# Solutions to Selected Problems

# for

# Quantum Mechanics for Scientists and Engineers

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# Introduction

Selected problems in the book *Quantum Mechanics for Scientists and Engineers* (Cambridge University Press, 2008) are marked with an asterisk (*), and solutions to these problems are collected here so that students can have access to additional worked examples.

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## 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,

$$\begin{aligned} P &= \int_{0.1}^{0.2} \left|\psi_1(z)\right|^2 dz = \int_{0.1}^{0.2} 2\sin^2(\pi z) dz \\ &= \int_{0.1}^{0.2} \left[1 - \cos(2\pi z)\right] dz \\ &= 0.1 - \int_{0.1}^{0.2} \cos(2\pi z) dz \\ &= 0.1 - \frac{1}{2\pi}\left[\sin(2\pi \times 0.2) - \sin(2\pi \times 0.1)\right] \\ &= 0.042 \end{aligned}$$

(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 $\pi$ radians.)

## 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 $x = 0$

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

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 $x = 0$,

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

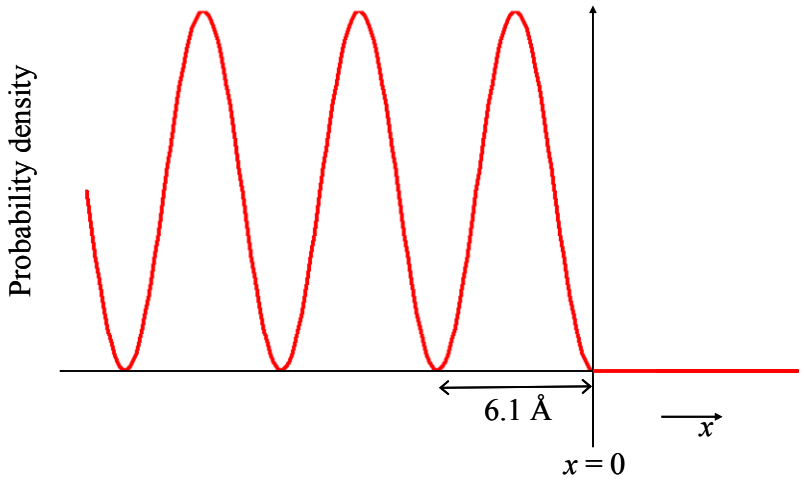
Thus, the wave function on the left hand side of the infinite barrier is a standing wave.

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

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

which has a period $\pi / k$.

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.)

## 2.8.3

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 $$k_L = \sqrt{\frac{2mE}{\hbar^2}} = 6.27\times10^9 \text{ m}^{-1} \quad \text{and} \quad k_R = \sqrt{\frac{2m(E-V_o)}{\hbar^2}} = 3.62\times10^9 \text{ m}^{-1}$$

Now applying boundary conditions

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

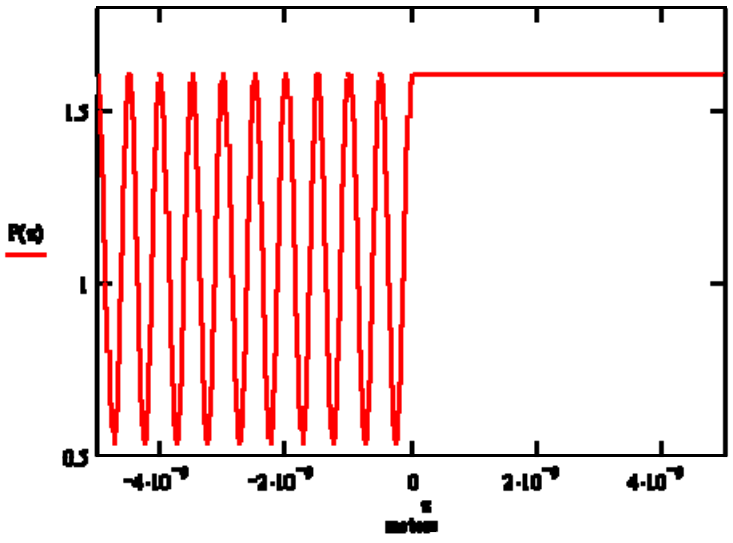
(b) continuity of the derivative of the wavefunction at $z$=0: $(C-D)k_L = k_R F$

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

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

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

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.



## 2.8.7

(i) The solution in the left half of the well is of the form

$$\sin\left(k_L z\right) \text{ with } k_L = \sqrt{\frac{2m_o E_S}{\hbar^2}}$$

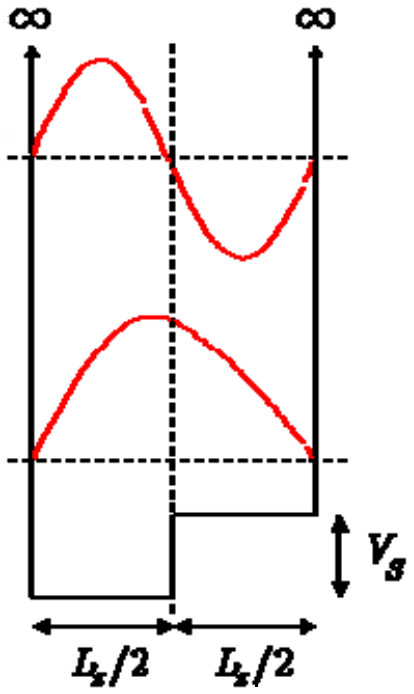
Note that this has a zero at the left wall as required.

The solution in the right half of the well is of the form

$$\sin\left(k_R\left(L_z - z\right)\right) \text{ (or } \sin\left(k_R\left(z - L_z\right)\right)\text{) with } k_R = \sqrt{\frac{2m_o\left(E_S - V_S\right)}{\hbar^2}}$$

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 $\left(\hbar^2/2m_o\right)\left(\pi/L_z\right)^2$, 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 $E_S > V_S$.

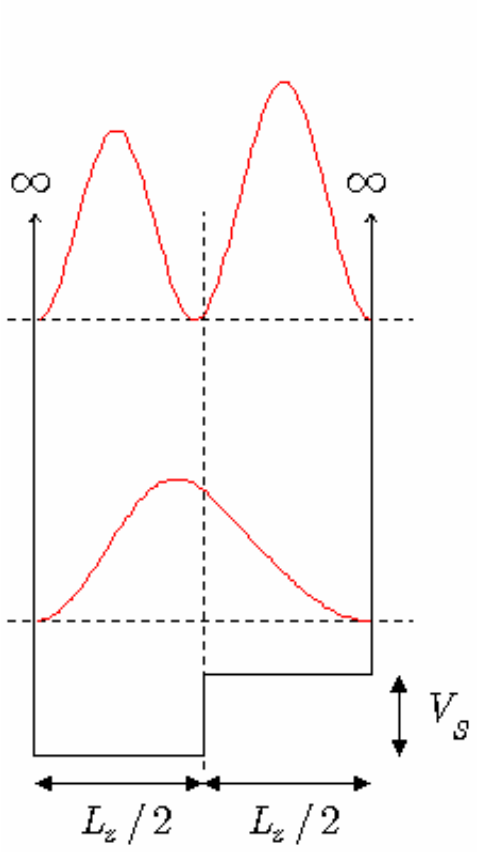



(ii) The lowest eigenstate we expect to have no zeros within the well. It will be sinusoidal in both halves, but will be more rapidly changing in the left half. This means that more than one quarter cycle will be in the left half, and less than one quarter cycle will be in the right half, hence the function 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.)

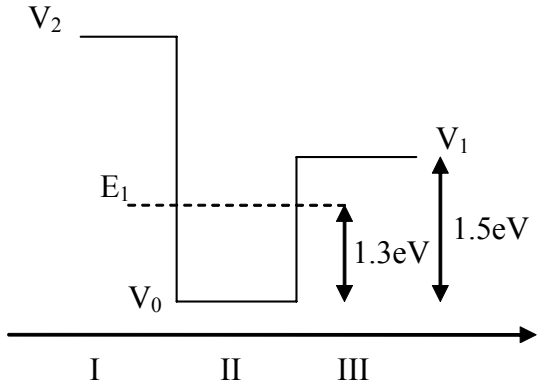
(The particular curves on the graphs here are actual solutions of such a stepped well problem for an electron, with $L_z$ = 1 nm and $V_S$ = 0.35 eV. The energy of the first state of a simple well of the same total thickness is $E_1$ = 0.376 eV. The energies of the first two solutions are 0.531 eV and 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

$$\begin{cases} k_1 = \dfrac{\sqrt{2m(E_1 - V_0)}}{\hbar} \\ \kappa_2 = \dfrac{\sqrt{2m(V_1 - E_1)}}{\hbar} \end{cases}$$

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

$$\psi_b(z) = F\exp(-\kappa_2 z)$$

## 2.11.1

For this problem, we use the expression for the eigenenergies in a linear varying potential

$$E_i = -\left(\frac{\hbar^2}{2m}\right)^{1/3} \left(e\mathsf{E}\right)^{2/3} \zeta_i$$

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.,

$$E_1 \simeq 3.65 \text{ eV}, \; E_2 \simeq 6.39 \text{ eV}, \text{ and } \; E_3 \simeq 8.62 \text{ eV}$$

## 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

$$\frac{\hbar^2k^2}{2m_o}\sin(kz-\omega t) = -i\hbar\omega\cos(kz-\omega t)$$

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

$$\frac{\hbar^2k^2}{2m_o}\exp(ikz) = 0$$

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

$$\frac{\hbar^2k^2}{2m_o}\exp[-i(\omega t+kz)] = i\hbar(-i\omega)\exp[-i(\omega t+kz)] = \hbar\omega\exp[-i(\omega t+kz)]$$

which is possible for real positive values of $k$ and $\omega$ provided $\frac{\hbar^2k^2}{2m_o} = \hbar\omega$.

(iv) $\exp\left[i(\omega t-kz)\right]$ is not a solution. Substituting it in, we would require

$$\frac{\hbar^2k^2}{2m_o}\exp[i(\omega t-kz)] = -\hbar\omega\exp[-i(\omega t+kz)]$$

which is impossible for positive, real values of $k$ and $\omega$. (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 $\omega$.)

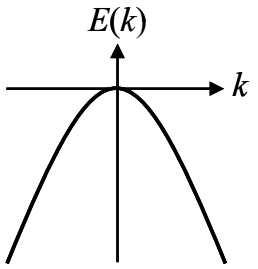
## 3.6.2

(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.

## 3.7.1

We are given that $E = -\frac{\hbar^2 k^2}{2b}$, where $b > 0$. This dispersion relation corresponds to a parabola with a peak at $k = 0$.




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")

## 3.12.1

(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

$$\langle p_z(t)\rangle$$

$$= \int_0^{L_z}\left(\frac{-i\hbar k}{L_z}\right)\left(\sin kz \exp(+i\omega_1 t) + \sin 2kz \exp(+i\omega_2 t)\right)\left(\cos kz \exp(-i\omega_1 t) + 2\cos 2kz \exp(-i\omega_2 t)\right) dz$$

$$= \left(\frac{-i\hbar k}{L_z}\right)\int_0^{L_z}\left(2\sin kz \cos 2kz \exp(-i(\omega_2 - \omega_1)t) + \cos kz \sin 2kz \exp(+i(\omega_2 - \omega_1)t)\right) dz$$

$$= \frac{\hbar}{iL_z}\left(2\left(-\frac{2}{3}\right)\exp(-i(\omega_2 - \omega_1)t) + \left(\frac{4}{3}\right)\exp(+i(\omega_2 - \omega_1)t)\right) = \frac{8\hbar}{3L_z}\sin((\omega_2 - \omega_1)t)$$

(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.

$$\sin kz \cos 3kz = \frac{1}{2}(\sin(kz + 3kz) + \sin(kz - 3kz))$$

$$k\int_0^{L_z} \sin kz \cos 3kz \, dz = \frac{1}{2}\left(-\frac{1}{4}[\cos 4kz]_0^{L_z} + \frac{1}{2}[\cos 2kz]_0^{L_z}\right) = 0$$

## 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.

## 4.11.4

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.

## 4.11.7

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

$$\begin{aligned}
\int g^*(x)\hat{M}f(x)dx &= \sum_{i,j} g_i^* f_j \int \psi_i^*(x)\,\hat{M}\psi_j(x)\,dx \\
&= \sum_{i,j} g_i^* f_j M_{ij} = \sum_{i,j} g_i^* f_j M_{ji}^* \\
&= \sum_{i,j} g_i^* f_j \left[\int \psi_j^*(x)\,\hat{M}\psi_i(x)\,dx\right]^* \\
&= \sum_{i,j} g_i^* f_j \int \left\{\hat{M}\psi_i(x)\right\}^* \psi_j(x)\,dx \\
&= \int \left\{\hat{M}\sum_i g_i\psi_i(x)\right\}\sum_j f_j\psi_j(x)\,dx \\
&= \int \left\{\hat{M}g(x)\right\}^* f(x)\,dx
\end{aligned}$$

as required.

## 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

$$\left(AB\right)^\dagger = B^\dagger A^\dagger = BA$$

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.

## 5.2.1

We are given that $\partial\hat{A}/\partial t = 0$, and we know that the expectation value of $\hat{A}$ is given by $\left\langle \hat{A} \right\rangle = \langle \psi | \hat{A} | \psi \rangle$. Consider the time derivative of the expectation value, which is

$$\frac{\partial}{\partial t}\left\langle \hat{A} \right\rangle = \left( \frac{\partial}{\partial t}\langle \psi | \right) \hat{A} | \psi \rangle + \langle \psi | \frac{\partial \hat{A}}{\partial t} | \psi \rangle + \langle \psi | \hat{A} \left( \frac{\partial}{\partial t} | \psi \rangle \right)$$
$$= \left( \left\langle \frac{\partial \psi}{\partial t} \right| \right) \hat{A} | \psi \rangle + \langle \psi | \hat{A} \left( \frac{\partial}{\partial t} | \psi \rangle \right)$$

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 $$\left( \left\langle \frac{\partial \psi}{\partial t} \right| \right) \hat{A} | \psi \rangle = \left\langle \frac{1}{i\hbar}\hat{H}\psi \right| \hat{A} | \psi \rangle = \langle \psi | \left( \frac{1}{i\hbar}\hat{H} \right)^{\dagger} \hat{A} | \psi \rangle = -\langle \psi | \frac{1}{i\hbar} \hat{H}^{\dagger} \hat{A} | \psi \rangle$$

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 $\partial \left\langle \hat{A} \right\rangle / \partial t = 0$

## 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

$$\begin{aligned}[\hat{z}, \hat{p}_z]|f\rangle &= -i\hbar z\frac{\partial f(z)}{\partial z} + i\hbar\frac{\partial}{\partial z}\{zf(z)\} \\ &= -i\hbar z\frac{\partial f(z)}{\partial z} + i\hbar z\frac{\partial f(z)}{\partial z} + i\hbar f(z)\frac{\partial z}{\partial z} \\ &= i\hbar|f\rangle\end{aligned}$$

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

$$\begin{aligned}[\hat{z}, \hat{p}_z]|g\rangle &= i\hbar\frac{\partial}{\partial k}\{kg(k)\} - i\hbar k\frac{\partial g(k)}{\partial k} \\ &= i\hbar k\frac{\partial g(k)}{\partial k} + i\hbar g(k)\frac{\partial k}{\partial k} - i\hbar k\frac{\partial g(k)}{\partial k} \\ &= i\hbar|g\rangle\end{aligned}$$

and hence in this representation we obtain the identical result $[\hat{z}, \hat{p}_z] = i\hbar$ .

## 6.3.1

(i) The perturbing Hamiltonian here is $H_p = eF\left(z - \frac{L_z}{2}\right)$, 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

$$\langle \psi_q | H_p | \psi_n \rangle = eF \langle \psi_q | z - \frac{L_z}{2} | \psi_n \rangle = eF \langle \psi_q | z - \frac{L_z}{2} | \psi_n \rangle (q \neq n)$$

$$= \frac{2}{L_z} \int_0^{L_z} \sin\left(\frac{\pi q z}{L_z}\right)\left(z - \frac{L_z}{2}\right)\sin\left(\frac{\pi n z}{L_z}\right) dz = \frac{2}{L_z}\left(\frac{L_z}{\pi}\right)^2 \int_0^{\pi}\left(\zeta - \frac{\pi}{2}\right)\sin(q\zeta)\sin(n\zeta)\, d\zeta$$

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

$$\langle \psi_q | z | \psi_n \rangle = -\frac{8L_z}{\pi^2}\frac{qn}{(n-q)^2(n+q)^2} \text{ for } n+q \text{ odd}$$

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

Hence, for $n = 2$, we have matrix elements

$$\langle \psi_1 | z | \psi_2 \rangle = -\frac{8L_z}{\pi^2}\frac{2}{1\times 9} = -\frac{16}{9}\frac{L_z}{\pi^2} = -1.778\frac{L_z}{\pi^2}$$

$$\langle \psi_3 | z | \psi_2 \rangle = -\frac{8L_z}{\pi^2}\frac{6}{1\times 25} = -\frac{48\,L_z}{25\pi^2} = -1.920\frac{L_z}{\pi^2}$$

$$\langle \psi_4 | z | \psi_2 \rangle = 0$$

$$\langle \psi_5 | z | \psi_2 \rangle = -\frac{8L_z}{\pi^2}\frac{10}{9\times 49} = -\frac{80_{\,z}}{9\times 49}\frac{L_z}{\pi^2} = -0.181\frac{L_z}{\pi^2}$$

$$\langle \psi_6 | z | \psi_2 \rangle = 0$$

$$\langle \psi_7 | z | \psi_2 \rangle = -\frac{8L_z}{\pi^2}\frac{14}{25\times 81}\frac{L_z}{\pi^2} = -\frac{112}{25\times 81}\frac{L_z}{\pi^2} = -0.055\frac{L_z}{\pi^2}$$

so, with $E_1$ as the energy of the unperturbed first state,

$$E_2^{(2)} \simeq \left(\frac{eFL_z}{\pi^2}\right)^2 \frac{1}{E_1}\left[\frac{(1.778)^2}{3} - \frac{(1.92)^2}{5} - \frac{(0.181)^2}{21} - \frac{(0.055)^2}{45} + \ldots\right]$$

$$\simeq \left(\frac{eFL_z}{\pi^2}\right)^2 \frac{1}{E_1}\left[1.053 - 0.737 - 0.002 - 0.000 + \ldots\right]$$

$$\simeq \left(\frac{eFL_z}{\pi^2}\right)^2 \frac{1}{E_1}\left[0.296\right]$$

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).

## 6.6.1

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).

## 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 $n$th level are given by, respectively,

$$E_n^{(0)} = \frac{n^2\hbar^2\pi^2}{2m_{eff}L_z^2} \quad \text{and} \quad \left|\psi_n{}^{(0)}\right\rangle = \sqrt{\frac{2}{L_z}}\sin(\frac{n\pi z}{L_z})$$

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

$$\dot{a}_2^{(1)}(t) = \frac{1}{i\hbar}\sum_n a_n^{(0)}\exp(i\omega_{2n}t)\left\langle\psi_2\left|\hat{H}_p(t)\right|\psi_n\right\rangle$$

Using (1), we have

$$\dot{a}_2^{(1)}(t) = \frac{1}{i\hbar}a_1^{(0)}\exp(i\omega_{21}t)\left\langle\psi_2\left|\hat{H}_p(t)\right|\psi_1\right\rangle$$

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

$$\hat{H}_p(t) = eF(t)\left(z - \frac{L_z}{2}\right) = eF_o\sin(\pi t/\Delta t)\left(z - \frac{L_z}{2}\right)$$

where we have chosen the potential origin in the middle of the well. So

$$\left\langle\psi_2\left|\hat{H}_p(t)\right|\psi_1\right\rangle = eF_o\sin(\pi t/\Delta t)\int_0^{L_z}\sqrt{\frac{2}{Lz}}\sin(\frac{2\pi z}{Lz})\left(z - \frac{L_z}{2}\right)\sqrt{\frac{2}{Lz}}\sin(\frac{\pi z}{Lz})dz$$

With a change of variable to $\zeta = \pi z/L_z$

$$\int_0^{L_z}\sqrt{\frac{2}{Lz}}\sin(\frac{2\pi z}{Lz})\left(z - \frac{L_z}{2}\right)\sqrt{\frac{2}{Lz}}\sin(\frac{\pi z}{Lz})dz = \frac{2}{L_z}\left(\frac{L_z}{\pi}\right)^2\int_0^{\pi}\left(\zeta - \frac{\pi}{2}\right)\sin(2\zeta)\sin(\zeta)\,d\zeta$$

$$= \frac{2}{L_z}\left(\frac{L_z}{\pi}\right)^2\left(-\frac{8}{9}\right) = \frac{-16L_z}{9\pi^2}$$

where we have used a standard result for the integral (see Appendix G of the book). That is,

$$\left\langle\psi_2\left|\hat{H}_p(t)\right|\psi_1\right\rangle = eF_o\sin(\pi t/\Delta t)\left(-\frac{16L_z}{9\pi^2}\right)$$

Now integrating over time to get the desired coefficient

$$
\begin{aligned}
a_2^{(1)}(t) &= \int_0^{\Delta t} \frac{1}{i\hbar} a_1^{(0)} \exp(i\omega_{21}t) \langle \psi_2 | \hat{H}_p(t) | \psi_1 \rangle dt \\
&= \int_0^{\Delta t} \frac{1}{i\hbar} \exp(i\omega_{21}t) eF_o \sin(\pi t/\Delta t) \left( -\frac{16L_z}{9\pi^2} \right) dt \\
&= \frac{1}{i\hbar} eF_o \left( -\frac{16L_z}{9\pi^2} \right) \int_0^{\Delta t} \exp(i\omega_{21}t) \sin(\pi t/\Delta t)\, dt \\
&= \frac{-1}{2\hbar} eF_o \left( -\frac{16L_z}{9\pi^2} \right) \int_0^{\Delta t} \exp(i\omega_{21}t) \left( \exp(i\pi t/\Delta t) - \exp(-i\pi t/\Delta t) \right) dt \\
&= \frac{1}{i\hbar} eF_o \left( \frac{16L_z}{9\pi} \right) \frac{\Delta t \left( 1 + \exp\left( i \frac{3E_1^{(0)}}{\hbar} \Delta t \right) \right)}{\left( \left( \frac{3E_1^{(0)}}{\hbar} \Delta t \right)^2 - \pi^2 \right)}
\end{aligned}
$$

(There are several relatively straightforward algebraic steps between the last two lines.) The probability of finding the electron in the second level is therefore

$$
\left| a_2^{(1)}(t) \right|^2 = \left( \frac{16 eF_o L_z \Delta t}{9\pi\hbar} \right)^2 \frac{4\cos^2\left( \frac{3E_1^{(0)}}{2\hbar} \Delta t \right)}{\left( \left( \frac{3E_1^{(0)}}{\hbar} \Delta t \right)^2 - \pi^2 \right)^2}
$$

where we used the identity $2\cos^2(\theta/2) = 1 + \cos\theta$.

(ii) For a GaAs semiconductor structure with $m_{eff} = 0.07 m_o$ 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, $\frac{3E_1^{(0)}}{2\hbar}\Delta t \simeq 12.25$ 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

$$F_o = \sqrt{\left|a_2^{(1)}(t)\right|^2}\frac{\left(\left(\frac{3E_1^{(0)}}{\hbar}\Delta t\right)^2 - \pi^2\right)}{2\left|\cos\left(\frac{3E_1^{(0)}}{2\hbar}\Delta t\right)\right|}\frac{9\pi\hbar}{16eL_z\Delta t}$$

$$= 0.1\times\frac{589.4}{1.87}\times\frac{9\pi\times1.055\times10^{-34}}{16\times1.602\times10^{-19}\times10^{-8}\times10^{-13}} = 3.67\times10^7 \text{ V/m}$$

which is therefore the minimum field required.

(iii) For a full cycle pulse the only mathematical difference is

$$a_2^{(1)}(t) = \frac{-1}{2\hbar}eF_o\left(-\frac{16L_z}{9\pi^2}\right)\int_0^{\Delta t}\exp\left(i\omega_{21}t\right)_o\left(\exp\left(2\pi it/\Delta t\right) - \exp\left(-2\pi it/\Delta t\right)\right)dt$$

$$= \frac{1}{i\hbar}eF_o\left(\frac{16L_z}{9\pi}\right)\frac{\Delta t\left(1-\exp\left(i\frac{3E_1^{(0)}}{\hbar}\Delta t\right)\right)}{\left(\left(\frac{3E_1^{(0)}}{\hbar}\Delta t\right)^2 - \pi^2\right)}$$

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 $\Delta t$, 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.

## 7.2.1

(i) We start with Fermi's Golden Rule.

$$W \propto \left|\langle final|\hat{H}_{p0}|initial\rangle\right|^2$$

For the electric dipole transitions we are considering here, we therefore have

$$W \propto \left|\langle final|z|initial\rangle\right|^2$$

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 $\langle final|z|initial\rangle$ 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.

[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 $\langle final|z-a|initial\rangle$ instead of $\langle final|z|initial\rangle$. But $\langle final|a|initial\rangle = a\langle final|initial\rangle = 0$ because the initial and final states are orthogonal, being energy eigenstates corresponding to different energy eigenvalues. So $\langle final|z-a|initial\rangle = \langle final|z|initial\rangle$.

## 8.6.1

We follow the derivation in the book of the effective mass Schrödinger equation, but instead of $E_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m_{eff}} + V$, 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

$$i\hbar \frac{\partial \Psi_{envnew}}{\partial t} = \sum_{\mathbf{k}_{new}} c_{\mathbf{k}_{new}} E_{\mathbf{k}_{new}} \exp(i\mathbf{k}_{new}.\mathbf{r}) \exp(-iE_{\mathbf{k}_{new}} t/\hbar)$$

$$= \frac{\hbar^2}{2m_{eff}} \sum_{\mathbf{k}_{new}} c_{\mathbf{k}_{new}} k_{new}^2 \exp(i\mathbf{k}_{new}.\mathbf{r}) \exp(-iE_{\mathbf{k}_{new}} t/\hbar)$$

$$+ V \sum_{\mathbf{k}_{new}} c_{\mathbf{k}_{new}} \exp(i\mathbf{k}_{new}.\mathbf{r}) \exp(-iE_{\mathbf{k}_{new}} t/\hbar)$$

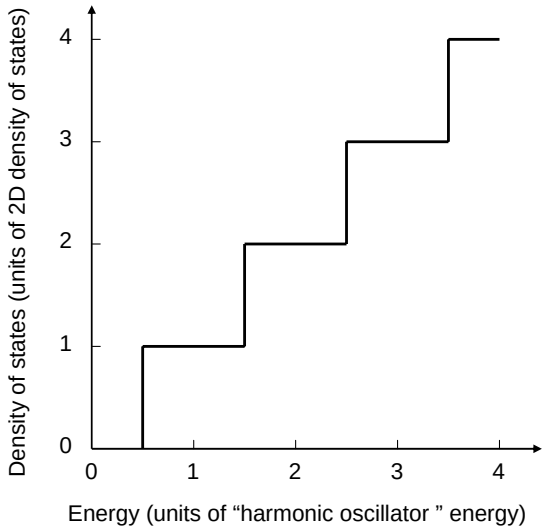
$$= \frac{\hbar^2}{2m_{eff}} \sum_{\mathbf{k}_{new}} \left[-c_{\mathbf{k}_{new}} \nabla^2 \exp(i\mathbf{k}_{new}.\mathbf{r})\right] \exp(-iE_{\mathbf{k}_{new}} t/\hbar) + V\Psi_{envnew}$$

so that, as required,

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

## 8.8.2

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.



## 9.2.1

$$\left[\nabla^2, \hat{L}_z\right] = -i\hbar^3\left[\nabla^2\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) - \left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\nabla^2\right]$$

$$= -i\hbar^3\left[\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) - \left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\right]$$

$$= -i\hbar^3\left[\frac{\partial}{\partial x}\left(\frac{\partial}{\partial y} + x\frac{\partial^2}{\partial x \partial y} - y\frac{\partial^2}{\partial x^2}\right) + \frac{\partial}{\partial y}\left(x\frac{\partial^2}{\partial y^2} - \frac{\partial}{\partial x} - y\frac{\partial^2}{\partial y dx}\right) + \frac{\partial^2}{\partial z^2}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\right.$$

$$\left. - x\frac{\partial}{\partial y}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + y\frac{\partial}{\partial x}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\right.$$

$$= -i\hbar^3\left[\frac{\partial^2}{\partial x \partial y} + \frac{\partial^2}{\partial x \partial y} + x\frac{\partial^3}{\partial x^2 \partial y} - y\frac{\partial^3}{\partial x^3} + x\frac{\partial^3}{\partial y^3} - \frac{\partial^2}{\partial x \partial y} - \frac{\partial^2}{\partial y \partial x} - y\frac{\partial^3}{\partial y^2 \partial x}\right.$$

$$\left. + x\frac{\partial^3}{\partial z^2 \partial y} - y\frac{\partial^3}{\partial z^2 \partial x} - x\frac{\partial^3}{\partial y \partial x^2} - x\frac{\partial^3}{\partial y^3} - x\frac{\partial^3}{\partial y \partial z^2} + y\frac{\partial^3}{\partial x^3} + y\frac{\partial^3}{\partial x \partial y^2} + y\frac{\partial^3}{\partial x \partial z^2}\right]$$

$$= 0$$

## 10.5.1

We are given $\nabla^2$ 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

$$\Phi(\phi)Z(z)\left[r\frac{\partial}{\partial r}r\frac{\partial}{\partial r}-\frac{r^2 2m_0 V(r)}{\hbar^2}\right]R(r)+R(r)Z(z)\frac{\partial^2\Phi(\phi)}{\partial\phi^2}$$

$$+r^2R(r)\Phi(\phi)\frac{\partial^2 Z(z)}{\partial z^2}+\frac{2m_0E_r^2R(r)\Phi(\phi)Z\left(z\right)}{\hbar^2}=0$$

We divide by $\psi$

$$\frac{1}{R(r)}\left[r\frac{\partial}{\partial r}r\frac{\partial}{\partial r}-\frac{r^2 2m_0V(r)}{\hbar^2}\right]R(r)+\frac{2m_0E_r^2}{\hbar^2}+\frac{r^2}{Z(z)}\frac{\partial^2 Z(z)}{\partial z^2}=-\frac{1}{\Phi}\frac{\partial^2\Phi(\phi)}{\partial\phi^2}=m^2$$

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 $\phi$ 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 $r^2$

$$\frac{1}{R(r)}\left[\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r}-\frac{2m_0V(r)}{\hbar^2}\right]R(r)+\frac{2mE}{\hbar^2}-\frac{m^2}{r^2}=-\frac{1}{Z(z)}\frac{\partial^2 Z(z)}{\partial z^2}=k_z^2$$

where $k_z^2$ is a separation constant. Hence the solution for $Z$ is (unnormalized)

$$Z(z)=\exp\left(ik_z z\right)$$

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

$$\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r}R\left(r\right)=\frac{1}{r}\frac{\partial}{\partial r}rR'=\frac{1}{r}R'+R''$$

We expect in the thin shell that the gradient $R'$ will change by $\sim\left|R'\right|$ 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

$$\left|\bar{R}''\right|\sim\frac{\left|\bar{R}'\right|}{L_r}>>\frac{\left|\bar{R}'\right|}{r_0}$$

because $r_0>>L_r$. 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 $\phi$ direction.

Hence, we have (neglecting normalization)

$$Z\left(z\right)=\exp\left(ik_zz\right)\ ,\ k_z\ \text{any real value}$$

$$\Phi(\phi) = \exp(im\phi) \ , \ m \text{ any integer}$$

$$R(r) = \sin\left(\frac{n\pi(r - r_o)}{L_r}\right) \text{ (for } r \text{ within the well), } n = 1, 2, 3, \ldots$$

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

$$-\frac{\hbar^2}{2m_0}\frac{d^2\chi(r)}{dr^2} + V(r)\chi(r) = E\chi(r)$$

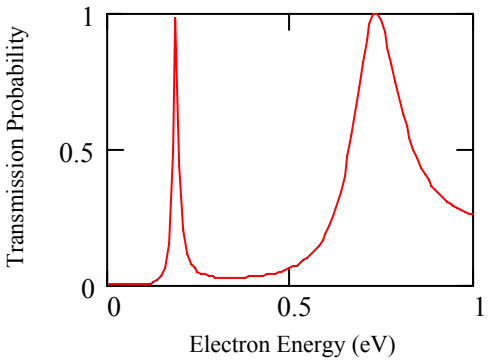
For the "infinite" potential well, we expect a boundary condition $\chi(r_0) = 0$, and we are reminded in the problem that $\chi(0) = 0$. Hence, this problem is mathematically like a simple one-dimensional quantum well of thickness $r_0$ (at least for all $l = 0$ states), and so we conclude that the lowest energy is

$$E_1 = \frac{\hbar^2}{2m_0}\left(\frac{\pi}{r_0}\right)^2$$

## 11.2.1

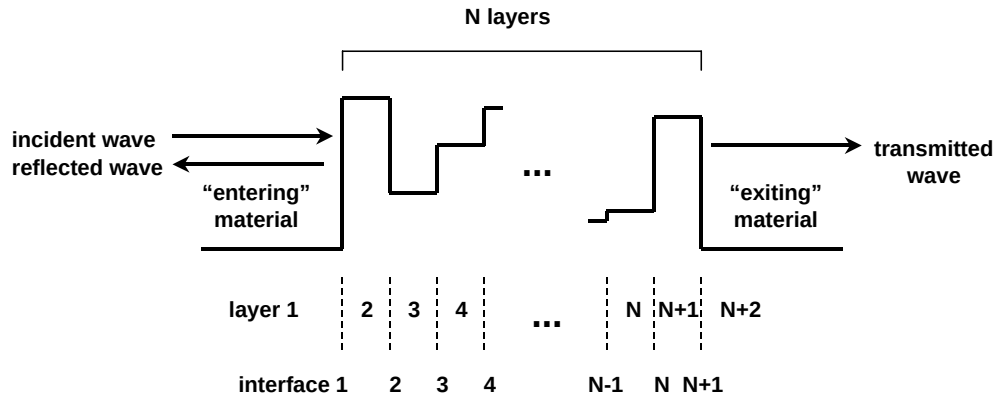
For this problem, one needs to set up an appropriate computer program for the transfer matrix method, using the formulae in the book. For example computer code, see the following Mathcad worksheet.

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 sig 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.

$$\text{hbar} := 1.055 \cdot 10^{-34} \qquad \text{mo} := 9.1095 \cdot 10^{-31} \qquad \text{q} := 1.602 \cdot 10^{-19}$$

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

$$\text{s} := \frac{2\text{q} \cdot \text{mo} \cdot 10^{-18}}{\text{hbar}^2} \qquad \text{which gives} \qquad \text{s} = 26.22299$$

Using this scaling parameter, we can write the formula for the wavevector as a function of the appropriate

$$\text{k}(\text{E}, \text{Vm}, \text{mfm}) := \sqrt{\text{s} \cdot \text{mfm} \cdot (\text{E} - \text{Vm})}$$

and the quantity

$$\Delta(\text{E}, \text{Vm}, \text{mfm}, \text{Vm1}, \text{mfm1}) := \text{k}(\text{E}, \text{Vm1}, \text{mfm1}) \cdot \frac{\text{mfm}}{\text{k}(\text{E}, \text{Vm}, \text{mfm}) \cdot \text{mfm1}}$$

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.

$mf_1 := 1 \quad Vm_1 := 0$

$mf_2 := 1 \quad Vm_2 := 1 \quad dm_2 := 0.3$

$mf_3 := 1 \quad Vm_3 := 0 \quad dm_3 := 1$

$mf_4 := 1 \quad Vm_4 := 1 \quad dm_4 := 0.3$

$mf_5 := 1 \quad Vm_5 := 0$

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.)

$$T(E) := D(E, Vm_1, mf_1, Vm_2, mf_2) \cdot \prod_{q=2}^{N+1} P(E, Vm_q, mf_q, dm_q) \cdot D(E, Vm_q, mf_q, Vm_{q+1}, mf_{q+1})$$

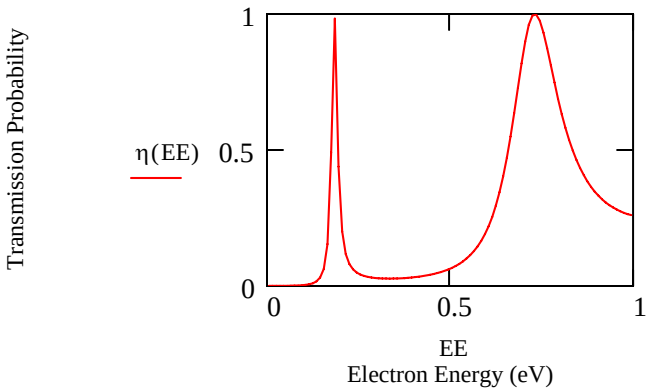
and we can define the transmission fraction by

$$\eta(E) := 1 - \frac{\left(\left|T(E)_{2,1}\right|\right)^2}{\left(\left|T(E)_{1,1}\right|\right)^2}$$

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 η(EE) is used as the vertical value plotted, hence giving the following graph.



## 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

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

## 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

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

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

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.)

## 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

$$\begin{aligned}
\rho_{HH} &= \langle\psi_H|\rho|\psi_H\rangle = P_1 + \frac{9}{25}P_2 = \frac{1}{5} + \frac{9}{25}\times\frac{4}{5} = \frac{25+36}{125} = \frac{61}{125} \\
\rho_{HV} &= \langle\psi_H|\rho|\psi_V\rangle = \frac{12i}{25}P_1 = -\frac{12i}{125} \\
\rho_{VV} &= \langle\psi_V|\rho|\psi_V\rangle = \frac{16}{25}P_2 = \frac{64}{125} \\
\rho_{VH} &= \langle\psi_V|\rho|\psi_H\rangle = \frac{12i}{25}P_2 = +\frac{12i}{125}
\end{aligned}$$

Hence the density matrix is

$$\rho = \begin{bmatrix} \frac{61}{125} & -\frac{12i}{125} \\ \frac{12i}{125} & \frac{64}{125} \end{bmatrix}$$

where $\rho_{HH}$ is the top left element in the matrix. (Note that this matrix is Hermitian, and does also have $Tr(\rho) = 1$. )

## 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.

## 15.6.2

The expected value of position is just the expectation value of the operator $\hat{\xi}_\lambda$, i.e.,

$$\left\langle \hat{\xi}_\lambda \right\rangle \equiv \overline{\xi}_\lambda = \frac{1}{\sqrt{2}} \left\langle \psi_{\lambda\overline{n}} \middle| \left( \hat{a}_\lambda + \hat{a}_\lambda^\dagger \right) \middle| \psi_{\lambda\overline{n}} \right\rangle = \frac{1}{\sqrt{2}} \left\{ \left\langle \psi_{\lambda\overline{n}} \middle| \hat{a}_\lambda \middle| \psi_{\lambda\overline{n}} \right\rangle + \left\langle \psi_{\lambda\overline{n}} \middle| \hat{a}_\lambda^\dagger \middle| \psi_{\lambda\overline{n}} \right\rangle \right\}$$

$$= \sqrt{\frac{\overline{n}}{2}} \exp\left(-i\omega_\lambda t\right) \left\langle \psi_{\lambda\overline{n}} \middle| \psi_{\lambda\overline{n}} \right\rangle + \sqrt{\frac{\overline{n}}{2}} \exp\left(i\omega_\lambda t\right) \left\langle \psi_{\lambda\overline{n}} \middle| \psi_{\lambda\overline{n}} \right\rangle$$

$$= \sqrt{\frac{\overline{n}}{2}} \left\{ \exp\left(-i\omega_\lambda t\right) + \exp\left(i\omega_\lambda t\right) \right\} = \sqrt{2\overline{n}} \cos\left(\omega_\lambda t\right)$$

Hence, the expected value of position is oscillating (co)sinusoidally at angular frequency $\omega_\lambda$.

## 16.1.1

Possible basis states are, in the order we will use them

$|0\rangle \equiv |0_1, 0_2\rangle$ no particles in either state

$|1_1, 0_2\rangle$ one particle in state 1

$|0_1, 1_2\rangle$ one particle in state 2

$|1_1, 1_2\rangle$ 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

$$\hat{b}_2^+ \left|0_1, 0_2\right\rangle = \left|0_1, 1_2\right\rangle$$
$$\hat{b}_2^+ \left|1_1, 0_2\right\rangle = \left|1_1, 1_2\right\rangle \quad (\textit{no swapping required})$$
$$\hat{b}_2^+ \left|0_1, 1_2\right\rangle = 0$$
$$\hat{b}_2^+ \left|1_1, 1_2\right\rangle = 0$$

For the state 2 annihilation operator

$$\hat{b}_2 \left|0_1, 0_2\right\rangle = 0 \quad (\textit{no swapping required})$$
$$\hat{b}_2 \left|1_1, 0_2\right\rangle = 0 \quad (\textit{no swapping required})$$
$$\hat{b}_2 \left|0_1, 1_2\right\rangle = \left|0_1, 0_2\right\rangle$$
$$\hat{b}_2 \left|1_1, 1_2\right\rangle = \left|1_1, 0_2\right\rangle$$

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

$$\hat{b}_2^+\hat{b}_2 + \hat{b}_2 b_2^+ = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}\begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

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

$$\hat{b}_1^+ b_1^+ = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

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

$$\hat{b}_1 b_1 + \hat{b}_1 \hat{b}_1 = 0$$

$$\hat{b}_2 \hat{b}_2 + \hat{b}_2 \hat{b}_2 = 0$$

## 16.3.3

(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

$$\begin{aligned}\hat{\mathbf{r}} &= \int \psi^{\dagger}\mathbf{r}\psi d^3\mathbf{r} \\ &= \int \sum_{m,n} \hat{b}_m^{+}\hat{b}_n \phi_m^{*}(\mathbf{r})\mathbf{r}\phi_n(\mathbf{r}) d^3\mathbf{r} \\ &= \sum_{m,n} r_{mn}\hat{b}_m^{+}\hat{b}_n\end{aligned} \tag{1}$$

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

$$\begin{aligned}r_{mn} &= \frac{2}{L}\left(\frac{L}{\pi}\right)^2 \int_0^{\pi}\left(\zeta - \frac{\pi}{2}\right)\sin(m\zeta)\sin(n\zeta) d\zeta \\ &= -\frac{L}{\pi^2}\frac{8nm}{(n-m)^2(n+m)^2} \text{ for } n+m \text{ odd} \\ &= 0 \text{ for } n+m \text{ even}\end{aligned} \tag{2}$$

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.)

## 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

$$\left| N_{fm}; N_{bm} \right\rangle = \hat{c}_\alpha^+ \hat{b}_\mu^+ \left| 0 \right\rangle$$
$$\left| N_{fq}; N_{bq} \right\rangle = \hat{c}_\beta^+ \hat{b}_v^+ \left| 0 \right\rangle$$

Then

$$M = \left\langle N_{fq}; N_{bq} \left| \hat{b}_j^+ \hat{c}_\lambda^+ \hat{b}_k \hat{c}_\mu \right| N_{fm}; N_{bm} \right\rangle$$
$$= \left\langle 0 \left| \hat{b}_v \hat{c}_\beta \hat{b}_j^+ \hat{c}_\lambda^+ \hat{b}_k \hat{c}_\mu \hat{c}_\alpha^+ \hat{b}_u^+ \right| 0 \right\rangle$$

Now using the fact that the operators for different particles commute, we can rewrite this as

$$M = \left\langle 0 \left| \hat{b}_v \hat{b}_j^+ \hat{c}_\beta \hat{c}_\lambda^+ \hat{c}_\mu \hat{c}_\alpha^+ \hat{b}_k \hat{b}_u^+ \right| 0 \right\rangle$$

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

$$M = \left\langle 0 \left| \left( \delta_{vj} - \hat{b}_j^+ \hat{b}_v \right) \left( \delta_{\beta\lambda} + \hat{c}_\lambda^+ \hat{c}_\beta \right) \left( \delta_{\mu\alpha} + \hat{c}_\alpha^+ \hat{c}_\mu \right) \left( \delta_{ku} - \hat{b}_k^+ \hat{b}_u \right) \right| 0 \right\rangle$$

i.e., since we have annihilation operators to the right in each case

$$M = \delta_{vj} \delta_{\beta\lambda} \delta_{\mu\alpha} \delta_{ku} \left\langle 0 \middle| 0 \right\rangle = \delta_{vj} \delta_{\beta\lambda} \delta_{\mu\alpha} \delta_{ku}$$

So

$$\left\langle N_{fq}; N_{bq} \left| H_{Cen} \right| N_{fm}; N_{bm} \right\rangle = H_{Cvu\beta\alpha}$$

## 18.3.3

From the definitions of the Bell states, we find

$$|\mathsf{H}\rangle_1|\mathsf{H}\rangle_2 = \frac{1}{\sqrt{2}}\left(|\Phi^+\rangle_{12} + |\Phi^-\rangle_{12}\right)$$

$$|\mathsf{V}\rangle_1|\mathsf{V}\rangle_2 = \frac{1}{\sqrt{2}}\left(|\Phi^+\rangle_{12} - |\Phi^-\rangle_{12}\right)$$

$$|\mathsf{H}\rangle_1|\mathsf{V}\rangle_2 = \frac{1}{\sqrt{2}}\left(|\Psi^+\rangle_{12} + |\Psi^-\rangle_{12}\right)$$

$$|\mathsf{V}\rangle_1|\mathsf{H}\rangle_2 = \frac{1}{\sqrt{2}}\left(|\Psi^+\rangle_{12} - |\Psi^-\rangle_{12}\right)$$

Hence the general two-particle state where each particle has two available basis states $|\mathsf{H}\rangle$ and $|\mathsf{V}\rangle$ can be written

$$\begin{aligned}
|\psi\rangle &= c_{\mathsf{HH}}|\mathsf{H}\rangle_1|\mathsf{H}\rangle_2 + c_{\mathsf{HV}}|\mathsf{H}\rangle_1|\mathsf{V}\rangle_2 + c_{\mathsf{VH}}|\mathsf{V}\rangle_1|\mathsf{H}\rangle_2 + c_{\mathsf{VV}}|\mathsf{V}\rangle_1|\mathsf{V}\rangle_2 \\
&= \frac{1}{\sqrt{2}}\left\{\begin{array}{l} c_{\mathsf{HH}}\left[|\Phi^+\rangle_{12} + |\Phi^-\rangle_{12}\right] + c_{\mathsf{HV}}\left[|\Psi^+\rangle_{12} + |\Psi^-\rangle_{12}\right] \\ +c_{\mathsf{VH}}\left[|\Psi^+\rangle_{12} - |\Psi^-\rangle_{12}\right] + c_{\mathsf{VV}}\left[|\Phi^+\rangle_{12} - |\Phi^-\rangle_{12}\right] \end{array}\right\} \\
&= \frac{c_{\mathsf{HH}} + c_{\mathsf{VV}}}{\sqrt{2}}|\Phi^+\rangle_{12} + \frac{c_{\mathsf{HH}} - c_{\mathsf{VV}}}{\sqrt{2}}|\Phi^-\rangle_{12} + \frac{c_{\mathsf{HV}} + c_{\mathsf{VH}}}{\sqrt{2}}|\Psi^+\rangle_{12} + \frac{c_{\mathsf{HV}} - c_{\mathsf{VH}}}{\sqrt{2}}|\Psi^-\rangle_{12}
\end{aligned}$$