psi_b\left(\mathbf{r}_2\right)+\psi_a\left(\mathbf{r}_2\right)\psi_b\left(\mathbf{r}_1\right)\right]$$

or in bra-ket form

$$\left|\psi_{tp}\right\rangle=\frac{1}{\sqrt{2}}\left(\left|1,a\right\rangle\left|2,b\right\rangle+\left|2,a\right\rangle\left|1,b\right\rangle\right)$$

Then

$$\left\langle E\right\rangle=\frac{1}{2}\left[\begin{array}{l}\left\langle 1,a\right|\left\langle 2,b\right|\hat{H}\left|1,a\right\rangle\left|2,b\right\rangle+\left\langle 2,a\right|\left\langle 1,b\right|\hat{H}\left|2,a\right\rangle\left|1,b\right\rangle\\+\left\langle 1,a\right|\left\langle 2,b\right|\hat{H}\left|2,a\right\rangle\left|1,b\right\rangle+\left\langle 2,a\right|\left\langle 1,b\right|\hat{H}\left|1,a\right\rangle\left|2,b\right\rangle\end{array}\right]$$

Hence the exchange energy, which is the sum of the last two terms, is

$$E_{EXab}=\frac{1}{2}\left(\left\langle 1,a\right|\left\langle 2,b\right|\hat{H}\left|2,a\right\rangle\left|1,b\right\rangle+\left[\left\langle 1,a\right|\left\langle 2,b\right|\hat{H}\left|2,a\right\rangle\left|1,b\right\rangle\right]^*\right)$$

$$=\text{Re}\left[\int\psi_a^*\left(\mathbf{r}_1\right)\psi_b^*\left(\mathbf{r}_2\right)\hat{H}\psi_a\left(\mathbf{r}_2\right)\psi_b\left(\mathbf{r}_1\right)d^3\mathbf{r}_1 d^3\mathbf{r}_2\right]$$

Note that the sign of this energy has now changed compared to the fermion case, but the energy is in general non-zero, and is therefore an example of exchange energy for interacting bosons.

13.4.2

(i)

$$E_T = R_{LT}E_L + T_{BT}E_B \ \text{ and } \ E_R = T_{LR}E_L + R_{BR}E_B$$

so

$$\left|E_T\right|^2 = \left|R_{LT}\right|^2\left|E_L\right|^2 + \left|T_{BT}\right|^2\left|E_B\right|^2 + R_{LT}T_{BT}^*E_LE_B^* + R_{LT}^*T_{BT}E_L^*E_B$$

and

$$\left|E_R\right|^2 = \left|T_{LR}\right|^2\left|E_L\right|^2 + \left|R_{BR}\right|^2\left|E_B\right|^2 + T_{LR}R_{BR}^*E_LE_B^* + T_{LR}^*R_{BR}E_L^*E_B$$

so the total output power is

$$\left|E_T\right|^2 + \left|E_R\right|^2 = \left(\left|R_{LT}\right|^2\left|T_{LR}\right|^2\right)\left|E_L\right|^2 + \left(\left|R_{BR}\right|^2 + \left|T_{BT}\right|^2\right)\left|E_B\right|^2 + \left(R_{LT}T_{BT}^* + R_{BR}^*T_{LR}\right)E_LE_B^* + c.c.$$

By conservation of power in this lossless beamsplitter, we have

$$\left|E_T\right|^2 + \left|E_R\right|^2 = \left|E_L\right|^2 + \left|E_B\right|^2$$

so

$$\left|E_L\right|^2 + \left|E_B\right|^2 = \left(\left|R_{LT}\right|^2\left|T_{LR}\right|^2\right)\left|E_L\right|^2 + \left(\left|R_{BR}\right|^2 + \left|T_{BT}\right|^2\right)\left|E_B\right|^2 + 2\operatorname{Re}\left\{\left(R_{LT}T_{BT}^* + R_{BR}^*T_{LR}\right)E_LE_B^*\right\} \qquad \text{(A)}$$

This relation (A) must hold for arbitrary E_L and E_B. Suppose then we hold the magnitudes of E_L and E_B constant, and vary only their relative phase. Then necessarily we will vary the phase of the term $\left(R_{LT}T_{BT}^* + R_{BR}^*T_{LR}\right)E_LE_B^*$ and so we will vary the real part of this term. But, all the other terms in (A) remain unchanged, and so the only way the Eq. (A) can remain satisfied for arbitrary relative phase of E_L and E_B is if

$$R_{LT}T_{BT}^* + R_{BR}^*T_{LR} = 0 \qquad \text{(B)}$$

which is our first condition for a lossless beamsplitter. With this condition, Eq. (A) becomes

$$\left|E_L\right|^2 + \left|E_B\right|^2 = \left(\left|R_{LT}\right|^2 + \left|T_{LR}\right|^2\right)\left|E_L\right|^2 + \left(\left|R_{BR}\right|^2 + \left|T_{BT}\right|^2\right)\left|E_B\right|^2 \qquad \text{(C)}$$

Now this relation (C) must hold for arbitrary $\left|E_L\right|^2$ and arbitrary $\left|E_B\right|^2$. In particular, it must hold for $\left|E_B\right|^2 = 0$, in which case we can deduce that

$$\left|R_{LT}\right|^2 + \left|T_{LR}\right|^2 = 1$$

and similarly considering the case of $\left|E_L\right|^2 = 0$

$$\left|R_{BR}\right|^2 + \left|T_{BT}\right|^2 = 1$$

13.4.3

(i) The appropriate symmetrized state is

$$|\psi_{in}\rangle = \frac{1}{\sqrt{2}}\left(|1,L\rangle|2,B\rangle + |1,B\rangle|2,L\rangle\right)$$

(ii)

$$|\psi_{out}\rangle = \left(\frac{1}{\sqrt{2}}\right)^3 \left[\left(i|1,T\rangle + |1,R\rangle\right)\left(|2,T\rangle + i|2,R\rangle\right)\right.$$
$$\left. + \left(|1,T\rangle + i|1,R\rangle\right)\left(i|2,T\rangle + |2,R\rangle\right)\right]$$
$$= \left(\frac{1}{\sqrt{2}}\right)^3 \left[i|1,T\rangle|2,T\rangle + |1,R\rangle|2,T\rangle + i|1,R\rangle|2,R\rangle - |1,T\rangle|2,R\rangle\right.$$
$$\left. + i|1,T\rangle|2,T\rangle - |1,R\rangle|2,T\rangle + i|1,R\rangle|2,R\rangle + |1,T\rangle|2,R\rangle\right]$$
$$= \frac{i}{\sqrt{2}}\left[|1,T\rangle|2,T\rangle + |1,R\rangle|2,R\rangle\right]$$

(iii) Finding one photon in the "top" mode means we have collapsed the state into one $\propto |1,T\rangle|2,T\rangle$, so we will find the other photon in the same "top" mode.

(iv) We always find both photons in the same output mode. (Finding one photon in the "right" mode will have collapsed the state to one $\propto |1,R\rangle|2,R\rangle$.) This is a remarkable, and completely quantum mechanical, property of the beam splitter for bosons. (It is also a general property of the 50:50 beamsplitter; any appropriate 50:50 beamsplitter matrix will give the same result of finding both photons in the same mode).

13.4.4

(i) The appropriately symmetrized input state will be

$$|\psi_{in}\rangle = \frac{1}{\sqrt{2}}\left(|1,L\rangle|2,B\rangle - |1,B\rangle|2,L\rangle\right)$$

(or minus this). The transformation rules remain the same as in the boson beamsplitter problem because the beamsplitter matrix is the same, that is, the effect of the beamsplitter on a given single particle incident state is the pair of transformations

$$|1,L\rangle \rightarrow \frac{1}{\sqrt{2}}\left(i|1,T\rangle + |1,R\rangle\right)$$

$$|1,B\rangle \rightarrow \frac{1}{\sqrt{2}}\left(|1,T\rangle + i|1,R\rangle\right)$$

so we have

$$|\psi_{out}\rangle = \left(\frac{1}{\sqrt{2}}\right)^3 \left[\left(i|1,T\rangle + |1,R\rangle\right)\left(|2,T\rangle + i|2,R\rangle\right) - \left(|1,T\rangle + i|1,R\rangle\right)\left(i|2,T\rangle + i|2,R\rangle\right)\right]$$

$$= \frac{1}{\sqrt{2}}\left[|1,R\rangle|2,T\rangle - |1,T\rangle|2,R\rangle\right]$$

(ii) The two electrons will always be found in different modes (single particle states). That is, if we measure the system and find an electron at the right port, we will always also find an electron on the top port; collapsing into either the first or second term in the above equation gives the same result in the measurement. (We know anyway that we cannot have two fermions in the same single particle states, and we see here that the action of the beamsplitter ensures this – the two input fermions always go into different output states.)

13.6.1

(i) For identical bosons, there is only one state

$$|1,a\rangle|2,b\rangle|3,c\rangle+|2,a\rangle|1,b\rangle|3,c\rangle+|1,a\rangle|3,b\rangle|2,c\rangle$$
$$+|2,a\rangle|3,b\rangle|1,c\rangle+|3,a\rangle|1,b\rangle|2,c\rangle+|3,a\rangle|2,b\rangle|1,c\rangle$$

(ii) For identical fermions, there is only one state

$$|1,a\rangle|2,b\rangle|3,c\rangle-|2,a\rangle|1,b\rangle|3,c\rangle-|1,a\rangle|3,b\rangle|2,c\rangle$$
$$+|2,a\rangle|3,b\rangle|1,c\rangle+|3,a\rangle|1,b\rangle|2,c\rangle-|3,a\rangle|2,b\rangle|1,c\rangle$$

(iii) For non-identical particles, there are six states

$$|1,a\rangle|2,b\rangle|3,c\rangle,\ |2,a\rangle|1,b\rangle|3,c\rangle,\ |1,a\rangle|3,b\rangle|2,c\rangle,$$
$$|2,a\rangle|3,b\rangle|1,c\rangle,\ |3,a\rangle|1,b\rangle|2,c\rangle,\ |3,a\rangle|2,b\rangle|1,c\rangle$$

Chapter 14 problem solutions

14.1.1

(i) Consider the pure spin state

$$|s_p\rangle = \frac{1}{\sqrt{3}}\left(|s_x\rangle + |s_y\rangle\right)$$

On the Bloch sphere, the state $|s_x\rangle$ has $\theta = \pi/2$ and $\phi = 0$, and the state $|s_y\rangle$ has $\theta = \pi/2$ and $\phi = \pi/2$, from which we can deduce, using the expression

$$|s\rangle = \cos\frac{\theta}{2}|\uparrow\rangle + \exp(i\phi)\sin\frac{\theta}{2}|\downarrow\rangle$$

that

$$|s_x\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle + |\downarrow\rangle\right) \quad \text{and} \quad |s_y\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle + i|\downarrow\rangle\right)$$

so

$$|s_p\rangle = \frac{1}{\sqrt{3}}\left[\frac{1}{\sqrt{2}}\left(|\uparrow\rangle + |\downarrow\rangle\right) + \frac{1}{\sqrt{2}}\left(|\uparrow\rangle + i|\downarrow\rangle\right)\right]$$

$$= \frac{1}{\sqrt{6}}\left(2|\uparrow\rangle + (1+i)|\downarrow\rangle\right)$$

(a)

$$\langle s_p|s_p\rangle = \frac{1}{6}\left[4 + (1+i)(1-i)\right] = 1$$

so the proposed pure state is normalized.

(b) Given that $\hat{\boldsymbol{\mu}}_e = g\mu_B\hat{\boldsymbol{\sigma}}$, we have

$$\langle\boldsymbol{\mu}_e\rangle = g\mu_B\langle s_p|\hat{\boldsymbol{\sigma}}|s_p\rangle = \frac{g\mu_B}{6}\begin{bmatrix}2 & 1-i\end{bmatrix}\hat{\boldsymbol{\sigma}}\begin{bmatrix}2 \\ 1+i\end{bmatrix}$$

$$= \frac{g\mu_B}{6}\begin{bmatrix}2 & 1-i\end{bmatrix}\left(\mathbf{i}\begin{bmatrix}0 & 1 \\ 1 & 0\end{bmatrix} + \mathbf{j}\begin{bmatrix}0 & -i \\ i & 0\end{bmatrix} + \mathbf{k}\begin{bmatrix}1 & 0 \\ 0 & -1\end{bmatrix}\right)\begin{bmatrix}2 \\ 1+i\end{bmatrix}$$

$$= \frac{g\mu_B}{6}\left(\mathbf{i}\begin{bmatrix}2 & 1-i\end{bmatrix}\begin{bmatrix}1+i \\ 2\end{bmatrix} + \mathbf{j}\begin{bmatrix}2 & 1-i\end{bmatrix}\begin{bmatrix}1-i \\ 2i\end{bmatrix} + \mathbf{k}\begin{bmatrix}2 & 1-i\end{bmatrix}\begin{bmatrix}2 \\ -1-i\end{bmatrix}\right)$$

$$= \frac{g\mu_B}{6}\left\{\mathbf{i}(2+2i+2-2i) + \mathbf{j}(2-2i+2i+2) + \mathbf{k}(4-(1-i)(1+i))\right\}$$

$$= \frac{g\mu_B}{6}\left\{4\mathbf{i} + 4\mathbf{j} + 2\mathbf{k}\right\} = \frac{g\mu_B}{3}\left\{2\mathbf{i} + 2\mathbf{j} + \mathbf{k}\right\}$$

(c) The magnitude of this magnetic moment is the length of the vector, which is

$$\left|\mathbf{\mu}_e\right| = g\mu_B\sqrt{\frac{1}{9}\left(4+4+1\right)}$$

$$= g\mu_B$$

(ii) Consider now the mixed spin state, with equal probabilities of electrons being in the x spin state $\left|s_x\right\rangle$ and y spin state $\left|s_y\right\rangle$, i.e., $P_x = 0.5$, $P_y = 0.5$.

(a) The resulting ensemble average expectation value is

$$\left\langle\mathbf{\mu}_e\right\rangle = g\mu_B\left[0.5\left\langle s_x\left|\hat{\boldsymbol{\sigma}}\right|s_x\right\rangle + 0.5\left\langle s_y\left|\hat{\boldsymbol{\sigma}}\right|s_y\right\rangle\right]$$

$$= \frac{g\mu_B}{4}\left(\begin{bmatrix}1 & 1\end{bmatrix}\hat{\boldsymbol{\sigma}}\begin{bmatrix}1\\1\end{bmatrix} + \begin{bmatrix}1 & -i\end{bmatrix}\hat{\boldsymbol{\sigma}}\begin{bmatrix}1\\i\end{bmatrix}\right)$$

$$= \frac{g\mu_B}{4}\left(\begin{bmatrix}1 & 1\end{bmatrix}\left\{\mathbf{i}\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix} + \mathbf{j}\begin{bmatrix}0 & -i\\i & 0\end{bmatrix} + \mathbf{k}\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}\right\}\begin{bmatrix}1\\1\end{bmatrix}\right.$$

$$\left. + \begin{bmatrix}1 & -i\end{bmatrix}\left\{\mathbf{i}\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix} + \mathbf{j}\begin{bmatrix}0 & -i\\i & 0\end{bmatrix} + \mathbf{k}\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}\right\}\begin{bmatrix}1\\i\end{bmatrix}\right)$$

$$= \frac{g\mu_B}{4}\left(2\mathbf{i} + 0\mathbf{j} + 0\mathbf{k} + 0\mathbf{i} + 2\mathbf{j} + 0\mathbf{k}\right)$$

$$= \frac{g\mu_B}{2}\left(\mathbf{i} + \mathbf{j}\right)$$

(b) The magnitude of this ensemble average magnetic moment is the length of the vector, which is

$$\left|\left\langle\mathbf{\mu}_e\right\rangle\right| = \frac{g\mu_B}{2}\sqrt{1^2 + 1^2} = \frac{g\mu_B}{\sqrt{2}}$$

(iii) The mixed state and the pure state have different directions of the magnetic moment. Specifically, the pure state has a component in the z-direction, and they have different magnitudes, with the mixed state giving an average value smaller by a factor of $1/\sqrt{2}$.

14.3.1

We have the linear polarization state

$$|\psi_1\rangle = |\psi_H\rangle$$

and the elliptical polarization state

$$|\psi_2\rangle = \frac{3}{5}|\psi_H\rangle + \frac{4i}{5}|\psi_V\rangle$$

with probabilities $P_1 = 0.2, P_2 = 0.8$. Hence, the density operator is, explicitly, in terms of $|\psi_H\rangle$ and $|\psi_V\rangle$

$$\begin{aligned}
\rho &= P_1|\psi_1\rangle\langle\psi_1| + P_2|\psi_2\rangle\langle\psi_2| \\
&= P_1|\psi_H\rangle\langle\psi_H| + P_2\left(\frac{3}{5}|\psi_H\rangle + \frac{4i}{5}|\psi_V\rangle\right)\left(\frac{3}{5}\langle\psi_H| - \frac{4i}{5}\langle\psi_V|\right) \\
&= P_1|\psi_H\rangle\langle\psi_H| + P_2\left(\frac{9}{25}|\psi_H\rangle\langle\psi_H|\right) - \frac{12i}{25}|\psi_H\rangle\langle\psi_V| \\
&\quad + \frac{12i}{25}|\psi_V\rangle\langle\psi_H| + \frac{16}{25}|\psi_V\rangle\langle\psi_V|
\end{aligned}$$

so, writing the density operator on the horizontal and vertical polarization basis gives

$$\rho_{HH} = \langle\psi_H|\rho|\psi_H\rangle = P_1 + \frac{9}{25}P_2 = \frac{1}{5} + \frac{9}{25}\times\frac{4}{5} = \frac{25+36}{125} = \frac{61}{125}$$

$$\rho_{HV} = \langle\psi_H|\rho|\psi_V\rangle = \frac{12i}{25}P_1 = -\frac{12i}{125}$$

$$\rho_{VV} = \langle\psi_V|\rho|\psi_V\rangle = \frac{16}{25}P_2 = \frac{64}{125}$$

$$\rho_{VH} = \langle\psi_V|\rho|\psi_H\rangle = \frac{12i}{25}P_2 = +\frac{12i}{125}$$

Hence the density matrix is

$$\rho = \begin{bmatrix} \dfrac{61}{125} & -\dfrac{12i}{125} \\[2mm] \dfrac{12i}{125} & \dfrac{64}{125} \end{bmatrix}$$

where ρ_{HH} is the top left element in the matrix. (Note that this matrix is Hermitian, and does also have $Tr(\rho) = 1$.)

14.3.2

(i) For the mixed state with equal probabilities of being in either of the spin states $|s_x\rangle$ and $|s_y\rangle$ (i.e., $(P_1 = 0.5, P_2 = 0.5)$ where

$$|s_x\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle + |\downarrow\rangle\right)$$

and

$$|s_y\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle + i|\downarrow\rangle\right)$$

the density operator is

$$\rho = 0.5|s_x\rangle\langle s_x| + 0.5|s_y\rangle\langle s_y|$$

$$= \frac{0.5}{2}\left(|\uparrow\rangle\langle\uparrow| + |\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|\right.$$

$$\left. + |\uparrow\rangle\langle\uparrow| - i|\uparrow\rangle\langle\downarrow| + i|\downarrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|\right)$$

$$= \frac{1}{4}\left(2|\uparrow\rangle\langle\uparrow| + (1-i)|\uparrow\rangle\langle\downarrow| + (1+i)|\downarrow\rangle\langle\uparrow| + 2|\downarrow\rangle\langle\downarrow|\right)$$

$$= \frac{1}{2}|\uparrow\rangle\langle\uparrow| + \frac{1}{2}|\downarrow\rangle\langle\downarrow| + \frac{1-i}{4}|\uparrow\rangle\langle\downarrow| + \frac{1+i}{4}|\downarrow\rangle\langle\uparrow|$$

(ii) Writing the density operator as a density matrix (on this z-spin basis), with the $|\uparrow\rangle\langle\uparrow|$ element in the top left of the matrix, gives

$$\rho = \begin{bmatrix} \dfrac{1}{2} & \dfrac{1-i}{4} \\ \dfrac{1+i}{4} & \dfrac{1}{2} \end{bmatrix}$$

(iii) The matrix elements of the spin magnetic dipole operator on this same z-spin basis become

$$\langle\uparrow|\hat{\boldsymbol{\mu}}_e|\uparrow\rangle = g\mu_B \begin{bmatrix} 1 & 0 \end{bmatrix}\left(\mathbf{i}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} + \mathbf{j}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} + \mathbf{k}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\right)\begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$= g\mu_B\left(0\mathbf{i} + 0\mathbf{j} + \mathbf{k}\right) = g\mu_B\mathbf{k}$$

Similarly,

$$\langle\downarrow|\hat{\boldsymbol{\mu}}_e|\downarrow\rangle = g\mu_B\left(o\mathbf{i} + o\mathbf{j} - \mathbf{k}\right) = -g\mu_B\mathbf{k}$$

Also

$$\langle \uparrow |\hat{\boldsymbol{\mu}}_e| \downarrow \rangle = g\mu_B \begin{bmatrix} 1 & 0 \end{bmatrix} \left(\mathbf{i} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} + \mathbf{j} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} + \mathbf{k} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \right) \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$= g\mu_B \left(\mathbf{i} - i\mathbf{j} + 0\mathbf{k} \right) = g\mu_B \left(\mathbf{i} - i\mathbf{j} \right)$$

$$\langle \downarrow |\hat{\boldsymbol{\mu}}_e| \uparrow \rangle = g\mu_B \begin{bmatrix} 0 & 1 \end{bmatrix} \left(\mathbf{i} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} + \mathbf{j} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} + \mathbf{k} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \right) \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$= g\mu_B \left(\mathbf{i} + i\mathbf{j} + 0\mathbf{k} \right) = g\mu_B \left(\mathbf{i} + i\mathbf{j} \right)$$

so on this basis $\hat{\boldsymbol{\mu}}_e$ is

$$\hat{\boldsymbol{\mu}}_e = g\mu_B \begin{bmatrix} \mathbf{k} & \mathbf{i} - i\mathbf{j} \\ \mathbf{i} + i\mathbf{j} & -\mathbf{k} \end{bmatrix}$$

(iv) Hence

$$\rho\hat{\boldsymbol{\mu}}_e = \frac{g\mu_B}{2} \begin{bmatrix} 1 & \dfrac{1-i}{2} \\ \dfrac{1+i}{2} & 1 \end{bmatrix} \begin{bmatrix} \mathbf{k} & \mathbf{i} - i\mathbf{j} \\ \mathbf{i} + i\mathbf{j} & -\mathbf{k} \end{bmatrix}$$

$$= \frac{g\mu_B}{2} \begin{bmatrix} \mathbf{k} + \left(\dfrac{1-i}{2}\right)(\mathbf{i} + i\mathbf{j}) & \mathbf{i} - i\mathbf{j} - \left(\dfrac{1-i}{2}\right)\mathbf{k} \\ \left(\dfrac{1+i}{2}\right)\mathbf{k} + \mathbf{i} + i\mathbf{j} & -\mathbf{k} + \left(\dfrac{1+i}{2}\right)(\mathbf{i} - i\mathbf{j}) \end{bmatrix}$$

so

$$\overline{\langle \boldsymbol{\mu}_e \rangle} = T_R \left(\rho\boldsymbol{\mu}_e \right) = \frac{g\mu_B}{4} \{ \mathbf{i} + i\mathbf{j} + \mathbf{i} - i\mathbf{j} - i\mathbf{i} + i\mathbf{i} + \mathbf{j} + \mathbf{j} \} = \frac{g\mu_B}{4} \{ 2\mathbf{i} + 2\mathbf{j} \}$$

i.e.,

$$\overline{\langle \boldsymbol{\mu}_e \rangle} = \frac{g\mu_B}{2} \{ \mathbf{i} + \mathbf{j} \}$$

14.5.1

To evaluate the polarization and the population difference, we first evaluate the behavior of the density matrix, in the approximation where we have relaxation time T_1 and T_2, and we can take $(\rho_{11} - \rho_{22})_0 = 1$ because the equilibrium condition is that the atoms would all be in their lower state (1).

(i) Since the system has been in steady state, we have the expressions Eqs. (14.47) and (14.49) for the off-diagonal density matrix elements (or their slowly-varying component β_{21}), and Eq. (14.46) for $\rho_{11} - \rho_{22}$, we obtain for the starting conditions at $t = 0$

$$\rho_{11} - \rho_{22} = \frac{1 + (\omega - \omega_{21})^2 T_2^2}{1 + (\omega - \omega_{21})^2 T_2^2 + 4\Omega^2 T_2 T_1} = \Delta\rho_0$$

where

$$\Omega = \mu_d E_0 / 2\hbar$$

and

$$\text{Im}\left(\beta_{21}(t=0)\right) = \frac{\Omega T_2}{1 + (\omega - \omega_{21})^2 T_2^2 + 4\Omega^2 T_2 T_1} \equiv \beta_{I0}$$

$$\text{Re}\left(\beta_{21}(t=0)\right) = \frac{(\omega_{21} - \omega)\Omega T_2^2}{1 + (\omega - \omega_{21})^2 T_2^2 + 4\Omega^2 T_2 T_1} \equiv \beta_{R0}$$

(Also, since $\exp(-i\omega t) = 1$ for $t = 0$, $\rho_{21}(t=0) = \beta_{R0} + i\beta_{I0}$.) Hence, from Eq. (14.45) with $t = 0$,

$$\overline{\langle\mu\rangle} = 2\mu_d \,\text{Re}(\beta_{21}) = \frac{2\mu d\,(\omega_{21} - \omega)\Omega T_2^2}{1 + (\omega - \omega_{21})^2 T_2^2 + 4\Omega^2 T_2 T_1} = 2\mu_d\beta_{R0} \equiv \overline{\mu}_0$$

(ii) From Eq. (14.43), with $E_0 = 0$, we now have

$$\frac{d}{dt}(\rho_{11} - \rho_{22}) = -\frac{(\rho_{11} - \rho_{22})}{T_1}$$

$$\rho_{11} - \rho_{22} = A\exp\left(-\frac{t}{T_1}\right) + C$$

i.e., fitting the boundary conditions of $(\rho_{11} - \rho_{22}) \to 1$, as $t \to \infty$ and $\Delta\rho_0$ at $t = 0$,

$$\rho_{11} - \rho_{22} = 1 - (1 - \Delta\rho_0)\exp\left(-\frac{t}{T_1}\right)$$

From Eq. (14.40), with $E_0 = 0$, we now have

$$\frac{d\rho_{21}}{dt} = -\left[i\omega_{21} + \frac{1}{T_2}\right]\rho_{21}$$

So

$$\rho_{21}(t) = (\beta_{R0} + i\beta_{I0})\exp(-i\omega_{21}t)\exp(-t/T_2)$$

Hence, from Eq. (14.35),

$$\langle \bar{\mu} \rangle = \mu_d(\rho_{12} + \rho_{21}) = \mu_d 2\,\mathrm{Re}(\rho_{21})$$

since ρ is Hermitian, with $\rho_{21}(t)$ as above.
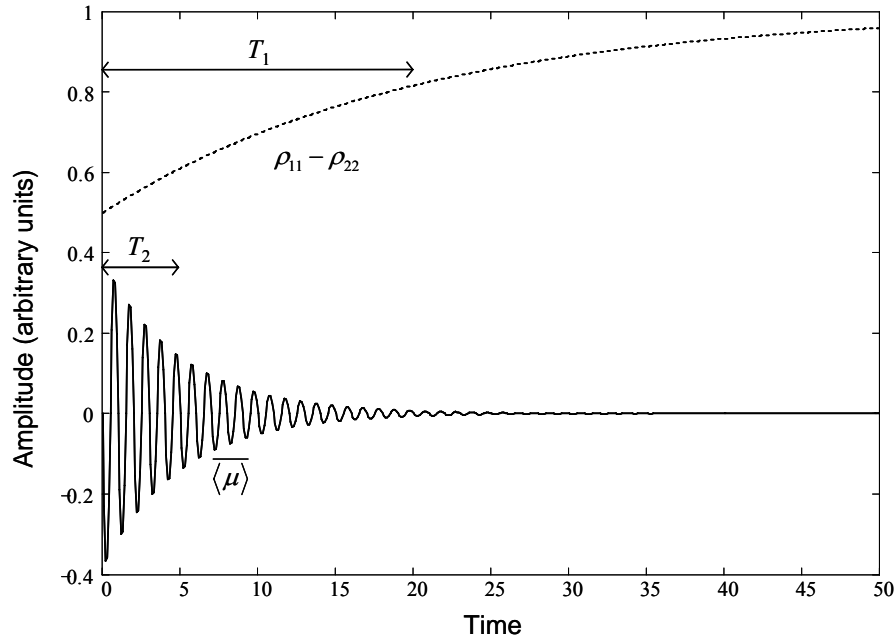
(iii) Far from resonance, $\beta_{R0} \simeq 0$, so

$$\rho_{21}(t) \simeq i\beta_{I0}\exp(-i\omega_{21}t)\exp(-t/T_2)$$

so

$$\overline{\langle \mu \rangle} \simeq -2\mu_d \beta_{I0}\exp(-t/T_2)\sin(\omega_{21}t)$$

The time units in the graph are in cycles of the ω_{21} frequency, i.e., $2\pi/\omega_{21}$. Hence the behavior is that (i) $\rho_{11} - \rho_{22}$ recovers exponentially to the population, all being in the lower state with time constant T_1, and (ii) the ensemble average of the polarization oscillates at frequency $\simeq \omega_{21}$ with the amplitude of that oscillation decaying exponentially with time constant T_2.

(iv) Remember that it is the ensemble average of the polarization that decays with time constant T_2. Individual atoms can still be emitting light; it is just that their phase is random relative to each other, so the ensemble average of the polarization can tend to vanish even if individual atoms are still emitting.

Chapter 15 problem solutions

15.1.1

Substituting, we have

$$\left[\hat{a},\hat{a}^{\dagger}\right]=\frac{1}{2}\left\{\left(\frac{d}{d\xi}+\xi\right)\left(-\frac{d}{d\xi}+\xi\right)-\left(-\frac{d}{d\xi}+\xi\right)\left(\frac{d}{d\xi}+\xi\right)\right\}$$

$$=\left\{\frac{d}{d\xi}\xi-\xi\frac{d}{d\xi}\right\}$$

Now, to complete this discussion, we need to formally imagine that this operator is operating on an arbitrary function, $f(\xi)$.

$$\left\{\frac{d}{d\xi}\xi-\xi\frac{d}{d\xi}\right\}f(\xi)=\frac{d}{d\xi}\left[\xi f(\xi)\right]-\xi\frac{d}{d\xi}f(\xi)$$

$$=f(\xi)\frac{d\xi}{d\xi}+\xi\frac{d}{d\xi}f(\xi)-\xi\frac{d}{d\xi}f(\xi)$$

$$=f(\xi)$$

In other words

$$\left[\hat{a},\hat{a}^{\dagger}\right]f(\xi)=f(\xi)$$

Since $f(\xi)$ is an arbitrary function, we can therefore say

$$\left[\hat{a},\hat{a}^{\dagger}\right]=1$$

as required (where, technically, the "1" on the right hand side is actually a unit (identity) operator).

15.1.2

Operate on both sides of the equation with $\hat{a}^\dagger$ and use the commutation relation to obtain

$$\hat{a}^\dagger \left(\hat{a}^\dagger \hat{a}\right)|\psi_n\rangle = \hat{a}^\dagger \left(\hat{a}\hat{a}^\dagger - 1\right)|\psi_n\rangle = n\hat{a}^\dagger |\psi_n\rangle$$

i.e.,

$$\hat{a}^\dagger \left(\hat{a}\hat{a}^\dagger\right)|\psi_n\rangle = (n+1)\hat{a}^\dagger |\psi_n\rangle$$

i.e.,

$$\hat{a}^\dagger \hat{a}\left(\hat{a}^\dagger |\psi_n\rangle\right) = (n+1)\left(\hat{a}^\dagger |\psi_n\rangle\right)$$

as required.

15.5.1

$$\left[\hat{\xi}_\lambda, \hat{\pi}_\lambda\right] = \frac{i}{2}\left\{\left(\hat{a}_\lambda + \hat{a}_\lambda^\dagger\right)\left(\hat{a}_\lambda^\dagger - \hat{a}_\lambda\right) - \left(\hat{a}_\lambda^\dagger - \hat{a}_\lambda\right)\left(\hat{a}_\lambda + \hat{a}_\lambda^\dagger\right)\right\}$$

$$= \frac{i}{2}\left\{\hat{a}_\lambda\hat{a}_\lambda^\dagger - \hat{a}_\lambda^\dagger\hat{a}_\lambda - \hat{a}_\lambda\hat{a}_\lambda + \hat{a}_\lambda^\dagger\hat{a}_\lambda^\dagger - \hat{a}_\lambda^\dagger\hat{a}_\lambda + \hat{a}_\lambda\hat{a}_\lambda^\dagger - \hat{a}_\lambda^\dagger\hat{a}_\lambda + \hat{a}_\lambda\hat{a}_\lambda^\dagger\right\}$$

$$= \frac{i}{2}\left\{\hat{a}_\lambda\hat{a}_\lambda^\dagger - \hat{a}_\lambda^\dagger\hat{a}_\lambda - \hat{a}_\lambda^\dagger\hat{a}_\lambda + \hat{a}_\lambda\hat{a}_\lambda^\dagger\right\}$$

$$= i\left\{\hat{a}_\lambda\hat{a}_\lambda^\dagger - \hat{a}_\lambda^\dagger\hat{a}_\lambda\right\}$$

$$= i$$

where we used the commutation relation $\left[\hat{a}, \hat{a}^\dagger\right] = \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} = 1$ in the last step.

15.6.1

We have the definition of the coherent state

$$\left| \psi_{\lambda \bar{n}} \right\rangle = \sum_{n_\lambda=0}^{\infty} C_{\lambda \bar{n} n} \exp\left[-i\left(n_\lambda + \frac{1}{2} \right) \omega_\lambda t \right] \left| n_\lambda \right\rangle$$

Hence

$$\hat{a}_\lambda \left| \psi_{\lambda \bar{n}} \right\rangle = \sum_{n_\lambda=0}^{\infty} \sqrt{\frac{\bar{n}^{n_\lambda} \exp(-\bar{n})}{n_\lambda !}} \exp\left[-i\left(n_\lambda + \frac{1}{2} \right) \omega_\lambda t \right] \hat{a}_\lambda \left| n_\lambda \right\rangle$$

Now

$$\hat{a}_\lambda \left| n_\lambda \right\rangle = \sqrt{n_\lambda} \left| n_\lambda - 1 \right\rangle$$

so

$$\hat{a}_\lambda \left| \psi_{\lambda \bar{n}} \right\rangle = \sum_{n_\lambda=1}^{\infty} \sqrt{\frac{\bar{n}^{n_\lambda} \exp(-\bar{n})}{n_\lambda !}} \exp\left[-i\left(n_\lambda + \frac{1}{2} \right) \omega_\lambda t \right] \sqrt{n_\lambda} \left| n_\lambda - 1 \right\rangle$$

where we have changed the lower limit on the sum to 1 from 0 because $\hat{a}_\lambda \left| 0 \right\rangle = 0$. Now we change the index of summation to $m_\lambda = n_\lambda - 1$ and write

$$\hat{a}_\lambda \left| \psi_{\lambda \bar{n}} \right\rangle = \sum_{m_\lambda=0}^{\infty} \sqrt{m_\lambda + 1} \sqrt{\frac{\bar{n}^{m_\lambda+1} \exp(-\bar{n})}{(m_\lambda + 1)!}} \exp\left[-i\left(m_\lambda + 1 + \frac{1}{2} \right) \omega_\lambda t \right] \left| m_\lambda \right\rangle$$

$$= \sqrt{\bar{n}} \exp(-i\,\omega_\lambda t) \sum_{m_\lambda=0}^{\infty} \sqrt{\frac{\bar{n}^{m_\lambda} \exp(-\bar{n})}{m_\lambda !}} \exp\left[-i\left(m_\lambda + \frac{1}{2} \right) \omega_\lambda t \right] \left| m_\lambda \right\rangle$$

$$= \sqrt{\bar{n}} \exp(-i\,\omega_\lambda t) \left| \psi_{\lambda \bar{n}} \right\rangle$$

Hence, $\left| \psi_{\lambda \bar{n}} \right\rangle$ is an eigenstate of $\hat{a}_\lambda$ with eigenvalue $\sqrt{\bar{n}} \exp(-i\omega_\lambda t)$

15.6.2

The expected value of position is just the expectation value of the operator $\hat{\xi}_\lambda$, i.e.,

$$\left\langle \hat{\xi}_\lambda \right\rangle \equiv \overline{\xi}_\lambda = \frac{1}{\sqrt{2}} \left\langle \psi_{\lambda\bar{n}} \left| \left(\hat{a}_\lambda + \hat{a}_\lambda^\dagger \right) \right| \psi_{\lambda\bar{n}} \right\rangle = \frac{1}{\sqrt{2}} \left\{ \left\langle \psi_{\lambda\bar{n}} \left| \hat{a}_\lambda \right| \psi_{\lambda\bar{n}} \right\rangle + \left\langle \psi_{\lambda\bar{n}} \left| \hat{a}_\lambda^\dagger \right| \psi_{\lambda\bar{n}} \right\rangle \right\}$$

$$= \sqrt{\frac{n}{2}} \exp\left(-i\omega_\lambda t\right) \left\langle \psi_{\lambda\bar{n}} \middle| \psi_{\lambda\bar{n}} \right\rangle + \sqrt{\frac{n}{2}} \exp\left(i\omega_\lambda t\right) \left\langle \psi_{\lambda\bar{n}} \middle| \psi_{\lambda\bar{n}} \right\rangle$$

$$= \sqrt{\frac{n}{2}} \left\{ \exp\left(-i\omega_\lambda t\right) + \exp\left(i\omega_\lambda t\right) \right\} = \sqrt{2n} \cos\left(\omega_\lambda t\right)$$

Hence, the expected value of position is oscillating (co)sinusoidally at angular frequency ω_λ.

15.6.3

(i) To deduce an uncertainty relation, we start with the commutator of the operators, i.e.,

$$\left[\hat{\xi}_\lambda, \hat{\pi}_\lambda\right] = i$$

as deduced in Prob. 14.4.1 above. We know in general that for a commutator $\left[\hat{A}, \hat{B}\right] = i\hat{C}$, the resulting uncertainty principle is $\overline{(\Delta A)^2}\,\overline{(\Delta B)^2} \geq \dfrac{\left(\overline{C}\right)^2}{4}$ (Eq. (5.23)) (or the square root of both sides if we prefer). Hence, the uncertainty relation for our operators here is

$$\Delta\pi_\lambda \Delta\xi_\lambda \geq \frac{1}{2}$$

(ii) We already know $\overline{\xi}_\lambda = \sqrt{2\overline{n}}\,\cos\left(\omega_\lambda t\right)$. Now let us evaluate $\left\langle \hat{\xi}_\lambda^2 \right\rangle$, noting first of all that

$$\hat{\xi}_\lambda^2 = \frac{1}{2}\left(\hat{a}_\lambda + \hat{a}_\lambda^\dagger\right)^2 = \frac{1}{2}\left(\hat{a}_\lambda^2 + \left(\hat{a}_\lambda^\dagger\right)^2 + \hat{a}_\lambda\hat{a}_\lambda^\dagger + \hat{a}_\lambda^\dagger\hat{a}_\lambda\right)$$

Now, this is still awkward, because it has a term $\hat{a}_\lambda\hat{a}_\lambda^\dagger$. We only know how to deal directly with $\hat{a}_\lambda\left|\psi_{\lambda\overline{n}}\right\rangle = \sqrt{\overline{n}}\,\exp\left(-i\omega_\lambda t\right)\left|\psi_{\lambda\overline{n}}\right\rangle$ or its Hermitian adjoint, $\left\langle\psi_{\lambda\overline{n}}\right|\hat{a}_\lambda^\dagger = \sqrt{\overline{n}}\,\exp\left(i\omega_\lambda t\right)\left\langle\psi_{\lambda\overline{n}}\right|$, but this term has the operators in the wrong order to allow us to use either of these results. So, we use the usual trick of substituting using the commutation relation $\hat{a}_\lambda\hat{a}_\lambda^\dagger - \hat{a}_\lambda^\dagger\hat{a}_\lambda = 1$ to obtain instead

$$\hat{\xi}_\lambda^2 = \frac{1}{2}\left(\hat{a}_\lambda^2 + \left(\hat{a}_\lambda^\dagger\right)^2 + 2\hat{a}_\lambda^\dagger\hat{a}_\lambda + 1\right)$$

and so

$$\left\langle \hat{\xi}_\lambda^2 \right\rangle = \frac{\overline{n}}{2}\left[\exp\left(-2i\omega_\lambda t\right) + \exp\left(2i\omega_\lambda t\right) + 2\right] + \frac{1}{2}$$

$$= \overline{n}\left[\cos\left(2\omega_\lambda t\right) + 1\right] + \frac{1}{2}$$

$$= 2\overline{n}\cos^2\left(\omega_\lambda t\right) + \frac{1}{2}$$

Hence, using the result for $\overline{\xi}_\lambda = \sqrt{2\overline{n}}\,\cos\left(\omega_\lambda t\right)$ from the preceding problem,

$$\left\langle \hat{\xi}_\lambda^2 \right\rangle - \overline{\xi}_\lambda^2 = \frac{1}{2}$$

But $\left\langle \hat{\xi}_\lambda^2 \right\rangle - \overline{\xi}_\lambda^2$ is just the statistical expression for the variance $\overline{(\Delta\xi_\lambda)^2}$ (the square of the standard deviation $\Delta\xi_\lambda$) (see Chapter 5, Eq. (5.16)), so we have

$$\sqrt{\overline{(\Delta\xi_\lambda)^2}} \equiv \Delta\xi_\lambda = \frac{1}{\sqrt{2}}$$

Note that this width of the distribution is constant, even as the average position oscillates.

(iii) For the "momentum" operator, the expected value is

$$\bar{\pi}_\lambda = \frac{i}{\sqrt{2}}\langle\psi_{\lambda\bar{n}}|\left(\hat{a}_\lambda^\dagger - \hat{a}_\lambda\right)|\psi_{\lambda\bar{n}}\rangle = \frac{i}{\sqrt{2}}\left\{\langle\psi_{\lambda\bar{n}}|\hat{a}_\lambda^\dagger|\psi_{\lambda\bar{n}}\rangle - \langle\psi_{\lambda\bar{n}}|\hat{a}_\lambda|\psi_{\lambda\bar{n}}\rangle\right\}$$

$$= i\sqrt{\frac{\bar{n}}{2}}\left\{\exp\left(i\omega_\lambda t\right) - \exp\left(-i\omega_\lambda t\right)\right\} = -\sqrt{2\bar{n}}\sin\left(\omega_\lambda t\right)$$

Now we write, analogously to before,

$$\hat{\pi}_\lambda^2 = \frac{-1}{2}\left(\hat{a}_\lambda^\dagger - \hat{a}_\lambda\right)^2 = \frac{-1}{2}\left(\hat{a}_\lambda^2 + \left(\hat{a}_\lambda^\dagger\right)^2 - \hat{a}_\lambda\hat{a}_\lambda^\dagger - \hat{a}_\lambda^\dagger\hat{a}_\lambda\right)$$

So, using the commutation relation $\hat{a}_\lambda\hat{a}_\lambda^\dagger - \hat{a}_\lambda^\dagger\hat{a}_\lambda = 1$, we obtain instead

$$\hat{\pi}_\lambda^2 = \frac{-1}{2}\left(\hat{a}_\lambda^2 + \left(\hat{a}_\lambda^\dagger\right)^2 - 2\hat{a}_\lambda^\dagger\hat{a}_\lambda - 1\right)$$

and so

$$\langle\hat{\pi}_\lambda^2\rangle = \frac{-\bar{n}}{2}\left[\exp\left(-2i\omega_\lambda t\right) + \exp\left(2i\omega_\lambda t\right) - 2\right] + \frac{1}{2}$$

$$= -\bar{n}\left[\cos\left(2\omega_\lambda t\right) - 1\right] + \frac{1}{2}$$

$$= 2\bar{n}\sin^2\left(\omega_\lambda t\right) + \frac{1}{2}$$

Hence,

$$\langle\hat{\pi}_\lambda^2\rangle - \bar{\pi}_\lambda^2 = \frac{1}{2}$$

so we have

$$\sqrt{\overline{\left(\Delta\pi_\lambda\right)^2}} \equiv \Delta\pi_\lambda = \frac{1}{\sqrt{2}}$$

(iv) Hence, finally, we have

$$\Delta\hat{\pi}_\lambda\Delta\hat{\xi}_\lambda = \frac{1}{2}$$

Comparing this with our uncertainty relation derived in part (i) above, we have shown that the coherent state has the minimum possible product of uncertainties of position and momentum.

Noting that our dimensionless position and momentum operators are scaled from actual position and momentum operators by factors of $1/\sqrt{\hbar}$, if we wish, we can restate this in the more conventional units of position x and momentum p as

$$\Delta p\Delta x = \frac{\hbar}{2}$$

15.7.1

Multiplying out the commutator, we have

$$\left[\hat{E}_x, \hat{B}_y\right] = \frac{i\hbar}{2}\sqrt{\frac{\mu_0}{\varepsilon_0}}\sum_{\lambda_1}\sum_{\lambda_2}\left[\left(\hat{a}_{\lambda_1} - \hat{a}_{\lambda_1}^\dagger\right)\left(\hat{a}_{\lambda_2} + \hat{a}_{\lambda_2}^\dagger\right) - \left(\hat{a}_{\lambda_2} + \hat{a}_{\lambda_2}^\dagger\right)\left(\hat{a}_{\lambda_1} - \hat{a}_{\lambda_1}^\dagger\right)\right]u_{x\lambda_1}(\mathbf{r})v_{y\lambda_2}(\mathbf{r})\sqrt{\omega_{\lambda_1}\omega_{\lambda_2}}$$

Now

$$\left(\hat{a}_{\lambda_1} - \hat{a}_{\lambda_1}^\dagger\right)\left(\hat{a}_{\lambda_2} + \hat{a}_{\lambda_2}^\dagger\right) - \left(\hat{a}_{\lambda_2} + \hat{a}_{\lambda_2}^\dagger\right)\left(\hat{a}_{\lambda_1} - \hat{a}_{\lambda_1}^\dagger\right)$$

$$= \left(\hat{a}_{\lambda_1}\hat{a}_{\lambda_2} - \hat{a}_{\lambda_2}\hat{a}_{\lambda_1}\right) + \left(\hat{a}_{\lambda_1}\hat{a}_{\lambda_2}^\dagger - \hat{a}_{\lambda_2}^\dagger\hat{a}_{\lambda_1}\right) - \left(\hat{a}_{\lambda_1}^\dagger\hat{a}_{\lambda_2} - \hat{a}_{\lambda_2}\hat{a}_{\lambda_1}^\dagger\right) - \left(\hat{a}_{\lambda_1}^\dagger\hat{a}_{\lambda_2}^\dagger - \hat{a}_{\lambda_2}^\dagger\hat{a}_{\lambda_1}^\dagger\right)$$

$$= 0 + \delta_{\lambda_1,\lambda_2} + \delta_{\lambda_1,\lambda_2} - 0$$

by the boson commutation relations. Hence

$$\left[\hat{E}_x, \hat{B}_y\right] = i\hbar\sqrt{\frac{\mu_0}{\varepsilon_0}}\sum_{\lambda}\omega_\lambda u_{x\lambda}(\mathbf{r})v_{y\lambda}(\mathbf{r})$$

Chapter 16 problem solutions

16.1.1

Possible basis states are, in the order we will use them

$$|0\rangle \equiv |0_1, 0_2\rangle \quad \text{no particles in either state}$$
$$|1_1, 0_2\rangle \qquad \text{one particle in state 1}$$
$$|0_1, 1_2\rangle \qquad \text{one particle in state 2}$$
$$|1_1, 1_2\rangle \qquad \text{one particle in state 1 and one in state 2}$$

We now proceed to evaluate the operator matrices examining the effect each one has on each basis state, allowing us to build up all the matrix elements.

Creation operator 1

We have the following results when this operator operates on each of the states

$$\hat{b}_1^+ |0\rangle = |1_1, 0_2\rangle$$
$$\hat{b}_1^+ |1_1, 0_2\rangle = 0$$
$$\hat{b}_1^+ |0_1, 1_2\rangle = -|1_1, 1_2\rangle$$

because, with our definition of standard order, we have to swap past the row corresponding to state 2, and

$$\hat{b}_1^+ |1_1, 1_2\rangle = 0$$

Hence

$$\hat{b}_1^+ \equiv \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{bmatrix}$$

Annihilation operator 1

$$\hat{b}_1 |0\rangle = 0$$
$$\hat{b}_1 |1_1, 0_2\rangle = |0\rangle$$

(there is only one "row" in the Slater determinant, so there is nothing to swap past)

$$\hat{b}_1 |0_1, 1_1\rangle = 0$$
$$\hat{b}_1 |1_1, 1_2\rangle = -|0_1, 1_2\rangle$$

we have to swap past the row corresponding to state 2.

Hence

$$\hat{b}_1 \equiv \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

We can verify the anticommutation relation for this pair

$$\hat{b}_1^+\hat{b}_1 + \hat{b}_1\hat{b}_1^+ = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{bmatrix}\begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \end{bmatrix}\begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{bmatrix}$$

as required.

For the state 2 creation operator

$$\hat{b}_2^+|0_1,0_2\rangle = |0_1,1_2\rangle$$
$$\hat{b}_2^+|1_1,0_2\rangle = |1_1,1_2\rangle \quad (no\ swapping\ required)$$
$$\hat{b}_2^+|0_1,1_2\rangle = 0$$
$$\hat{b}_2^+|1_1,1_2\rangle = 0$$

For the state 2 annihilation operator

$$\hat{b}_2|0_1,0_2\rangle = 0 \quad (no\ swapping\ required)$$
$$\hat{b}_2|1_1,0_2\rangle = 0 \quad (no\ swapping\ required)$$
$$\hat{b}_2|0_1,1_2\rangle = |0_1,0_2\rangle$$
$$\hat{b}_2|1_1,1_2\rangle = |1_1,0_2\rangle$$

Hence

$$\hat{b}_2^+ \equiv \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

$$\hat{b}_2 \equiv \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

The anticommutation relation for this pair of operators is

$$\hat{b}_2^+ \hat{b}_2 + \hat{b}_2 \hat{b}_2^+ = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

as required.

For other anticommutation relations, we have

$$\hat{b}_1^+ \hat{b}_2^+ + \hat{b}_2^+ \hat{b}_1^+ = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} = 0$$

and similarly for

$$\hat{b}_1 \hat{b}_2 + \hat{b}_2 \hat{b}_1 = 0$$

Also

$$\hat{b}_1^+\hat{b}_1^+ = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{bmatrix}\begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

so

$$\hat{b}_1^+\hat{b}_1^+ + \hat{b}_1^+\hat{b}_1^+ = 0$$

and similarly for

$$\hat{b}_2^+\hat{b}_2^+ + \hat{b}_2^+\hat{b}_2^+ = 0$$

and also

$$\hat{b}_1 b_1 + \hat{b}_1 \hat{b}_1 = 0$$

$$\hat{b}_2\hat{b}_2 + \hat{b}_2\hat{b}_2 = 0$$

16.1.2

Follow similar steps as in the derivation of $\hat{b}_j^\dagger \hat{b}_k^\dagger + \hat{b}_k^\dagger \hat{b}_j^\dagger = 0$ in the chapter. Explicitly, we have the following argument.

For the sake of definiteness of illustration, let us suppose that we start with the state in which single-particle states b, k, and m are occupied but all other states are not. As in the chapter, we ignore the factorial normalization factors that should precede the determinants; we concentrate on the signs and orderings only. Then we have

$$\hat{b}_k \begin{Vmatrix} |1,b\rangle & |2,b\rangle & |3,b\rangle \\ |1,k\rangle & |2,k\rangle & |3,k\rangle \\ |1,m\rangle & |2,m\rangle & |3,m\rangle \end{Vmatrix} = \hat{b}_k \left(- \begin{Vmatrix} |1,b\rangle & |2,b\rangle & |3,b\rangle \\ |1,m\rangle & |2,m\rangle & |3,m\rangle \\ |1,k\rangle & |2,k\rangle & |3,k\rangle \end{Vmatrix} \right)$$

$$= -\hat{b}_k \begin{Vmatrix} |1,b\rangle & |2,b\rangle & |3,b\rangle \\ |1,m\rangle & |2,m\rangle & |3,m\rangle \\ |1,k\rangle & |2,k\rangle & |3,k\rangle \end{Vmatrix} = - \begin{Vmatrix} |1,b\rangle & |2,b\rangle \\ |1,m\rangle & |2,m\rangle \end{Vmatrix} \qquad (A)$$

So

$$\hat{b}_m \hat{b}_k \begin{Vmatrix} |1,b\rangle & |2,b\rangle & |3,b\rangle \\ |1,k\rangle & |2,k\rangle & |3,k\rangle \\ |1,m\rangle & |2,m\rangle & |3,m\rangle \end{Vmatrix} = -\hat{b}_m \begin{Vmatrix} |1,b\rangle & |2,b\rangle \\ |1,m\rangle & |2,m\rangle \end{Vmatrix} = -\begin{Vmatrix} |1,b\rangle \end{Vmatrix} \; (\equiv -|1,b\rangle) \qquad (B)$$

But

$$\hat{b}_m \begin{Vmatrix} |1,b\rangle & |2,b\rangle & |3,b\rangle \\ |1,k\rangle & |2,k\rangle & |3,k\rangle \\ |1,m\rangle & |2,m\rangle & |3,m\rangle \end{Vmatrix} = \begin{Vmatrix} |1,b\rangle & |2,b\rangle \\ |1,k\rangle & |2,k\rangle \end{Vmatrix} \qquad (C)$$

so

$$\hat{b}_k \hat{b}_m \begin{Vmatrix} |1,b\rangle & |2,b\rangle & |3,b\rangle \\ |1,k\rangle & |2,k\rangle & |3,k\rangle \\ |1,m\rangle & |2,m\rangle & |3,m\rangle \end{Vmatrix} = \hat{b}_k \begin{Vmatrix} |1,b\rangle & |2,b\rangle \\ |1,k\rangle & |2,k\rangle \end{Vmatrix} = \begin{Vmatrix} |1,b\rangle \end{Vmatrix} \; (\equiv |1,b\rangle) \qquad (D)$$

The results for $\hat{b}_m \hat{b}_k$ and $\hat{b}_k \hat{b}_m$ differ by a factor of -1 because there is always one more swap required in one case than the other.

This behavior of obtaining opposite signs for the result if the particles are annihilated in opposite order is a general one and it does not matter what the initial state is or what specific states the particles are being annihilated from (as long as the particles are being annihilated from states that are different and that are initially occupied). Hence, we have the result, valid for the operators operating on any state in which single-particle states j and k are initially occupied

$$\hat{b}_j \hat{b}_k + \hat{b}_k \hat{b}_j = 0 \qquad (E)$$

In fact, this relation in Eq. (E) is universally true for any state. To see this, we note first that for any state in which state k is initially empty, the result $\hat{b}_j \hat{b}_k + \hat{b}_k \hat{b}_j = 0$ holds trivially because

$$\hat{b}_k \left| \ldots, 0_k, \ldots \right\rangle = 0 \tag{F}$$

because we cannot annihilate a fermion from a single particle state that is already empty (and, of course, the operator $\hat{b}_j$ does not create a particle in state k).

Hence, our relation Eq. (E) still works here because each individual term is zero. We get an exactly similar result if the initial state is such that the single-particle state j is empty. We also trivially get the same result for any initial state if $j = k$ because we are trying to annihilate two fermions from the same single-particle state, which is impossible, so we also get zero for both terms. Hence, we conclude that Eq. (E) is valid for any starting state.

16.2.1

Substituting using the wavefunction operator

$$\hat{\psi}\left(\underline{r}_1,\underline{r}_2\right)\left|...,1_k,...1_m,...\right\rangle = \hat{\psi}\left(\underline{r}_1,\underline{r}_2\right)\hat{b}_k^\dagger\,\hat{b}_m^\dagger\left|0\right\rangle$$

$$= \frac{1}{\sqrt{2}}\sum_{j,n}\phi_j\left(\underline{r}_1\right)\phi_n\left(\underline{r}_2\right)\hat{b}_n\hat{b}_j\hat{b}_k^\dagger\hat{b}_m^\dagger\left|0\right\rangle$$

Now, progressively using the anticommutation relation $\hat{b}_p^\dagger\hat{b}_q + \hat{b}_q\hat{b}_p^\dagger = \delta_{pq}$ to push the annihilation operators to the right

$$\hat{b}_n\hat{b}_j\hat{b}_k^\dagger\,\hat{b}_m^\dagger = \hat{b}_n\left(\delta_{jk} - \hat{b}_k^\dagger\,\hat{b}_j\right)\hat{b}_m^\dagger$$

$$= \delta_{jk}\hat{b}_n\hat{b}_m^\dagger - \hat{b}_n\hat{b}_k^\dagger\,\hat{b}_j\hat{b}_m^\dagger$$

$$= \delta_{jk}\left(\delta_{nm} - \hat{b}_m^\dagger\hat{b}_n\right) - \hat{b}_n\hat{b}_k^\dagger\left(\delta_{jm} - \hat{b}_m^\dagger\hat{b}_j\right)$$

$$= \delta_{jk}\delta_{jm} - \delta_{jk}\hat{b}_m^\dagger\hat{b}_n - \left(\delta_{nk} - \hat{b}_k^\dagger\hat{b}_n\right)\left(\delta_{jm} - \hat{b}_m^\dagger\hat{b}_j\right)$$

$$= \delta_{jk}\delta_{nm} - \delta_{nk}\delta_{jm}$$

$$- \delta_{jk}\hat{b}_m^\dagger\hat{b}_n + \delta_{jm}\hat{b}_k^\dagger\hat{b}_n + \delta_{nk}\hat{b}_m^\dagger\hat{b}_j - \hat{b}_k^\dagger\hat{b}_n\hat{b}_m^\dagger\hat{b}_j$$

Note that we have arranged that all the terms containing any of the annihilation and creation operators have an annihilation operator on the far right. Hence, when any of these terms operate on $\left|0\right\rangle$, we get a null result. All that is left are the two Kronecker delta terms, i.e.,

$$\hat{b}_n\hat{b}_j\hat{b}_k^\dagger\hat{b}_m^\dagger\left|0\right\rangle = \left(\delta_{jk}\delta_{nm} - \delta_{nk}\delta_{jm}\right)\left|0\right\rangle$$

Hence

$$\hat{\psi}\left(\underline{r}_1,\underline{r}_2\right)\left|...,1_k,...1_m,...\right\rangle$$

$$= \frac{1}{\sqrt{2}}\sum_{j,n}\phi_j\left(\underline{r}_2\right)\phi_n\left(\underline{r}_2\right)\left(\delta_{jk}\delta_{nm} - \delta_{nk}\delta_{jm}\right)\left|0\right\rangle$$

$$= \frac{1}{\sqrt{2}}\left[\phi_k\left(\underline{r}_1\right)\phi_m\left(\underline{r}_2\right) - \phi_m\left(\underline{r}_1\right)\phi_k\left(\underline{r}_2\right)\right]\left|0\right\rangle$$

16.3.1

$$\langle 0|\hat{b}_m\hat{b}_k\hat{b}_a^\dagger\hat{b}_b^\dagger\hat{b}_d\hat{b}_c\hat{b}_k^\dagger\hat{b}_m^\dagger|0\rangle$$

$$= \langle 0|\hat{b}_m\left(\delta_{ak}-\hat{b}_a^\dagger\hat{b}_k\right)\hat{b}_b^\dagger\hat{b}_d\left(\delta_{kc}-\hat{b}_k^\dagger\hat{b}_c\right)\hat{b}_m^\dagger|0\rangle$$

$$= \langle 0|\delta_{ak}\delta_{kc}\hat{b}_m\hat{b}_b^\dagger\hat{b}_d\hat{b}_m^\dagger|0\rangle - \langle 0|\delta_{ak}\hat{b}_m\hat{b}_b^\dagger\hat{b}_d\hat{b}_k^\dagger\hat{b}_c\hat{b}_m^\dagger|0\rangle$$

$$- \langle 0|\delta_{kc}\hat{b}_m\hat{b}_a^\dagger\hat{b}_k\hat{b}_b^\dagger\hat{b}_d\hat{b}_m^\dagger|0\rangle + \langle 0|\hat{b}_m\hat{b}_a^\dagger\hat{b}_k\hat{b}_b^\dagger\hat{b}_d\hat{b}_k^\dagger\hat{b}_c\hat{b}_m^\dagger|0\rangle$$

$$= \langle 0|\delta_{ak}\delta_{kc}\left(\delta_{bm}-\hat{b}_b^\dagger\hat{b}_m\right)\left(\delta_{dm}-\hat{b}_m^\dagger\hat{b}_d\right)|0\rangle$$

$$- \langle 0|\delta_{ak}\left(\delta_{bm}-\hat{b}_b^\dagger\hat{b}_m\right)\left(\delta_{dk}-\hat{b}_k^\dagger\hat{b}_d\right)\left(\delta_{cm}-\hat{b}_m^\dagger\hat{b}_c\right)|0\rangle$$

$$- \langle 0|\delta_{kc}\left(\delta_{am}-\hat{b}_a^\dagger\hat{b}_m\right)\left(\delta_{bk}-\hat{b}_b^\dagger\hat{b}_k\right)\left(\delta_{dm}-\hat{b}_m^\dagger\hat{b}_d\right)|0\rangle$$

$$+ \langle 0|\left(\delta_{am}-\hat{b}_a^\dagger\hat{b}_m\right)\left(\delta_{bk}-\hat{b}_b^\dagger\hat{b}_k\right)\left(\delta_{dk}-\hat{b}_k^\dagger\hat{b}_d\right)\left(\delta_{mc}-\hat{b}_m^\dagger\hat{b}_c\right)|0\rangle$$

$$= \langle 0|\left[\delta_{ak}\delta_{kc}\delta_{bm}\delta_{dm} + \delta_{am}\delta_{bk}\delta_{dk}\delta_{mc} - \delta_{kc}\delta_{am}\delta_{bk}\delta_{dm} - \delta_{ak}\delta_{bm}\delta_{dk}\delta_{cm}\right]|0\rangle$$

$$= \delta_{ak}\delta_{bm}\delta_{ck}\delta_{dm} + \delta_{cm}\delta_{bk}\delta_{cm}\delta_{dk} - \delta_{am}\delta_{bk}\delta_{ck}\delta_{dm} - \delta_{ak}\delta_{bm}\delta_{cm}\delta_{dk}$$

16.3.2

(i) The **r** form of the Hamiltonian is

$$\hat{H}_{\mathbf{r}}\left(\mathbf{r}_e,\mathbf{r}_h\right) = -\frac{\hbar^2}{2m_e}\nabla_{\mathbf{r}_e}^2 - \frac{\hbar^2}{2m_p}\nabla_{\mathbf{r}_h}^2 - \frac{e^2}{2\pi\varepsilon_0\left|\mathbf{r}_e - \mathbf{r}_p\right|}$$

where e and p refer to the electron and proton, respectively. We have now an electron single-particle wavefunction operator

$$\hat{\psi}_e(\mathbf{r}_e) = \sum_j \hat{b}_j \phi_{ej}(\mathbf{r}_e)$$

and a proton single particle wave function operator

$$\hat{\psi}_p(\mathbf{r}_p) = \sum_k \hat{c}_k \phi_{pk}(\mathbf{r}_p)$$

where now we use the notation $\hat{c}_k$ for the proton annihilation operator.

Note that, because these are different particles, the annihilation and creation operators for the different particles all commute, as also do the wave function operators. Hence, we have, transforming with both wave function operators

$$\hat{H} = \iint \hat{\psi}_e^\dagger \hat{\psi}_p^\dagger H_{\mathbf{r}}(\mathbf{r}_e,\mathbf{r}_h)\hat{\psi}_e\hat{\psi}_p \, d^3\mathbf{r}_e d^3\mathbf{r}_h$$

$$= \iint \sum_{a,b,c,d} \hat{b}_a^\dagger \phi_{ea}^*(\mathbf{r}_e)\hat{c}_b^\dagger \phi_{pb}^*(\mathbf{r}_p)\hat{H}_{\mathbf{r}}(\mathbf{r}_e,\mathbf{r}_h)\hat{b}_c\,\phi_{ec}(\mathbf{r}_e)\hat{c}_d\phi_{pd}(\mathbf{r}_p) \, d^3\mathbf{r}_e d^3\mathbf{r}_p$$

$$= \sum_{a,b,c,d} H_{abcd}\hat{b}_a^\dagger \hat{b}_c\,\hat{c}_b^\dagger \hat{c}_d$$

(ii) Suppose the system is in a given state as suggested, with the electron in state k and the proton in state m. The state, therefore, is

$$\left|\psi\right> = \hat{b}_k^\dagger \hat{c}_m^\dagger \left|0\right>$$

Then the expectation value of the energy in that state is

$$\left<E\right> = \left<\psi\left|\hat{H}\right|\psi\right> = \sum_{a,b,c,d} H_{abcd}\left<0\left|\hat{c}_m\hat{b}_k\hat{b}_a^\dagger \hat{b}_c\,\hat{c}_b^\dagger \hat{c}_d\hat{b}_k^\dagger \hat{c}_m^\dagger\right|0\right>$$

Now

$$\hat{c}_m\hat{b}_k\hat{b}_a^\dagger \hat{b}_c\,\hat{c}_b^\dagger \hat{c}_d\hat{b}_k^\dagger \hat{c}_m^\dagger \left|0\right> = \hat{b}_k\hat{b}_a^\dagger \hat{b}_c\,\hat{b}_k^\dagger \hat{c}_m\hat{c}_b^\dagger \hat{c}_d\hat{c}_m^\dagger \left|0\right>$$

$$= \left(\delta_{ak} - \hat{a}_a^\dagger \hat{a}_k\right)\left(\delta_{ck} - \hat{a}_k^\dagger \hat{a}_c\right)\left(\delta_{bm} - \hat{c}_b^\dagger \hat{c}_m\right)\left(\delta_{dm} - \hat{c}_m^\dagger \hat{c}_d\right)\left|0\right>$$

$$= \delta_{ak}\delta_{ck}\delta_{bm}\delta_{dm}\left|0\right>$$

(Note there is only one string of Kronecker δ's here, not four). Hence

$$\left<E\right> = H_{kmkm} = \int \phi_{ek}^*(\mathbf{r}_e)\phi_{pm}^*(\mathbf{r}_p)\hat{H}_{\mathbf{r}}(\mathbf{r}_e,\mathbf{r}_p)\phi_{ek}(\mathbf{r}_e)\phi_{pm}(\mathbf{r}_p) \, d^3\mathbf{r}_e d^3\mathbf{r}_p$$

which has no exchange terms in it. For example, the Coulomb potential contribution to this energy would be

$$-\frac{e^2}{4\pi\varepsilon_0}\int\frac{\left|\phi_{eh}\left(\mathbf{r}_e\right)\right|^2\left|\phi_{pm}\left(\mathbf{r}_p\right)\right|^2}{\left(\mathbf{r}_e-\mathbf{r}_h\right)}d^3\mathbf{r}_e d^3\mathbf{r}_h$$

which has no exchange component to it.

16.3.3

(i) To find the representation of the position operator $\hat{\mathbf{r}}$ for a fermion in terms of fermion creation and annihilation operators, we use the wavefunction operator $\hat{\psi}$ in the single particle case, i.e., we write

$$\hat{\mathbf{r}} = \int \psi^\dagger \mathbf{r} \psi \, d^3\mathbf{r}$$
$$= \int \sum_{m,n} \hat{b}_m^+ \hat{b}_n \, \phi_m^*(\mathbf{r}) \mathbf{r} \phi_n(\mathbf{r}) \, d^3\mathbf{r} \tag{1}$$
$$= \sum_{m,n} r_{mn} \hat{b}_m^+ \hat{b}_n$$

where

$$r_{mn} = \int \phi_m^*(\mathbf{r}) \mathbf{r} \phi_n(\mathbf{r}) \, d^3\mathbf{r}$$

(ii) For the case of a particle in a one-dimensional box of width L, the wavefunctions are

$$\phi_m(z) = \sqrt{\frac{2}{L}} \sin\left(\frac{m\pi z}{L}\right)$$

so, if we are referring the position operator to the center of the well, we will have matrix elements for position relative to the center of the well of

$$r_{mn} = \frac{2}{L} \int_0^L \left(z - \frac{L}{2}\right) \sin\left(\frac{m\pi z}{L}\right) \sin\left(\frac{n\pi z}{L}\right) dz$$

Changing variables to $\zeta = \dfrac{\pi z}{L}$, we have

$$r_{mn} = \frac{2}{L}\left(\frac{L}{\pi}\right)^2 \int_0^\pi \left(\zeta - \frac{\pi}{2}\right) \sin(m\zeta)\sin(n\zeta) \, d\zeta$$
$$= -\frac{L}{\pi^2} \frac{8nm}{(n-m)^2 (n+m)^2} \quad \text{for } n+m \text{ odd} \tag{2}$$
$$= 0 \text{ for } n+m \text{ even}$$

which then becomes the r_{mn} in formula (1) above, i.e., we have, for this one-dimensional position operator

$$\hat{z} = \sum_{m,n} r_{mn} \hat{b}_m^\dagger \hat{b}_n$$

with r_{mn} given by formula (2) above.

(We could have chosen the position operator relative to the position of the left of the well. In that case, we would just end up adding $L/2$ to all of the "diagonal" (i.e., $m = n$) matrix elements.)

Chapter 17 problem solutions

17.2.1

(i) This process corresponds to the absorption of a photon from the plane wave state with wavevector $\mathbf{k}_3$, and changing a proton from the plane wave state with wavevector $\mathbf{k}_2$ to that with wavevector $\mathbf{k}_1$.

(ii) This process corresponds to the absorption of two photons both originally in the plane wave state with wavevector $\mathbf{k}_3$, and changing an electron from the plane wave state with wavevector $\mathbf{k}_2$ to that with wavevector $\mathbf{k}_1$. (This would be a two-photon absorption process, which is a possible non-linear optical process, and it does not violate Pauli exclusion because it is quite legal to have two photons in a given mode.)

(iii) This process corresponds to two protons scattering off each other (e.g., from the Coulomb interaction between them). Explicitly, two incident protons with initial wavevectors $\mathbf{k}_3$ and $\mathbf{k}_4$ scatter to give two protons with wavevectors $\mathbf{k}_1$ and $\mathbf{k}_2$.

(iv) This process would correspond to two electrons with initial wavevectors $\mathbf{k}_3$ and $\mathbf{k}_4$ scattering off one another to give two electrons in the same state with wavevector $\mathbf{k}_1$. This process, however, is forbidden by the Pauli exclusion principle, so it will never happen.

(v) This process corresponds to an electron with wavevector $\mathbf{k}_3$ and a proton wavevector $\mathbf{k}_4$ scattering off one another to give the electron and proton both with wavevector $\mathbf{k}_1$. (This process is not forbidden by Pauli exclusion because it is two different fermions that each occupy basis states with the same $\mathbf{k}$.)

(vi) This process corresponds to an electron initially with wavevector $\mathbf{k}_3$ and a photon initially with wavevector $\mathbf{k}_4$ scattering off of one another to give an electron with wavevector $\mathbf{k}_1$ and a photon with wavevector $\mathbf{k}_2$. (This is called Compton scattering.)

17.3.1

We have

$$H_{Cen} = \sum H_{Cjk\lambda\mu} \hat{b}_j^+ \hat{c}_\lambda^+ \hat{b}_k \hat{c}_\mu$$

and we can write

$$\left| N_{fm}; N_{bm} \right\rangle = \hat{c}_\alpha^+ \hat{b}_\mu^+ \left| 0 \right\rangle$$

$$\left| N_{fq}; N_{bq} \right\rangle = \hat{c}_\beta^+ \hat{b}_\nu^+ \left| 0 \right\rangle$$

Then

$$M = \left\langle N_{fq}; N_{bq} \left| \hat{b}_j^+ \hat{c}_\lambda^+ \hat{b}_k \hat{c}_\mu \right| N_{fm}; N_{bm} \right\rangle$$

$$= \left\langle 0 \left| \hat{b}_\nu \hat{c}_\beta \hat{b}_j^+ \hat{c}_\lambda^+ \hat{b}_k \hat{c}_\mu \hat{c}_\alpha^+ \hat{b}_u^+ \right| 0 \right\rangle$$

Now using the fact that the operators for different particles commute, we can rewrite this as

$$M = \left\langle 0 \left| \hat{b}_\nu \hat{b}_j^+ \hat{c}_\beta \hat{c}_\lambda^+ \hat{c}_\mu \hat{c}_\alpha^+ \hat{b}_k \hat{b}_u^+ \right| 0 \right\rangle$$

Now we use the anticommutation relation for identical fermions

$$\hat{b}_r \hat{b}_s^+ + \hat{b}_s^+ \hat{b}_r = \delta_{rs}$$

i.e.,

$$\hat{b}_r \hat{b}_s^+ = \delta_{rs} - \hat{b}_s^+ \hat{b}_r$$

and the commutation relation for identical bosons

$$\hat{c}_\rho \hat{c}_\sigma^+ - \hat{c}_\sigma^+ \hat{c}_\rho = \delta_{\rho\sigma}$$

i.e.,

$$\hat{c}_\rho \hat{c}_\sigma^+ = \delta_{\rho\sigma} + \hat{c}_\sigma^+ \hat{c}_\rho$$

to rewrite M, obtaining

$$M = \left\langle 0 \left| \left(\delta_{\nu j} - \hat{b}_j^+ \hat{b}_\nu \right) \left(\delta_{\beta\lambda} + \hat{c}_\lambda^+ \hat{c}_\beta \right) \left(\delta_{\mu\alpha} + \hat{c}_\alpha^+ \hat{c}_\mu \right) \left(\delta_{ku} - \hat{b}_k^+ \hat{b}_u \right) \right| 0 \right\rangle$$

i.e., since we have annihilation operators to the right in each case

$$M = \delta_{\nu j} \delta_{\beta\lambda} \delta_{\mu\alpha} \delta_{ku} \left\langle 0 \middle| 0 \right\rangle = \delta_{\nu j} \delta_{\beta\lambda} \delta_{\mu\alpha} \delta_{ku}$$

So

$$\left\langle N_{fq}; N_{bq} \left| H_{Cen} \right| N_{fm}; N_{bm} \right\rangle = H_{C\nu u\beta\alpha}$$

17.4.1

For an electron in state m (which we will choose later to be 1 or 2, depending on the part of the problem we are solving)

$$\left| N_{fs}; N_{bs} \right\rangle = \frac{1}{\sqrt{n_{\lambda 1}!}} \hat{b}_m^\dagger \left(\hat{a}_{\lambda_1}^\dagger \right)^{n_{\lambda 1}} \left| 0 \right\rangle$$

and we are interested in

$$\hat{H}_p \left| N_{fs}; N_{bs} \right\rangle = \sum_{j,k,\lambda} H_{ed\lambda jk} \hat{b}_j^\dagger \hat{b}_k \left(\hat{a}_\lambda - \hat{a}_\lambda^\dagger \right) \left| N_{fs}; N_{bs} \right\rangle$$

Now

$$\hat{b}_j^\dagger \hat{b}_k \left(\hat{a}_\lambda - \hat{a}_\lambda^\dagger \right) \hat{b}_m^\dagger \left(\hat{a}_{\lambda 1}^\dagger \right)^{n_{\lambda 1}} \left| 0 \right\rangle$$

$$= \hat{b}_j^\dagger \hat{b}_k \hat{b}_m^\dagger \left[\hat{a}_\lambda \left(\hat{a}_{\lambda 1}^\dagger \right)^{n_{\lambda 1}} - \hat{a}_\lambda^\dagger \left(\hat{a}_{\lambda 1}^\dagger \right)^{n_{\lambda 1}} \right] \left| 0 \right\rangle$$

$$= \hat{b}_j^\dagger \left(\delta_{km} - \hat{b}_m^\dagger \hat{b}_k \right) \left[\hat{a}_\lambda \left(\hat{a}_{\lambda 1}^\dagger \right)^{n_{\lambda 1}} - \hat{a}_\lambda^\dagger \left(\hat{a}_{\lambda 1}^\dagger \right)^{n_{\lambda 1}} \right] \left| 0 \right\rangle$$

Also

$$\hat{a}_\lambda \left(\hat{a}_{\lambda 1}^\dagger \right)^{n_{\lambda 1}} = \hat{a}_\lambda \hat{a}_{\lambda 1}^\dagger \left(\hat{a}_{\lambda 1}^\dagger \right)^{(n_{\lambda 1} - 1)} = \left(\delta_{\lambda \lambda_1} + \hat{a}_{\lambda 1}^\dagger \hat{a}_\lambda \right) \left(\hat{a}_{\lambda 1}^\dagger \right)^{(n_{\lambda 1} - 1)}$$

$$= \delta_{\lambda \lambda_1} \left(\hat{a}_{\lambda 1}^\dagger \right)^{(n_{\lambda 1} - 1)} + \hat{a}_{\lambda 1}^\dagger \hat{a}_\lambda \hat{a}_{\lambda 1}^\dagger \left(\hat{a}_{\lambda 1}^\dagger \right)^{(n_{\lambda 1} - 2)}$$

$$= \delta_{\lambda \lambda_1} \left(\hat{a}_{\lambda 1}^\dagger \right)^{(n_{\lambda 1} - 1)} + \delta_{\lambda \lambda_1} \left(\hat{a}_{\lambda 1}^\dagger \right)^{(n_{\lambda 1} - 1)} + \left(\hat{a}_{\lambda 1}^\dagger \right)^2 \hat{a}_\lambda \left(\hat{a}_{\lambda 1}^\dagger \right)^{(n_{\lambda 1} - 2)}$$

$$= n_{\lambda 1} \delta_{\lambda \lambda_1} \left(\hat{a}_{\lambda 1}^\dagger \right)^{(n_{\lambda 1} - 1)} + \left(\hat{a}_{\lambda 1}^\dagger \right)^{n_{\lambda 1}} \hat{a}_\lambda$$

and, so, eliminating terms with annihilation operators on the far right

$$\hat{H}_p \left| N_{fs}; n_{bs} \right\rangle = \frac{1}{\sqrt{n_{\lambda 1}!}} \sum_{j,k,\lambda} H_{ed\lambda jk} \delta_{km} \hat{b}_j^\dagger \left[n_{\lambda 1} \delta_{\lambda \lambda_1} \left(\hat{a}_{\lambda 1}^\dagger \right)^{(n_{\lambda 1} - 1)} - \hat{a}_\lambda^\dagger \left(\hat{a}_{\lambda 1}^\dagger \right)^{n_{\lambda 1}} \right] \left| 0 \right\rangle$$

$$= \sum_j \sqrt{n_{\lambda 1}} H_{ed\lambda_1 jm} \frac{1}{\sqrt{(n_{\lambda 1} - 1)!}} \hat{b}_j^\dagger \left(\hat{a}_{\lambda 1}^\dagger \right)^{(n_{\lambda 1} - 1)} \left| 0 \right\rangle - \sum_{j,\lambda} H_{ed\lambda jm} \frac{1}{\sqrt{n_{\lambda 1}!}} \hat{b}_j^\dagger \hat{a}_\lambda^\dagger \left(\hat{a}_{\lambda 1}^\dagger \right)^{(n_{\lambda 1})} \left| 0 \right\rangle$$

The only three possible final states for which we will get non-zero results for $\left\langle N_{fq}; N_{bq} \left| \hat{H}_p \right| N_{fs}; N_{bs} \right\rangle$ will be the following states.

(a)
$$\frac{1}{\sqrt{(n_{\lambda 1} - 1)!}} \hat{b}_j^\dagger \left(\hat{a}_{\lambda 1}^\dagger \right)^{(n_{\lambda 1} - 1)} \left| 0 \right\rangle$$

which we call state q_{abs}. It corresponds to an absorption transition with one photon removed from mode λ_1, and has energy $E_j + (n_{\lambda 1} - 1)\hbar\omega_{\lambda 1}$.

(b)
$$\frac{1}{\sqrt{(n_{\lambda 1} + 1)!}} \hat{b}_j^\dagger \left(\hat{a}_{\lambda 1}^\dagger \right)^{(n_{\lambda 1} + 1)} \left| 0 \right\rangle$$

which is for the particular case where $\lambda = \lambda_1$ and which we call q_{stim}. It corresponds to a stimulated emission transition with one photon added to mode λ_1, and has energy $E_j + (n_{\lambda 1} + 1)\hbar\omega_{\lambda 1}$.

(c)
$$\frac{1}{\sqrt{n_{\lambda 1}!}} \hat{b}_j^\dagger \hat{a}_\lambda^\dagger \left(\hat{a}_{\lambda 1}^\dagger\right)^{n_{\lambda 1}} |0\rangle$$

which is for the case $\lambda \neq \lambda_1$ and which we call q_{spon}. It corresponds to a spontaneous emission transition, with one photon added to mode λ, and has energy $E_j + \hbar\omega_\lambda + n_{\lambda 1}\hbar\omega_{\lambda 1}$.

(i) Considering the electron initially in state 2 (i.e., $m = 2$) and $\lambda = \lambda_1$, we have from time-dependent perturbation theory

$$\dot{c}_{qstim} = \frac{1}{i\hbar}\exp\left[i\left(E_j - E_2 + \hbar\omega_{\lambda 1}\right)t_0/\hbar\right] H_{ed\lambda_1 j2}\langle 0|\frac{1}{\sqrt{(n_{\lambda 1}+1)!}}\left(\hat{a}_{\lambda 1}\right)^{(n_{\lambda 1}+1)}\hat{b}_j\frac{1}{\sqrt{n_{\lambda 1}!}}\hat{b}_j^\dagger\left(\hat{a}_{\lambda 1}^\dagger\right)^{(n_{\lambda 1}+1)}|0\rangle$$

To get a properly normalized state with $n_{\lambda 1} + 1$ photons, we should have $1/\sqrt{(n_{\lambda 1}+1)!}$ instead of $1/\sqrt{n_{\lambda 1}!}$ inside the bra-ket expression, so we have to add a factor $\sqrt{(n_{\lambda 1}+1)}$ on the top line as we make this change on the bottom line. In other words, the bra-ket expression evaluates to $\sqrt{(n_{\lambda 1}+1)}$. Hence, we have

$$\dot{c}_{qstim} = \frac{1}{i\hbar}\exp\left[i\left(E_j - E_2 + \hbar\omega_{\lambda 1}\right)t_0/\hbar\right]\sqrt{n_{\lambda 1}+1}\; H_{ed\lambda_1 jZ}$$

which leads to a transition rate

$$w_{qstim} = \frac{2\pi}{\hbar}(n_{\lambda 1}+1)\left|H_{ed\lambda_1 j2}\right|^2 \delta\left(E_j - E_2 + \hbar\omega_{\lambda 1}\right)$$

The only choice of state, for which we can get the δ-function to be non-zero for any finite $\omega_{\lambda 1}$ is $j = 1$, and so we have

$$w_{qstim} = \frac{2\pi}{\hbar}(n_{\lambda 1}+1)\left|H_{ed\lambda_1 12}\right|^2 \delta\left(E_1 - E_2 + \hbar\omega_{\lambda 1}\right)$$

(ii) With the electron in state 2 (i.e., $m = 2$), and $\lambda \neq \lambda_1$, we have from time-dependent perturbation theory

$$\dot{c}_{qspon} = \frac{1}{i\hbar}\exp\left[i\left(E_j + \hbar\omega_\lambda - E_2\right)t_0/\hbar\right] H_{ed\lambda j2}\langle 0|\frac{1}{\sqrt{n_{\lambda 1}!}}\left(\hat{a}_{\lambda 1}\right)^{n_{\lambda 1}}\hat{a}_\lambda\hat{b}_j\frac{1}{\sqrt{n_{\lambda 1}!}}\hat{b}_j^\dagger\hat{a}_\lambda^\dagger\left(\hat{a}_{\lambda 1}^\dagger\right)^{n_{\lambda 1}}|0\rangle$$

The expression $\langle 0|...|0\rangle$ is in the form of the inner product of two identical normalized states, so we have

$$\dot{c}_{qspon} = \frac{1}{i\hbar}\exp\left[i\left(E_j + \hbar\omega_\lambda - E_2\right)t_0/\hbar\right] H_{ed\lambda j2}$$

which leads to the transition rate

$$w_{qspon} = \frac{2\pi}{\hbar}\left|H_{ed\lambda j2}\right|^2 \delta\left(E_j + \hbar\omega_\lambda - E_2\right)$$

The only choice of state j for which we can get the δ-function to be non-zero for finite ω_λ is $j = 1$, so we have

$$w_{qspon} = \frac{2\pi}{\hbar}\left|H_{ed\lambda 12}\right|^2 \delta\left(E_1 - E_2 + \hbar\omega_\lambda\right)$$

(iii) For the electron initially in state 1 with $n_{\lambda 1}$ photons in the mode we have from time-dependent perturbation theory

$$\dot{c}_{qabs} = \frac{1}{i\hbar}\exp\left[i\left(E_j - \hbar\omega_{\lambda 1} - E_1\right)t_0 / \hbar\right]\sqrt{n_{\lambda 1}}H_{ed\lambda_1 j1}$$

$$\times \left\langle 0\left|\frac{1}{\sqrt{(n_{\lambda 1}-1)!}}\left(\hat{a}_{\lambda 1}\right)^{(n_{\lambda 1}-1)}\hat{b}_j\frac{1}{\sqrt{(n_{\lambda 1}-1)!}}\hat{b}_j^\dagger\left(\hat{a}_{\lambda 1}^\dagger\right)^{(n_{\lambda 1}-1)}\right|0\right\rangle$$

The expression $\left\langle 0\left|...\right|0\right\rangle$ is in the form of the inner product of two identical normalized states, so we have

$$\dot{c}_{qabs} = \frac{1}{i\hbar}\exp\left[i\left(E_j - \hbar\omega_{\lambda 1} - E_1\right)t_0 / \hbar\right]\sqrt{n_{\lambda 1}}H_{ed\lambda_1 j1}$$

which leads to the transition rate

$$w_{qabs} = \frac{2\pi}{\hbar}n_{\lambda 1}\left|H_{ed\lambda_1 j1}\right|^2 \delta\left(E_j - E_1 - \hbar\omega_{\lambda 1}\right)$$

The only choice of state j for which we can get the δ-function to be non-zero for any finite $\omega_{\lambda 1}$ is $j = 2$, and so we have

$$w_{qabs} = \frac{2\pi}{\hbar}n_{\lambda 1}\left|H_{ed\lambda_1 Z1}\right|^2 \delta\left(E_2 - E_1 - \hbar\omega_{\lambda 1}\right)$$

Now

$$H_{ed\lambda_1 21} = H_{ed\lambda_1 12}{}^*$$

Also, we were asked here to consider not the state with $n_{\lambda 1}$ photons in the mode, but the state with $n_{\lambda 1} + 1$. Hence, finally we have

$$w_{qabs} = \frac{2\pi}{\hbar}\left(n_{\lambda 1} + 1\right)\left|H_{ed\lambda_1 12}\right|^2 \delta\left(E_2 - E_1 - \hbar\omega_{\lambda 1}\right)$$

which is identical to the rate for the stimulated emission from electron state 2 to state 1 with $n_{\lambda 1}$ photons originally in mode λ_1 (since $\delta(E_2 - E_1 - \hbar\omega_{\lambda 1}) = \delta(E_1 - E_2 + \hbar\omega_{\lambda 1})$).

17.4.2

(i) The classical Hamiltonian of this system is

$$\hat{H}_c = \frac{p^2}{2m} + \frac{1}{2}m\Omega^2(z-z_0)^2$$

Thus, we get the quantum mechanical Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + \frac{1}{2}m\Omega^2(z-z_0)^2$$

Using now the dimensionless position coordinate

$$\xi = \sqrt{\frac{m\Omega}{\hbar}}(z-z_0)$$

We can rewrite the Hamiltonian as

$$\hat{H} = \frac{\hbar\Omega}{2}\left(-\frac{d^2}{d\xi^2} + \xi^2\right) = \hbar\Omega\left(\hat{d}^\dagger\hat{d} + \frac{1}{2}\right)$$

where $\hat{d}$ is the annihilation operator for quanta of this oscillator and $\hat{d}^\dagger$ is the creation operator, each given by, respectively

$$\hat{d}^\dagger = \frac{1}{\sqrt{2}}\left(-\frac{d}{d\xi} + \xi\right)$$

$$\hat{d} = \frac{1}{\sqrt{2}}\left(\frac{d}{d\xi} + \xi\right)$$

(ii) From (i) and the standard theory for harmonic oscillators, we obtain the dimensionless position operator as

$$\xi = \frac{1}{\sqrt{2}}\left(\hat{d}^\dagger + \hat{d}\right)$$

and hence the operator for the real position ($z - z_0$) is

$$(z-z_0) = \sqrt{\frac{\hbar}{2m\Omega}}\left(\hat{d}^\dagger + \hat{d}\right)$$

(iii) For a mass with charge q, the electric dipole energy will be, classically, for a displacement from position z_0

$$H_{ed} = -q\mathbf{E}\cdot\boldsymbol{\zeta}(z-z_0)$$

where $\boldsymbol{\zeta}$ is a unit vector in the z-direction, and $\mathbf{E}$ is the classical electric field. Now we can postulate the quantized version, using the multimode electric field operator to substitute for $\mathbf{E}$,

$$\hat{\mathbf{E}}(\mathbf{r},t) = i\sum_\lambda\left(\hat{a}_\lambda - \hat{a}_\lambda^\dagger\right)\sqrt{\frac{\hbar\omega_\lambda}{2\varepsilon_o}}\mathbf{u}_\lambda(\mathbf{r})$$

and the position operator from (ii) to substitute for z - z_0, giving

$$\hat{H}_{ed} = -qi\sqrt{\frac{\hbar}{2m\Omega}}\sqrt{\frac{\hbar}{2\varepsilon_0}}\sum_{\lambda}\left(\hat{a}_{\lambda} - \hat{a}_{\lambda}^{\dagger}\right)\left(\hat{d}^{\dagger} + \hat{d}\right)\sqrt{\omega_{\lambda}}\mathbf{u}_{\lambda}(\mathbf{r}_0)\cdot\boldsymbol{\zeta}$$

where we have made the suggested simplification of substituting $\mathbf{u}_{\lambda}(\mathbf{r}_0)$ for $\mathbf{u}_{\lambda}(\mathbf{r})$, where $\mathbf{r}_0$ is the (equilibrium) position of the oscillating mass. We make this simplification because the electromagnetic wave, by assumption, varies very little over the size of the oscillating system.

(iv) We consider $\hat{H}_{ed}$ as a perturbing Hamiltonian. We consider also now states $|n_{vm};N_{bm}\rangle$. n_{vm} is the number of quanta in the vibrating mode of the mass when the entire system is in state m. N_{bm} is the list of occupation numbers for all of the electric field modes.

In looking at the transition rate from a state m of the system to a state q, we have

$$w_{mq} = \frac{2\pi}{\hbar}\left|\left\langle n_{vq};N_{bq}\left|\hat{H}_{ed}\right|n_{vm};N_{bm}\right\rangle\right|^2\delta\left(E_q - E_m\right)$$

We consider the initial state to be one with a photon in the plane wave mode polarized by assumption for this part of the problem in the $\boldsymbol{\zeta}$ direction (i.e., the z direction) , with (1) a corresponding mode function

$$\mathbf{u}_{\lambda}(\mathbf{r}) = \frac{1}{\sqrt{V_b}}\boldsymbol{\zeta}\exp\left[i\mathbf{k}_{\lambda}\cdot\mathbf{r}\right]$$

where V_b is the volume of the "box" for the wave, so

$$\mathbf{u}_{\lambda}(\mathbf{r}_0) = \frac{1}{\sqrt{V_b}}\boldsymbol{\zeta}\exp\left[i\mathbf{k}_{\lambda}\cdot\mathbf{r}_0\right]\quad(\equiv\boldsymbol{\zeta}u_{\lambda}(\mathbf{r}_0))$$

and (2) no quanta in the vibrating system.

Hence, the initial state is

$$|n_{vs};N_{bs}\rangle = \hat{a}_{\lambda 1}^{\dagger}|0\rangle$$

which has energy $E_g = \hbar\omega_{\lambda}$. Hence, with the mode polarized in the z direction by assumption for this part of the problem (so $\mathbf{u}_{\lambda}(\mathbf{r}_0)\cdot\boldsymbol{\zeta} = u_{\lambda}(\mathbf{r}_0)$)

$$\hat{H}_{ed}|n_{vs};N_{bs}\rangle = \sum_{\lambda}C_{\lambda}\sqrt{\omega_{\lambda}}\left(\hat{a}_{\lambda} - \hat{a}_{\lambda}^{\dagger}\right)\left(\hat{d}^{\dagger} + \hat{d}\right)\hat{a}_{\lambda 1}^{\dagger}|0\rangle$$

where

$$C_{\lambda} = -qi\sqrt{\frac{\hbar^2}{4m\Omega\varepsilon_0 V_b}}\exp\left(i\mathbf{k}_{\lambda}\cdot\mathbf{r}_0\right)$$

(Note here that, because of our simplifying assumption that the wavelength is much larger than the oscillator, C_{λ} is just a number for any given mode λ. It is not a function of position. This means that, when we have to evaluate a matrix element like $\left\langle n_{vq};N_{bq}\left|\hat{H}_{ed}\right|n_{vs};N_{bs}\right\rangle$ below, the results are particularly simple. Formally, such a matrix element does involve an integration over space, but the only integrals actually required will reduce to the normalization or orthogonality integrals with basis

functions. Those integrals are by definition trivial (being just Kronecker deltas), and the answers are basically already built in to our formalism.)

Now proceeding to consider the explicit effects of the operators, we have

$$
\begin{aligned}
\left(\hat{a}_\lambda - \hat{a}_\lambda^\dagger\right)\left(\hat{d}^\dagger + \hat{d}\right)\hat{a}_{\lambda 1}^\dagger\,|0\rangle &= \left(\hat{a}_\lambda - \hat{a}_\lambda^\dagger\right)\hat{a}_{\lambda 1}^\dagger\left(\hat{d}^\dagger + \hat{d}\right)|0\rangle \\
&= \hat{a}_\lambda \hat{a}_{\lambda 1}^\dagger \hat{d}^\dagger\,|0\rangle - \hat{a}_\lambda^\dagger \hat{a}_{\lambda 1}^\dagger \hat{d}^\dagger\,|0\rangle \\
&= \left(\delta_{\lambda,\lambda 1} - \hat{a}_{\lambda 1}^\dagger \hat{a}_\lambda\right)\hat{d}^\dagger\,|0\rangle - \hat{a}_\lambda^\dagger \hat{a}_{\lambda 1}^\dagger \hat{d}^\dagger\,|0\rangle \\
&= \delta_{\lambda,\lambda 1}\hat{d}^\dagger\,|0\rangle - \hat{a}_\lambda^\dagger \hat{a}_{\lambda 1}^\dagger \hat{d}^\dagger\,|0\rangle
\end{aligned}
$$

There are therefore two possible states to give finite matrix elements $\left\langle n_{vq}; N_{bq}\left|\hat{H}_{ed}\right|n_{vs}; N_{bs}\right\rangle$, which are

(a) $\left|n_{vq}; N_{bq}\right\rangle = \delta_{\lambda,\lambda 1}\hat{d}^\dagger\,|0\rangle$

which has energy $E_q = \hbar\Omega$.

(b) $\left|n_{vq}; N_{bq}\right\rangle = \hat{a}_\lambda^\dagger \hat{a}_{\lambda 1}^\dagger \hat{d}^\dagger\,|0\rangle$

which has energy $E_q = \hbar\Omega + \hbar\omega_\lambda + \hbar\omega_{\lambda 1}$. This second state (b) can be discarded because

$$
E_q - E_m = \hbar\Omega + \hbar\omega_{\lambda 1}
$$

can never be zero and so the δ-function in Fermi's Golden Rule is always zero. Hence we are left only with state (a). So, the transition rate is

$$
w_{mq} = \frac{2\pi}{\hbar}\left|C_{\lambda 1}\right|^2 \omega_{\lambda 1}\delta\left(\hbar\Omega - \hbar\omega_{\lambda 1}\right)
$$

or, explicitly

$$
w_{mq} = \frac{2\pi}{\hbar}\frac{q^2\hbar^2\omega_{\lambda 1}}{4m\Omega\varepsilon_0 V_b}\delta\left(\hbar\Omega - \hbar\omega_{\lambda 1}\right)
$$

Hence the absorption spectrum is very simple; there is one optical absorption line, and it is for photon energy $\hbar\omega_{\lambda 1} = \hbar\Omega$, i.e., the frequency of the light has to match the natural oscillation frequency of the vibrating system.

(v) The analysis of spontaneous emission proceeds very similarly to the electron-photon case, except we have a slightly different form for the matrix element.

We take the initial state to be one with no photons and with the vibrating system in its first excited state

$$
\left|n_{vs}; N_{bs}\right\rangle = \hat{d}^\dagger\,|0\rangle
$$

and we will consider each different possible final state corresponding to a photon in a mode λ and the vibrating system in its lowest state, without any quanta, i.e.,

$$
\left|n_{vq}; N_{bq}\right\rangle = \hat{a}_\lambda^\dagger\,|0\rangle
$$

Hence, the matrix element becomes, for a photon mode polarized in the direction $\mathbf{e}_\lambda$ (i.e., $\mathbf{u}_\lambda(\mathbf{r}) = \dfrac{1}{\sqrt{V_b}} \mathbf{e}_\lambda \exp(\imath k_\lambda \cdot \mathbf{r})$).

$$C_\lambda \sqrt{\omega_\lambda} \mathbf{e}_\lambda \cdot \zeta \langle 0| \hat{a}_\lambda \left(\hat{a}_\lambda - \hat{a}_\lambda^\dagger \right)\left(\hat{d}^\dagger + \hat{d} \right)\hat{d}^\dagger |0\rangle$$

$$= C_\lambda \sqrt{\omega_\lambda} \mathbf{e}_\lambda \cdot \zeta \Big[\langle 0|(\hat{a}_\lambda)^2(\hat{d}^\dagger)^2|0\rangle - \langle 0|\hat{a}_\lambda \hat{a}_\lambda^\dagger(\hat{d}^\dagger)^2|0\rangle + \langle 0|(\hat{a}_\lambda)^2\hat{d}\hat{d}^\dagger|0\rangle - \langle 0|\hat{b}_\lambda \hat{b}_\lambda^\dagger \hat{d}\hat{d}^\dagger|0\rangle \Big]$$

The first three terms are all zero; there are several equivalent ways of looking at why, but in each case we are left with at least one annihilation operator operating on $|0\rangle$ or a creation operator "operating to the left" on $\langle 0|$.

We note that

$$\hat{a}_\lambda \hat{a}_\lambda^\dagger \hat{d}\hat{d}^\dagger |0\rangle = \left(1 + \hat{a}_\lambda^\dagger \hat{a}_\lambda\right)\left(1 + \hat{d}^\dagger \hat{d}\right)|0\rangle = |0\rangle$$

Hence we have

$$\left\langle n_{vq}; N_{bq} \left| \hat{H}_{ed} \right| n_{vs}; N_{bs} \right\rangle = C_\lambda \sqrt{\omega_\lambda} \mathbf{e}_\lambda \cdot \zeta$$

We will therefore, in general, have a total spontaneous emission transition rate of

$$W_{spon} = \frac{2\pi}{\hbar} \sum_\lambda \left| \left\langle n_{vq}; N_{bq} \left| \hat{H}_{ed} \right| n_{vs}; N_{bs} \right\rangle \right|^2 \delta\left(\hbar\omega_\lambda - \hbar\Omega\right)$$

i.e.,

$$W_{spon} = \frac{2\pi}{\hbar} \sum_\lambda |C_\lambda|^2 \, \omega_\lambda \left(\mathbf{e}_\lambda \cdot \zeta\right)^2 \delta\left(\hbar\omega_\lambda - \hbar\Omega\right)$$

As in the electron photon case, we choose our polarization directions for the plane wave modes to be either perpendicular to the plane of ζ and $\mathbf{k}_\lambda$, in which case there is no interaction ($\mathbf{e}_\lambda \cdot \zeta = 0$), or we choose them in the plane of ζ and $\mathbf{k}_\lambda$, in which case, for an angle θ between $\mathbf{k}_\lambda$ and ζ, since $\mathbf{e}_\lambda$ is perpendicular to $\mathbf{k}_\lambda$

$$\mathbf{e}_\lambda \cdot \zeta = \sin\theta$$

Changing from a sum to an integral

$$\sum_\lambda \to \int \frac{V_b}{\left(2\pi\right)^3} d^3\mathbf{k}_\lambda$$

leads to

$$W_{spon} = \frac{2\pi}{\hbar} \frac{V_b}{\left(2\pi\right)^3} |C|^2 \int \omega_\lambda \sin^2\theta \, \delta\left(\hbar\omega_\lambda - \hbar\Omega\right)d^3\mathbf{k}_\lambda$$

where the absolute value of C_λ is independent of λ. We have

$$|C_\lambda|^2 = |C|^2 = \frac{q^2\hbar^2}{4m\Omega\varepsilon_0 V_b}$$

Also

$$\int \omega_\lambda \sin^2\theta\, \delta\left(\hbar\omega_\lambda - \hbar\Omega\right) d^3\mathbf{k}_\lambda = \int\limits_{k_\lambda=0}^{\infty} \int\limits_{\theta=0}^{\pi} \omega_\lambda \sin^2\theta\, \delta\left(\hbar\omega_\lambda - \hbar\Omega\right) 2\pi \sin\theta\, d\theta\, dk_\lambda^2 dk_\lambda$$

$$= \frac{2\pi}{\hbar^4 c^3} \int_0^\pi \sin^3\theta\, d\theta \int\limits_{\hbar ck_\lambda=0}^{\infty} \hbar ck_\lambda\, \delta(\hbar ck_\lambda - \hbar\Omega)(\hbar ck_\lambda)^2\, d\hbar ck_\lambda$$

$$= \frac{2\pi}{\hbar^4 c^3} \frac{4}{3}(\hbar\Omega)^3 = \frac{8\pi}{3\hbar c^3}\Omega^3$$

Thus, we obtain the total spontaneous emission rate

$$W_{spon} = \frac{2\pi}{\hbar} \frac{V_b}{\left(2\pi\right)^3} \frac{q^2\hbar^2}{4m\Omega\varepsilon_0 V_b} \frac{8\pi\Omega^3}{3\hbar c^3}$$

$$= \frac{2\pi \times 8\pi}{3\times 8\pi^3 \times 4} \frac{q^2\Omega^2}{m\varepsilon_0 c^3}$$

$$= \frac{1}{6\pi} \frac{q^2\Omega^2}{m\varepsilon_0 c^3}$$

(vi) Hence for $m = 10^{-26}\, kg$, $\Omega = 2\pi \times 10^{14}\, s^{-1}$, $q = 1.602 \times 10^{-19}\, C$

$$W_{spon} = \frac{1}{6\pi} \times \frac{(1.602)^2(2\pi)^2}{8.85\times 27} \times 10^{-19-19+14+14+26+12-24}$$

$$= 0.0225\times 10^4 = 2.25\times 10^2\ \text{s}^{-1}$$

Therefore, the natural lifetime of this state is

$$\tau = \frac{1}{W_{spon}} = 4.4\,\text{ms}$$

The electromagnetic modes themselves are uniformly distributed in angle, but their interaction with the vibration is not. Those modes propagating along the z-axis have an electric field perpendicular to the motion of the mass and cannot interact with it, so there is no emission along the z-axis. The emission probability increases steadily as we move to modes whose propagation is perpendicular to the z-axis, where the emission probability is maximum. The emission probability is cylindrically symmetric around the z-axis. (The actual relative strength is $\alpha \sin^2\theta$, coming from $\left|(\mathbf{u}_\lambda \cdot \boldsymbol{\zeta})\right|^2$, where θ is the angle between the propagation direction and the z direction).

Chapter 18 problem solutions

18.3.1

(i) This is not entangled, because it can be rewritten as

$$\frac{1}{\sqrt{2}}\left(|H\rangle_1|V\rangle_2 - |H\rangle_1|H\rangle_2\right) = |H\rangle_1 \frac{1}{\sqrt{2}}\left(|V\rangle_2 - |H\rangle_2\right)$$

(ii) This is entangled

(iii) This is not entangled, because it can be written as

$$\left(\frac{3}{5}|H\rangle_1 + \frac{4i}{5}|V\rangle_1\right)|V\rangle_2$$

(iv) This is not entangled, because it can be written as

$$\frac{1}{2}\left(|H\rangle_1|H\rangle_2 + |H\rangle_1|V\rangle_2 + |V\rangle_1|H\rangle_2 + |V\rangle_1|V\rangle_2\right)$$

$$= \frac{1}{\sqrt{2}}\left(|H\rangle_1 + |V\rangle_1\right)\frac{1}{\sqrt{2}}\left(|H\rangle_2 + |V\rangle_2\right)$$

18.3.2

$$\left(\left\langle \Psi^+ \right|_{12} \right) \left| \Phi^- \right\rangle_{12} = \frac{1}{2} \left(\left\langle H \right|_1 \left\langle V \right|_2 + \left\langle V \right|_1 \left\langle H \right|_2 \right) \left(\left| H \right\rangle_1 \left| H \right\rangle_2 - \left| V \right\rangle_1 \left| V \right\rangle_2 \right)$$

$$= \frac{1}{2} \left(\left\langle H \right|_1 \left| H \right\rangle_1 \left\langle V \right|_2 \left| H \right\rangle_2 + \left\langle H \right|_2 \left| H \right\rangle_2 \left\langle V \right|_1 \left| H \right\rangle_1 - \left\langle V \right|_2 \left| V \right\rangle_2 \left\langle H \right|_1 \left| V \right\rangle_1 - \left\langle V \right|_1 \left| V \right\rangle_1 \left\langle H \right|_2 \left| V \right\rangle_2 \right)$$

$$= \frac{1}{2} \left(\left\langle V \right|_2 \left| H \right\rangle_2 + \left\langle V \right|_1 \left| H \right\rangle_1 - \left\langle H \right|_1 \left| V \right\rangle_1 - \left\langle H \right|_2 \left| V \right\rangle_2 \right)$$

$$= \frac{1}{2} \left(0 + 0 - 0 - 0 \right)$$

$$= 0$$

18.3.3

From the definitions of the Bell states, we find

$$|H\rangle_1 |H\rangle_2 = \frac{1}{\sqrt{2}}\left(|\Phi^+\rangle_{12} + |\Phi^-\rangle_{12}\right)$$

$$|V\rangle_1 |V\rangle_2 = \frac{1}{\sqrt{2}}\left(|\Phi^+\rangle_{12} - |\Phi^-\rangle_{12}\right)$$

$$|H\rangle_1 |V\rangle_2 = \frac{1}{\sqrt{2}}\left(|\Psi^+\rangle_{12} + |\Psi^-\rangle_{12}\right)$$

$$|V\rangle_1 |H\rangle_2 = \frac{1}{\sqrt{2}}\left(|\Psi^+\rangle_{12} - |\Psi^-\rangle_{12}\right)$$

Hence the general two-particle state where each particle has two available basis states $|H\rangle$ and $|V\rangle$ can be written

$$|\psi\rangle = c_{HH}|H\rangle_1|H\rangle_2 + c_{HV}|H\rangle_1|V\rangle_2 + c_{VH}|V\rangle_1|H\rangle_2 + c_{VV}|V\rangle_1|V\rangle_2$$

$$= \frac{1}{\sqrt{2}}\left\{ \begin{array}{l} c_{HH}\left[|\Phi^+\rangle_{12} + |\Phi^-\rangle_{12}\right] + c_{HV}\left[|\Psi^+\rangle_{12} + |\Psi^-\rangle_{12}\right] \\ + c_{VH}\left[|\Psi^+\rangle_{12} - |\Psi^-\rangle_{12}\right] + c_{VV}\left[|\Phi^+\rangle_{12} - |\Phi^-\rangle_{12}\right] \end{array} \right\}$$

$$= \frac{c_{HH} + c_{VV}}{\sqrt{2}}|\Phi^+\rangle_{12} + \frac{c_{HH} - c_{VV}}{\sqrt{2}}|\Phi^-\rangle_{12} + \frac{c_{HV} + c_{VH}}{\sqrt{2}}|\Psi^+\rangle_{12} + \frac{c_{HV} - c_{VH}}{\sqrt{2}}|\Psi^-\rangle_{12}$$

18.3.4

(i) Consider the Bell state

$$\left|\Phi^-\right\rangle_{12} = \frac{1}{\sqrt{2}}\left(\left|H\right\rangle_1\left|H\right\rangle_2 - \left|V\right\rangle_1\left|V\right\rangle_2\right)$$

Now consider a new set of axes at +45° and -45°. In terms of the corresponding states

$$\left|+45\right\rangle = \frac{1}{\sqrt{2}}\left(\left|H\right\rangle + \left|V\right\rangle\right) \quad \left|-45\right\rangle = \frac{1}{\sqrt{2}}\left(\left|H\right\rangle - \left|V\right\rangle\right)$$

we can write

$$\left|H\right\rangle = \frac{1}{\sqrt{2}}\left(\left|+45\right\rangle + \left|-45\right\rangle\right) \quad \left|V\right\rangle = \frac{1}{\sqrt{2}}\left(\left|+45\right\rangle - \left|-45\right\rangle\right)$$

Hence, rewriting $\left|\Phi^-\right\rangle$ in terms of these new states, we have

$$\left|\Phi^-\right\rangle = \left(\frac{1}{\sqrt{2}}\right)^3 \left[\left(\left|+45\right\rangle_1 + \left|-45\right\rangle_1\right)\left(\left|+45\right\rangle_2 + \left|-45\right\rangle_2\right) - \left(\left|+45\right\rangle_1 - \left|-45\right\rangle_1\right)\left(\left|+45\right\rangle_2 - \left|-45\right\rangle_2\right)\right]$$

$$= \frac{1}{2}\frac{1}{\sqrt{2}}\left[\left|+45\right\rangle_1\left|+45\right\rangle_2 + \left|-45\right\rangle_1\left|-45\right\rangle_2 + \left|+45\right\rangle_1\left|-45\right\rangle_2 + \left|-45\right\rangle_1\left|+45\right\rangle_2\right.$$

$$\left. - \left|+45\right\rangle_1\left|+45\right\rangle_2 - \left|-45\right\rangle_1\left|-45\right\rangle_2 + \left|+45\right\rangle_1\left|-45\right\rangle_2 + \left|-45\right\rangle_1\left|+45\right\rangle_2\right]$$

$$= \frac{1}{\sqrt{2}}\left|+45\right\rangle_1\left|-45\right\rangle_2 + \left|-45\right\rangle_1\left|+45\right\rangle_2$$

which is still a Bell state.

(ii) Consider the Bell state

$$\left|\Phi^+\right\rangle_{12} = \frac{1}{\sqrt{2}}\left(\left|H\right\rangle_1\left|H\right\rangle_2 + \left|V\right\rangle_1\left|V\right\rangle_2\right)$$

Similarly we can rewrite $\left|\Phi^+\right\rangle_{12}$ in the $\left|+45\right\rangle$ and $\left|-45\right\rangle$ states, obtaining

$$\left|\Phi^+\right\rangle_{12} = \left(\frac{1}{\sqrt{2}}\right)^3 \left[\left(\left|+45\right\rangle_1 + \left|-45\right\rangle_1\right)\left(\left|+45\right\rangle_2 + \left|-45\right\rangle_2\right) + \left(\left|+45\right\rangle_1 - \left|-45\right\rangle_1\right)\left(\left|+45\right\rangle_2 - \left|-45\right\rangle_2\right)\right]$$

$$= \frac{1}{2}\frac{1}{\sqrt{2}}\left[\left|+45\right\rangle_1\left|+45\right\rangle_2 + \left|-45\right\rangle_1\left|-45\right\rangle_2 + \left|+45\right\rangle_1\left|-45\right\rangle_2 + \left|-45\right\rangle_1\left|+45\right\rangle_2\right.$$

$$\left. + \left|+45\right\rangle_1\left|+45\right\rangle_2 + \left|-45\right\rangle_1\left|-45\right\rangle_2 - \left|+45\right\rangle_1\left|-45\right\rangle_2 - \left|-45\right\rangle_1\left|-45\right\rangle_2\right]$$

$$= \frac{1}{\sqrt{2}}\left[\left|+45\right\rangle_1\left|+45\right\rangle_2 + \left|-45\right\rangle_1\left|-45\right\rangle_2\right]$$

which is not only a Bell state, but is the same form of Bell state as the original version of state $\left|\Phi^+\right\rangle_{12}$.

Chapter 19 problem solutions

19.1.1

(i) Consider axes at angles rotated by θ relative to the horizontal.
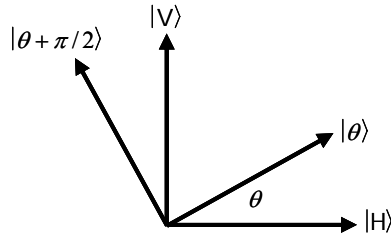
Then

$$|V\rangle = \sin\theta|\theta\rangle + \cos\theta\left|\theta + \frac{\pi}{2}\right\rangle$$

$$|H\rangle = \cos\theta|\theta\rangle - \sin\theta\left|\theta + \frac{\pi}{2}\right\rangle$$

So, on these new axes, we can rewrite

$$
\begin{aligned}
\left|\Phi^+\right\rangle_{12} &= \frac{1}{\sqrt{2}}\left[\left(\cos\theta|\theta\rangle_1 - \sin\theta\left|\theta+\frac{\pi}{2}\right\rangle_1\right)\left(\cos\theta|\theta\rangle_2 - \sin\theta\left|\theta+\frac{\pi}{2}\right\rangle_2\right)\right.\\
&\quad \left.+\left(\sin\theta|\theta\rangle_1 + \cos\theta\left|\theta+\frac{\pi}{2}\right\rangle_1\right)\left(\sin\theta|\theta\rangle_2 + \cos\theta\left|\theta+\frac{\pi}{2}\right\rangle_2\right)\right]\\
&= \frac{1}{\sqrt{2}}\left[\cos^2\theta|\theta\rangle_1|\theta\rangle_2 + \sin^2\theta\left|\theta+\frac{\pi}{2}\right\rangle_1\left|\theta+\frac{\pi}{2}\right\rangle_2\right.\\
&\quad -\sin\theta\cos\theta\left|\theta+\frac{\pi}{2}\right\rangle_1|\theta\rangle_2 - \cos\theta\sin\theta|\theta\rangle_1\left|\theta+\frac{\pi}{2}\right\rangle_2\\
&\quad +\sin^2\theta|\theta\rangle_1|\theta\rangle_2 + \cos^2\theta\left|\theta+\frac{\pi}{2}\right\rangle_1\left|\theta+\frac{\pi}{2}\right\rangle_2\\
&\quad \left.+\sin\theta\cos\theta|\theta\rangle_1\left|\theta+\frac{\pi}{2}\right\rangle_2 + \cos\theta\sin\theta\left|\theta+\frac{\pi}{2}\right\rangle_1|\theta\rangle_2\right]\\
&= \frac{1}{\sqrt{2}}\left[|\theta\rangle_1|\theta\rangle_2 + \left|\theta+\frac{\pi}{2}\right\rangle_1\left|\theta+\frac{\pi}{2}\right\rangle_2\right]
\end{aligned}
$$

(ii) If one photon is measured with a polarizer at angle θ and is found to pass, then the state has been collapsed to $|\theta\rangle_1|\theta\rangle_2$, and the other photon will be found also to pass a polarizer at angle θ. A similar argument follows for polarizers at $\theta + \pi/2$. Hence, the two photons always emerge on the same arm of aligned polarization splitters, regardless of the orientation of the polarizers, because θ is an arbitrary angle.

19.3.1

Write

$$\psi(\mathbf{r},t) = R(\mathbf{r},t)\exp\big(iS(\mathbf{r},t)\big)$$

where S and R are real (this is sufficient for describing any complex ψ). ψ obeys the Schrödinger wave equation. Differentiating gives

$$\nabla\psi = \nabla R\exp(iS) + iR\nabla S\exp(iS)$$

$$\nabla^2\psi = \big[\nabla^2 R + 2i\nabla R\nabla S + iR\nabla^2 S - R(\nabla S)^2\big]\exp(iS)$$

and

$$\frac{\partial\psi}{\partial t} = \left[\frac{\partial R}{\partial t} + iR\frac{\partial S}{\partial t}\right]\exp(iS)$$

So the the Schrödinger wave equation gives us

$$-\frac{\hbar^2}{2m}\Big[\nabla^2 R - R(\nabla S)^2\Big]\exp(iS) + VR\exp(iS) - \frac{\hbar^2 i}{2m}\Big[2\nabla R\nabla S + R\nabla^2 S\exp(iS)\Big]$$

$$= i\hbar\left[\frac{\partial R}{\partial t} + iR\frac{\partial S}{\partial t}\right]\exp(iS) = \left[-R\frac{\partial S}{\partial t} + i\hbar\frac{\partial R}{\partial t}\right]\exp(iS)$$

Dividing by $\exp(iS)$ and then separately equating real and imaginary parts, we have, for the real part

$$-\frac{\hbar^2}{2m}\nabla^2 R + \frac{R(\nabla S)^2}{2m} + VR = -\frac{R\partial S}{\partial t}$$

Dividing by R and rearranging, we have

$$\frac{\partial S}{\partial t} + \frac{(\nabla S)^2}{2m} + V - \frac{\hbar^2}{2m}\frac{\nabla^2 R}{R} = 0$$

which is the required solution for part (i).

From the imaginary part we have

$$-\frac{\hbar\partial R}{\partial t} - \frac{\hbar}{m}\nabla R\nabla S - \frac{\hbar R\nabla^2 S}{2m} = 0$$

that is,

$$\frac{\partial R}{\partial t} + \frac{\nabla R\nabla S}{m} + \frac{R\nabla^2 S}{2m} = 0 \tag{A}$$

Now consider

$$\frac{\partial R^2}{\partial t} + \nabla\cdot\left(\frac{R^2\nabla S}{m}\right) = 0$$

After taking the divergence, we have

$$2R\frac{\partial R}{\partial t} + 2R\nabla R\frac{\nabla S}{m} + \frac{R^2\nabla^2 S}{m} = 0$$

Dividing by $2R$ gives Eq. (A) above, so we have proved (A), the required result for part (ii).