Example Examinations

for

Quantum Mechanics for Scientists and Engineers

David A. B. Miller
Stanford University

Introduction

Two examinations and solutions are given here. These examinations use problems not found in the book.

The first examination can be used as a “midterm” exam. It examines material in Chapters 2 and 3. It is intended as a closed book exam. Examinees are expected to have memorized the formulae in the Memorization List at the end of the book for Chapters 2 and 3. (It does not examine the optional material in Section 2.11.) If this examination is given at 50 minutes duration, students will have to execute the problems very efficiently, and it will test their speed. At 60 minutes to 75 minutes duration, it will test their understanding of the concepts with less emphasis on speed.

The second examination is a test of approximately half the material in the book, explicitly Chapters 2 – 7, and Chapters 9 and 10. (It does not examine on the optional material in these Chapters.) The intention with this examination is that the students would compile one sheet of paper (both sides) with whatever notes they wish (such as formulae from the Memorization List for these Chapters), but would bring no other material into the examination. At three hours duration, the students need to be reasonably fast in their execution of the material. For a less demanding examination, it is likely better to omit some question or questions rather than prolonging an examination beyond three hours.

For examination on the material in other Chapters, I have typically not used timed examinations, relying on two to three take-home assignments spaced out over the term instead, such as the problems marked as substantial assignments in the book. I have also typically assigned one such take-home assignment during the term as part of the assessment of the students understanding of the material in Chapters 2 – 7 and Chapters 9 and 10.

David A. B. Miller

Stanford, California

March 2008

Examination on Chapters 2 and 3

1 hour duration

This exam is intended as "closed book". Examinees should not bring any notes or books into the exam. A simple calculator may be required for some questions.

This exam has 6 questions for a total of 50 points.

1. (6 points) Based on the definition of normalization for wavefunctions in quantum mechanics, state whether the following functions are normalized, justifying your answers briefly.

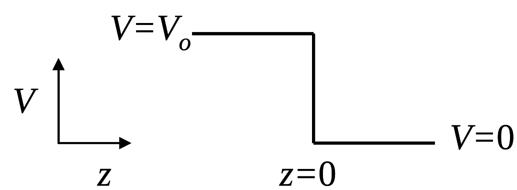
(a) $\sqrt{2}\sin(\pi s)$ over the interval from $s=0$ to $s=1$

(b) x^2 over the interval from $x=-1$ to $x=1$

(c) $\sqrt{3/2}\,x$ over the interval from $x=-1$ to $x=1$

(d) $\frac{1}{5}\sqrt{\frac{2}{L_z}}\left[3\sin\left(\frac{\pi z}{L_z}\right)+4\sin\left(\frac{4\pi z}{L_z}\right)\right]$ over the interval from $z=0$ to $z=L_z$

2. (10 points) Consider the potential step shown in the figure. The potential drops from V_o to 0 at the position z = 0. An electron is incident from the left with an energy E greater than V_o.



(a) Find an expression, as a function of E (for $E > V_o$), for the probability that the electron will be reflected from the step.

(b) For V_o = 1 eV, and for an incident electron energy of 1.1 eV, what is the probability that the electron will be reflected from the step?

3. (8 points) For an electron in an infinitely deep potential well,

(i) state the following wavefunctions in a form so that they are normalized solutions of the time-*dependent* Schrödinger equation (take the zero of the energy to be at the bottom of the potential well)

(a) the first state of an electron in the well

(b) the second state of an electron in the well.

(c) an equal linear superposition of the first and second states of an electron in the well

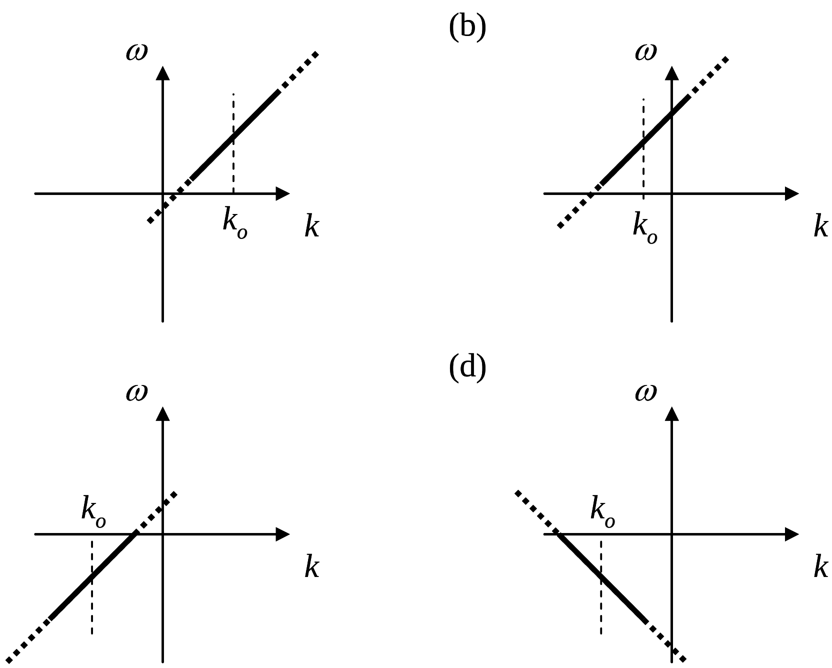
(ii) For each of the states (a) and (b) in part (i), state the expectation value of the position of the electron [you need not formally calculate this expectation value – stating it with some justification is sufficient]

(iii) For state (c) in part (i), describe in words what now will be the behavior in time of the expectation value of position, giving explicit expressions for any frequency or frequencies involved. [you need not formally calculate this expectation value – describing its behavior is sufficient].

4. (8 points) Consider the dispersion relations in the figures below. In each of these figures, the axes cross at the point where $k = 0$ and $\omega = 0$. In each case, the dispersion, i.e., the relation between the angular frequency ω and the wavevector magnitude k, is approximately linear near the wavevector magnitude k_o of interest, as shown by the straight lines in each case. For each of the cases (a) through (d), state

(i) whether the phase velocity for waves of wavevector magnitude k_o and the group velocity for wavepackets centered near k_o are in the same or opposite directions, and

(ii) whether the magnitude of this group velocity is greater than the magnitude of this phase velocity.



5. (10 points) Consider an electron in an infinitely deep potential well of thickness L_z. At some specific time, the (normalized) wavefunction of the electron is $\psi(z) = \sqrt{\frac{30}{L_z}}\left[\frac{1}{4} - \frac{z^2}{L_z^2}\right]$, where z is the distance from the *center* of the well.

(i) What is the expectation value of the energy for this electron? (Take the energy origin to be the potential at the bottom of the well.)

(ii) How does this energy compare with the energy of the lowest energy eigenstate of the well?

6. (8 points) State whether the following pairs of functions are orthogonal, justifying your answers briefly. [Hint: you may be able to do this problem without formally evaluating any integrals.]

(a) $\sin(\pi y)$ and $\sin(2\pi y)$ over the interval $y = 0$ to $y = 1$

(b) x and x^2 over the interval $x = -1$ to $x = 1$

(c) z and $\sin(\pi z)$ over the interval $z = 0$ to $z = 1$

(d) $z - (1/2)$ and $\cos(\pi z)$ over the interval $z = 0$ to $z = 1$

Solutions to Examination on Chapters 2 and 3

1(a) Yes, this is normalized. It is the known normalized $n=1$ "particle in a box" wavefunction taking the thickness $L_z = 1$ unit.

(b)

$$\int_{-1}^{1} (x^2)^2\,dx = \int_{-1}^{1} x^4 dx = \frac{1}{5}\left[x^5\right]_{-1}^{1} = \frac{1}{5} - \left(-\frac{1}{5}\right)$$
$$= \frac{2}{5} \neq 1, \text{so this is not normalized}$$

(c)

$$\frac{3}{2}\int_{-1}^{1} x^2 dx = \frac{3}{2}\frac{1}{3}\left[x^3\right]_{-1}^{1} = \frac{3}{2}\frac{2}{3} = 1 \ \text{ so this is normalized}$$

(d)

$$I = \frac{2}{25L_z}\int_0^{L_z}\left[3\sin\left(\frac{\pi_z}{L_z}\right) + 4\sin\left(\frac{4\pi_z}{L_z}\right)\right]^2 dz$$
$$= \frac{1}{25}\frac{2}{L_z}\int_0^{L_z}\left[9\sin^2\left(\frac{\pi_z}{L_z}\right) + 16\sin^2\left(\frac{4\pi_z}{L_z}\right)\right] dz$$

The cross-terms disappeared in the above integral by orthogonality of the different sine functions. Since we know also that

$$\sqrt{\frac{Z}{L_z}}\sin\left(\frac{\pi_z}{L_z}\right)$$

and

$$\sqrt{\frac{Z}{L_z}}\sin\left(\frac{4\pi_z}{L_z}\right)$$

are normalized, then

$$I = \frac{9}{25} + \frac{16}{25} = 1$$

So this function is normalized.

2 (a) The wave on the left can be written

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

while that on the right can be written

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

where

$$k_L = \sqrt{\frac{2m}{\hbar^2}(E - V_0)}$$

and

$$k_R = \sqrt{\frac{2m}{\hbar^2}E}$$

Equating the waves at z = 0 gives

$$A + B = C \tag{1}$$

Equating the derivatives gives

$$k_L(A - B) = k_R C$$

i.e.,

$$\frac{k_L}{k_R}(A - B) = C \tag{2}$$

Subtracting (2) from (1) gives

$$A\left(1 - \frac{k_L}{k_R}\right) + B\left(1 + \frac{k_L}{k_R}\right) = 0$$

or

$$A(k_R - k_L) + B(k_R + k_L) = 0$$

i..e.,

$$B = \left(\frac{k_L - k_R}{k_R + k_L}\right)A$$

The probability of reflection is

$$P = \frac{|B|^2}{|A|^2} = \left(\frac{k_L - k_R}{k_R + k_L}\right) = \left(\frac{\sqrt{E - V_0} - \sqrt{E}}{\sqrt{E - V_0} + \sqrt{E}}\right)^2$$

(b) For E = 1.1 eV, V_0 = 1 eV, we have the reflection probability

$$P = \left(\frac{\sqrt{0.1} - \sqrt{1.1}}{\sqrt{0.1} + \sqrt{1.1}} \right)^2 = \left(\frac{0.3162 - 1.0488}{0.3162 + 1.0488} \right)^2$$

$$= \left(\frac{0.7326}{1.365} \right)^2 = 0.288 = 28.8\%$$

3 (i) (a)

$$\sqrt{\frac{2}{L_z}} \exp\left[-\frac{i\hbar\pi^2 t}{2mL_z^2} \right] \sin\left(\frac{\pi z}{L_z} \right)$$

(b)

$$\sqrt{\frac{2}{L_z}} \exp\left[-i\frac{4\hbar\pi^2 t}{2mL_z^2} \right] \sin\left(\frac{2\pi z}{L_z} \right)$$

(c)

$$\sqrt{\frac{1}{L_z}} \exp\left[-\frac{i\hbar\pi^2 t}{2mL_z^2} \right] \sin\left(\frac{\pi z}{L_z} \right) + \sqrt{\frac{1}{L_z}} \exp\left[-\frac{i4\hbar\pi^2 t}{2mL_z^2} \right] \sin\left(\frac{2\pi z}{L_z} \right)$$

(We had to divide each part by $\sqrt{2}$ to keep the combination normalized).

(ii) For both of the states (a) and (b), the expectation value of position is $\langle z \rangle = \frac{L_z}{2}$ because both of the probability distributions are symmetric about the center of the well.

(iii) Because the electron is in a linear superposition of two energy eigenstates, the resulting probability distribution will oscillate in time, at the difference (angular) frequency

$$\omega = \frac{E_2 - E_1}{\hbar}$$

i.e., at

$$\omega = \frac{3\hbar\pi^2}{2m_0 L_z^2}$$

This will be an oscillation from left to right and back again, as the positive and negative parts of the second wavefunction beat with the (positive) first wavefunction.

4. (a) (i) same directions

(ii) group velocity larger magnitude than phase velocity

(b) (i) opposite directions

(ii) phase velocity larger magnitude than group velocity

(c) (i) same directions

(ii) group velocity larger magnitude than phase velocity

(d) (i) opposite directions

(ii) group velocity larger magnitude than phase velocity

5. (i) For this problem, the key is to use the expression

$$\langle E\rangle = \int \psi^*(z)\hat{H}\psi(z)dz$$

for the expectation value.

Here, within the well

$$\begin{aligned}
\langle \hat{H}\rangle &= -\frac{\hbar^2}{2m_0}\frac{30}{L_z}\int_{-L_z/2}^{L_z/2}\left(\frac{1}{4}-\frac{z^2}{L_z^2}\right)\frac{d^2}{dz^2}\left(\frac{1}{4}-\frac{z^2}{L_z^2}\right)dz \\
&= -\frac{30\hbar^2}{2m_0L_z}\int_{-L_z/2}^{L_z/2}\left(\frac{1}{4}-\frac{z^2}{L_z^2}\right)\frac{d}{dz}\left(-2\frac{z}{L_z^2}\right)dz \\
&= \frac{60\hbar^2}{2m_0L_z^3}\int_{-L_z/2}^{L_z/2}\left(\frac{1}{4}-\frac{z^2}{L_z^2}\right)dz = \frac{60\hbar^2}{2m_0L_z^3}\left\{\left[\frac{z}{4}\right]_{-L_z/2}^{L_z/2}-\frac{1}{3}\left[\frac{z^3}{L_z^2}\right]_{-L_z/2}^{L_z/2}\right\} \\
&= \frac{60\hbar^2}{2m_0L_z^3}\left\{\frac{L_z}{4}-\frac{1}{3}\frac{L_z}{4}\right\} \\
&= \frac{60\hbar^2}{2m_0L_z^2}\times\frac{2}{3}\times\frac{1}{4} \\
&= \frac{10\hbar^2}{2m_0L_z^2}
\end{aligned}$$

(ii) It is slightly larger than the lowest energy eigen state, by a factor of $10/\pi^2$.

6. (a) Yes, they are orthogonal. One function is odd $(\sin(2\pi y))$ and the other is even $(\sin(\pi y))$ over this interval (reflecting about the middle of the interval).

(b) Yes, they are orthogonal, because x is even and x^2 is odd on this interval.

(c) These are *not* orthogonal over this interval. Both are positive functions throughout this interval.

(d) No, these are *not* orthogonal, because, with respect to the point $z = \frac{1}{2}$, both are odd.

Examination on Chapters 2 – 7, 9, and 10

3 hours duration. You may consult notes on one sheet of paper. Other notes or books are prohibited. A calculator is not required for this examination.

You may need the following expressions: For integers n and m of value 1 or greater,

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

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

$$\int_0^{\pi}(x-\pi/2)\sin(nx)\sin(mx)\,dx=\int_0^{\pi}x\sin(nx)\sin(mx)\,dx \text{ when } n \text{ and } m \text{ are different}$$

There are 8 questions for a total of 100 points.

1. (6 points) Prove that a unitary transformation $\hat{U}$ from one representation to another does not change the "length" (i.e., $\sqrt{\langle\psi|\psi\rangle}$) of a vector $|\psi\rangle$.

2. (6 points) By considering the matrix elements $A_{mn}=\langle\psi_m|\hat{A}|\psi_n\rangle$ of some operator $\hat{A}$ and some complete orthonormal basis set $|\psi_p\rangle$, show that the sum of the modulus squared of these matrix elements is equal to the sum of the diagonal elements of the operator $\hat{A}^\dagger\hat{A}$, i.e.,

$$\sum_{m,n}|A_{mn}|^2=\sum_n\langle\psi_n|\hat{A}^\dagger\hat{A}|\psi_n\rangle$$

3. (8 points) (i) For the hydrogen atom, how many states are there with principal quantum number n = 3?

(ii) How many of these states have the same energy?

4. (11 points) In certain semiconductor materials, the relation between the electron eigenenergies E and the effective wavevector k in the z direction can take the form

$$k=\left[\frac{2m_{eff}E}{\hbar^2}\left(1+\frac{E}{E_G}\right)\right]^{1/2}$$

where m_{eff} and E_G are constants (they happen to represent the effective mass of the electron at zero momentum, and the bandgap energy, respectively).

(i) Obtain an expression for the group velocity as a function of energy E for this electron.

(ii) Describe in words what happens to the group velocity in the limit of very large E.

(iii) What can you say about the dispersion (i.e., the tendency to spread out as it propagates) of a wavepacket formed from states of eigenenergies just round about some very large energy E?

(iv) In the limit of very large E, describe in words the comparison between the phase velocity and group velocity of such an electron wave.

[Note: For parts (ii), (iii), and (iv) above, you may well first be obtaining an algebraic result, but you are asked also to interpret the meaning of the result in words.]

5. (11 points) (i) For the position operators $\hat{x}$, $\hat{y}$, and $\hat{z}$ corresponding to the usual *x*, *y*, and *z* directions, and for the momentum operators $\hat{p}_x$, $\hat{p}_y$, and $\hat{p}_z$ associated respectively with those same directions, state which pairs of such operators do *not* commute.

(ii) Starting from the definitions for the angular momentum operators

$$\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y \, , \; \hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z \, , \; \hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$$

and the commutation relations between all six of the operators $\hat{x}$, $\hat{y}$, $\hat{z}$, $\hat{p}_x$, $\hat{p}_y$, and $\hat{p}_z$, prove that

$$\left[\hat{L}_x, \hat{L}_y\right] = i\hbar \hat{L}_z$$

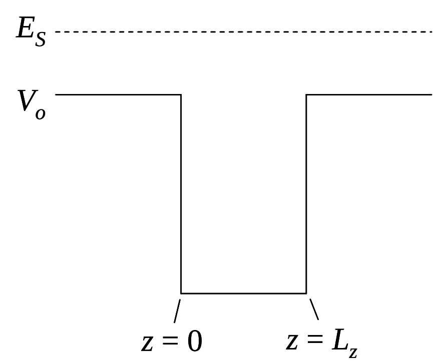
6. (18 points) Suppose we have an infinitely deep potential well of width L_z in the *z* direction, and we have an electron initially in the lowest state of the well. Then for some finite amount of time t_o we apply a uniform electric field *F* across the well (i.e., in the *z* direction), giving a simple time-dependent perturbation to this system.

(i) Derive an expression for the probability that the electron will be found in the second energy state at the end of this experiment (presuming the field *F* is relatively weak).

(ii) For any value of t_o, what is the largest possible value of this probability

(iii) What is the probability that the electron will be found in the third energy state at the end of this experiment?

7. (20 points) Consider a one-dimensional potential well of width L_z and of finite depth V_o, as shown in the diagram. An electron of energy $E_S > V_o$ is incident from the left.



(i) Derive an expression for the transmission probability from left to right for such an electron as a function of energy E_S. (Express your energies relative to the energy of the bottom of the potential well.)

(ii) What is the maximum possible transmission?

(iii) What are the electron energies corresponding to any maxima in the transmission?

[Notes: (a) In such a problem, with a right-going incident wave of amplitude *A*, and a (necessarily) right-going transmitted wave of amplitude *E*, the transmission probability of the structure is $|E/A|^2$. (b) In analyzing such problems, it is often more convenient to start the analysis from the right interface, and work back to the left interface, because there is only a right-going wave to the right of the structure.]

8. (20 points) Consider an electron in the lowest energy state of an infinitely deep one-dimensional potential well of width L_z. We apply a constant electric field *F* to this well in the (positive) *z* direction. Derive an approximate expression, valid to lowest order in *F* (i.e., up to the lowest power of *F* that gives a non-zero expression) for the expectation value of the position of the electron relative to the center of the well as a function of *F*.

[Note: If you find that you have to sum a series to obtain a result, you may truncate that summation once you judge that the subsequent terms are becoming relatively small in magnitude (e.g., < 10%) compared to the first non-zero term.]

Solutions to Examination on Chapters 2 – 7, 9, and 10

1.

$$\left|\psi_{new}\right\rangle = \hat{U}\left|\psi_{old}\right\rangle$$
$$\left\langle\psi_{new}|\psi_{new}\right\rangle = \left\langle\psi_{old}\left|\hat{U}^{+}\hat{U}\right|\psi_{old}\right\rangle$$

But, by definition, for a unitary operator

$$U^{+}U = I \ \text{(i.e., the identity operator)}$$

so

$$\left\langle\psi_{new}|\psi_{new}\right\rangle = \left\langle\psi_{old}|\psi_{old}\right\rangle$$

so

$$\sqrt{\left\langle\psi_{new}|\psi_{new}\right\rangle} = \sqrt{\left\langle\psi_{old}|\psi_{old}\right\rangle}$$

so the length of a vector is not changed by a unitary transformation.

2.

$$\begin{aligned}
\sum_{m,n}\left|A_{mn}\right|^2 &= \sum_{m,n}\left|\left\langle\psi_m\left|\hat{A}\right|\psi_n\right\rangle\right|^2 \\
&= \sum_{m,n}\left\langle\psi_n\left|\hat{A}^{+}\right|\psi_m\right\rangle\left\langle\psi_m\left|\hat{A}\right|\psi_n\right\rangle \\
&= \sum_{n}\left\langle\psi_n\left|\hat{A}^{+}\left(\sum_{m}\left|\psi_m\right\rangle\left\langle\psi_m\right|\right)\hat{A}\right|\psi_n\right\rangle \\
&= \sum_{n}\left\langle\psi_n\left|\hat{A}^{+}\hat{I}\hat{A}\right|\psi_n\right\rangle \\
&= \sum_{n}\left\langle\psi_n\left|\hat{A}^{+}\hat{A}\right|\psi_n\right\rangle
\end{aligned}$$

since $\sum_{m}\left|\psi_m\right\rangle\left\langle\psi_m\right|$ is the identity operator $\hat{I}$.

3. (i) We have, for the principal quantum number n, and the orbital quantum number ℓ ,

$$n \geq \ell + 1$$

so

$$\ell \leq n - 1$$

For n = 3, therefore, we can have

$$\ell = 0,1,2$$

For $\ell = 0$, there is only one possible value of the magnetic quantum number m, giving, trivially, one state.

For $\ell = 1$, we can have $m = -1,0,1$, giving 3 states.

For $\ell = 2$, we can have $m = -2,-1,0,1,2$, giving 5 states.

So, altogether, there are nine states with principal quantum number n = 3. (If we include spin, this number doubles to 18. Either answer is acceptable here).

(ii) Since the energy of a hydrogen atom state is

$$E_n = -\frac{R_y}{h^2}$$

all the states have the same energy, so there are nine such states (or 18, including spin) with the same energy.

4. (i) Group velocity, v_g is

$$v_g = \frac{dk}{d\omega}$$

and the quantum mechanical energy is

$$E = \hbar\omega$$

So

$$v_g = \frac{d\omega}{dk} = \frac{1}{dk/d\omega} = \frac{1}{\hbar dk/dE}$$

$$\frac{dk}{dE} = \frac{1}{2}\frac{1}{\left[\frac{2m_{eff}E}{\hbar^2}\left(1+\frac{E}{E_G}\right)\right]^{1/2}} \times \left[\frac{2m_{eff}}{\hbar^2}\left(1+\frac{2E}{E_G}\right)\right]$$

$$= \frac{1}{\hbar}\sqrt{\frac{m_{eff}}{2}}\frac{\left(1+\frac{2E}{E_G}\right)}{\left[E\left(1+\frac{E}{E_G}\right)\right]^{1/2}}$$

so

$$v_g = \sqrt{\frac{2}{m_{eff}}}\frac{\left[E\left(1+\frac{E}{E_G}\right)\right]^{1/2}}{\left(1+\frac{2E}{E_G}\right)}$$

(ii) For very large values of energy E

$$v_g \to \sqrt{\frac{2}{m_{eff}} \frac{E}{\sqrt{E_G}} \frac{E_G}{2E}} = \sqrt{\frac{E_G}{2m_{eff}}}$$

i.e., v_g tends to a constant value.

(iii) Because the group velocity is becoming a constant for large E, the group velocity dispersion is also vanishing and so, for large E, the wavepacket will tend not to disperse.

(iv) The phase velocity is

$$\begin{aligned} v_p &= \frac{\omega}{k} = \frac{1}{\hbar}\frac{E}{k} \\ &= \frac{E}{\hbar}\left[\frac{\hbar^2}{2m_{eff}E}\frac{1}{\left(1+\frac{E}{E_G}\right)}\right]^{1/2} \end{aligned}$$

For large E

$$\begin{aligned} v_p &\to \frac{E}{\hbar}\left[\frac{\hbar^2}{2m_{eff}}\frac{E_G}{E^2}\right]^{1/2} \\ &= \frac{\hbar}{\hbar\sqrt{2m_{eff}}}\sqrt{E_G} \\ &= \sqrt{\frac{E_G}{2m_{eff}}} \end{aligned}$$

So the group velocity and the phase velocity tend to the same value.

5. (i) $\hat{x}$ and $\hat{p}_x$, $\hat{y}$ and $\hat{p}_y$, and $\hat{z}$ and $\hat{p}_z$ are the pairs that do not commute.

(ii) We are given

$$\begin{aligned} \hat{L}_x &= \hat{y}\hat{p}_z - \hat{z}\hat{p}_y \\ \hat{L}_y &= \hat{z}\hat{p}_x - \hat{x}\hat{p}_z \\ \hat{L}_z &= \hat{x}\hat{p}_y - \hat{y}\hat{p}_x \end{aligned}$$

Hence

$$
\begin{aligned}
\left[\hat{L}_x,\hat{L}_y\right] &= \left(\hat{y}\hat{p}_z-\hat{z}\hat{p}_y\right)\left(\hat{z}\hat{p}_x-\hat{x}\hat{p}_z\right)-\left(\hat{z}p_x-\hat{x}\hat{p}_z\right)\left(\hat{y}p_z-\hat{z}p_y\right)\\
&= \hat{y}\hat{p}_z\hat{z}\hat{p}_x-\hat{y}\hat{p}_z\hat{x}p_z-\hat{z}p_y\hat{z}\hat{p}_x+\hat{z}\hat{p}_y\hat{x}\hat{p}_z-\hat{z}p_x\hat{y}\hat{p}_z+\hat{z}\hat{p}_x\hat{z}\hat{p}_y+\hat{x}\hat{p}_z\hat{y}\hat{p}_z-\hat{x}\hat{p}_z\hat{z}\hat{p}_y\\
&= \hat{x}\hat{p}_y\left(\hat{z}\hat{p}_z-\hat{p}_z\hat{z}\right)+\hat{y}\hat{p}_x\left(\hat{p}_z\hat{z}-\hat{z}\hat{p}_z\right)\\
&= i\hbar\left(\hat{x}\hat{p}_y-\hat{y}\hat{p}_x\right)\quad\text{since}\quad \hat{p}_z\hat{z}-\hat{z}\hat{p}_z=\left[\hat{p}_z,\hat{z}\right]=-i\hbar
\end{aligned}
$$

so

$$\left[\hat{L}_x,\hat{L}_x\right]=i\hbar\hat{L}_z$$

6. (i) For a system initially in state $\left|\psi_1\right\rangle$, the expansion coefficient of this state is 1 and all others are zero. We have

$$a_q^{(1)}(t)=\frac{1}{i\hbar}\exp\left(i\omega_{q1}t\right)\left\langle\psi_q\left|\hat{H}_p(t)\right|\psi_1\right\rangle$$

for the rate of change of the expansion coefficient a_q of state $\left|\psi_q\right\rangle$, where

$$\omega_{q1}=\frac{E_q-E_1}{\hbar}$$

and in this problem our perturbing Hamiltonian is

$$
\begin{aligned}
\hat{H}_p(t)&=0 && t<0\\
&=eF_z && 0\le t\le t_0\\
&=0 && t>t_0
\end{aligned}
$$

So, with

$$z_{q1}=\left\langle\psi_q\left|z\right|\psi_1\right\rangle$$

we have

$$
\begin{aligned}
a_q^{(1)}(t>t_0) &= \frac{eFz_{q1}}{i\hbar}\int_0^{t_0}\exp\left(i\omega_{q1}t\right)dt\\
&= -\frac{eFz_{q1}}{\hbar\omega_{q1}}\left[\exp\left(i\omega_{q1}t_0\right)-1\right]\\
&= -\frac{eFz_{q1}}{E_q-E_1}\exp\left(\frac{i\omega_{q1}t_0}{2}\right)\left[\exp\left(\frac{i\omega_{q1}t_0}{2}\right)-\exp\left(-\frac{i\omega_{q1}t_0}{2}\right)\right]\\
&= -\frac{2ieFz_{q1}}{E_q-E_1}\exp\left(\frac{i\omega_{q1}t_0}{2}\right)\sin\left(\frac{\omega_{q1}t_0}{2}\right)
\end{aligned}
$$

Now, for our infinitely deep potential well,

$$\left|\psi_n\right\rangle = \sqrt{\frac{z}{L_z}}\sin\left(\frac{n\pi z}{L_z}\right) \qquad \text{and} \qquad E_n = \frac{\hbar^2}{2m_0}\left(\frac{n\pi}{L_z}\right)^2$$

so

$$z_{21} = \frac{z}{L_z}\int_0^{L_z} z\sin\left(\frac{2\pi z}{L_z}\right)\sin\left(\frac{\pi z}{L_z}\right)dz$$

Change variables to $x = \frac{\pi z}{L_z}$ (so $z = \frac{L_z}{\pi}x$).

$$z_{21} = \frac{z}{L_z}\left(\frac{L_z}{\pi}\right)^2\int_0^{\pi} x\sin 2x\sin x\,dx$$

Given that

$$\begin{aligned}\int_0^{\pi}\left(x-\frac{\pi}{2}\right)\sin nx\sin mx\,dx &= -\frac{4nm}{(n-m)^2(n+m)^2} \quad \text{for n + m odd}\\ &= 0 \quad \text{for n + m even}\end{aligned}$$

then

$$\int_0^{\pi} x\sin 2x\sin x\,dx = -\frac{8}{9}+\frac{\pi}{2}\int_0^{\pi}\sin 2x\sin x\,dx = -\frac{8}{9}$$

(we are given this equivalence $\int_0^{\pi}\left(x-\frac{\pi}{2}\right)\sin nx\sin mx\,dx = \int_0^{\pi} x\sin nx\sin mx\,dx$ for different *n* and *m*, though that is also easily proved, since $\int_0^{\pi}\sin nx\sin mx\,dx = 0$ because the two sines are orthogonal because they are different eigenfunctions of an appropriate operator), and so

$$z_{21} = -\frac{16L_z}{9\pi^2}$$

Hence

$$a_2(t>t_0) = \frac{64im_0eFL_z^3}{27\pi^4 3\hbar^2}\exp\left(\frac{i\omega_{21}t_0}{2}\right)\sin\left(\frac{\omega_{21}t_0}{2}\right)$$

So the probability of finding the electron in the second state of the well for times $t > t_0$ is

$$P_2 = \left|a_2\left(t > t_0\right)\right|^2 = \left(\frac{64}{27\pi^4}\right)^2 \frac{m_0^2 e^2 F^2 L_z^6}{\hbar^4} \sin^2\left(\frac{3\hbar^2\pi^2 t_0}{4m_0 L_z^2}\right)$$

(ii) The largest possible value of $\sin^2\left(\theta\right)$ is 1, so the answer is the above expression with the $\sin^2$ term replaced by 1, i.e.,

$$P_{2\max} = \left(\frac{64}{27\pi^4}\right)^2 \frac{m_0^2 e^2 F^2}{\hbar^4} L_z^6$$

(iii) The matrix element $\langle\psi_3|z|\psi_1\rangle = 0$ by parity relative to the center of the well (note

$$\langle\psi_3|\frac{L_z}{2}|\psi_1\rangle = \frac{L_z}{2}\langle\psi_3|\psi_1\rangle = 0$$

by orthogonality, so

$$\langle\psi_3|z|\psi_1\rangle = \langle\psi_3|\frac{z - L_z}{z}|\psi_1\rangle = 0$$

by parity).

So, the electron will not be found in the third state, i.e., that probability is zero.

7. On the left of the well, the wave can be written

$$\psi_L(z) = A\exp\left(ik_s z\right) + B\exp\left(-ik_s z\right)$$

where

$$k_s = \sqrt{\frac{2m_0\left(E_s - V_0\right)}{\hbar^2}}$$

In the well, the wave can be written

$$\psi_w(z) = C\exp(ik_w z) + D\exp\left(-ik_w z\right)$$

where

$$kw = \sqrt{\frac{2m_0 E_s}{\hbar^2}}$$

On the right of the well, the wave can be written

$$\psi_R(z) = E\exp\left(ik_s\left(z - L_z\right)\right)$$

The boundary conditions we use at the interfaces are continuity of ψ and continuity of $d\psi/dz$.

At the right interface, we have from ψ

$$C\exp\left(ik_w L_z\right) - k_w D\exp\left(-ik_w L_z\right) = E \tag{1}$$

and from $d\psi / dz$.

$$k_w C\exp\left(ik_w L_z\right) - k_w D\exp\left(-ik_w L_z\right) = k_s E$$

i.e.,

$$C\exp\left(ik_w L_z\right) - D\exp\left(-ik_w L_z\right) = \frac{k_s}{k_w} E \tag{2}$$

Adding (1) and (2) gives

$$2C\exp\left(ik_w L_z\right) = \left(1 + \frac{k_s}{k_w}\right) E$$

i.e.,

$$C = \frac{1}{2}\left(1 + \frac{k_s}{k_w}\right)\exp\left(-ik_w L_z\right) E$$

Subtracting (2) from (1) gives

$$2D\exp\left(-ik_w L_z\right) = \left(1 - \frac{k_s}{k_w}\right) E$$

i.e.,

$$D = \frac{1}{2}\left(1 - \frac{k_s}{k_w}\right)\exp\left(ik_w L_z\right) E$$

Rewriting the wave in the well, we now have

$$\psi_w(z) = \frac{E}{2}\left[\left(1 + \frac{k_s}{k_w}\right)\exp\left(ik_w\left(z - L_z\right)\right) + \left(1 - \frac{k_s}{k_w}\right)\exp\left(-ik_w\left(z - L_z\right)\right)\right]$$

At the left interface (z = 0), matching ψ , we therefore have

$$A + B = \frac{E}{2}\left[\left(1 + \frac{k_s}{k_w}\right)\exp\left(-ik_w L_z\right) + \left(1 - \frac{k_s}{k_w}\right)\exp\left(ik_w L_z\right)\right] \tag{3}$$

and matching $d\psi / dz$

$$A - B = \frac{Ek_w}{2k_s}\left[\left(1 + \frac{k_s}{k_w}\right)\exp\left(-ik_w L_z\right) - \left(1 - \frac{k_s}{k_w}\right)\exp\left(ik_w L_z\right)\right] \tag{4}$$

Adding (3) and (4) gives

$$A=\frac{E}{4}\left[\left(1+\frac{k_w}{k_s}\right)\left(1+\frac{k_s}{k_w}\right)\exp\left(-ik_wL_z\right)+\left(1-\frac{k_w}{k_s}\right)\left(1-\frac{k_s}{k_w}\right)\exp\left(ik_wL_z\right)\right]$$

i.e.,

$$A=\frac{E}{4k_sk_w}\left[\left(k_s+k_w\right)^2\exp\left(-ik_wL_z\right)-\left(k_s-k_w\right)^2\exp\left(ik_wL_z\right)\right]$$

so

$$|A|^2=\frac{|E|^2}{16k_s^2k_w^2}\left[\left(k_s+k_w\right)^4+\left(k_s-k_w\right)^4-2\left(k_s+k_w\right)^2\left(k_s-k_w\right)^2\cos\left(2k_wL_z\right)\right]$$

So the transmission of the structure is

$$T=\frac{|E|^2}{|A|^2}=\frac{16k_s^2k_w^2}{\left(k_s+k_w\right)^4+\left(k_s-k_w\right)^4-2\left(k_s+k_w\right)^2\left(k_s-k_w\right)^2\cos\left(2k_wL_z\right)}$$

(ii) For $2k_wL_z=2n\pi$ for some integer n

$$\cos(2k_wL_z)=1$$

and then

$$\begin{aligned}T&=\frac{16k_s^2k_w^2}{\left(k_s+k_w\right)^4+\left(k_s-k_w\right)^4-2\left(k_s+k_w\right)^2\left(k_s-k_w\right)^2}\\&=\frac{16k_s^2k_w^2}{\left[\left(k_s+k_w\right)^2-\left(k_s-k_w\right)^2\right]^2}\\&=\frac{16k_s^2k_w^2}{\left(k_s^2+k_w^2+2k_sk_w-k_s^2-k_w^2+2k_sk_w\right)^2}\\&=1\quad\text{(which is the largest possible transmission)}\end{aligned}$$

(iii) The transmission has maxima for

$$k_wL_z=2\pi$$

i.e.,

$$\sqrt{\frac{2m_eE_s}{\hbar^2}}L_z=2\pi$$

i.e.,

$$E_s = \frac{\hbar^2}{2m_0}\left(\frac{n\pi}{L_z}\right)^2$$

8. We will approach this problem by perturbation theory. Since we need to find an expectation value, we will need to find a perturbation correction to the wavefunction. We have, in general, for the first order correction to the first state

$$\left|\phi_1^{(1)}\right\rangle = \sum_{n=2}^{\infty} \frac{\langle \psi_n | \hat{H}_p | \psi_1 \rangle |\psi_n\rangle}{E_1 - E_n} \tag{1}$$

$\hat{H}_p$ here is

$$\hat{H}_p = eFz$$

(The sign corresponds to the increase in energy that an electron would experience if it were to be moved to positive z in the presence of a field in the positive z direction, because such a field pushes the electron in the negative z direction, i.e., the electron would be being pushed against the electrostatic force).

The wavefunctions are

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

and the unperturbed energies are

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

where

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

Hence

$$\langle \psi_n | \hat{H}_p | \psi_1 \rangle = \frac{2eF}{L_z} \int_0^{L_z} z \sin\left(\frac{n\pi z}{L_Z}\right) \sin\left(\frac{\pi z}{L_Z}\right) dz$$

Changing variables to $x = \frac{\pi z}{L_z}$, i.e., so $z = \frac{L_x}{\pi}$, we have (for *n* not equal to 1)

$$\langle \psi_n | \hat{H}_p | \psi_1 \rangle = \frac{2eF}{L_z}\left(\frac{L_z}{\pi}\right)^2 \int_0^{\pi} x\sin(nx)\sin(x)dx$$

$$= -\frac{8eFL_z}{\pi^2}\frac{n}{(n-1)^2(n+1)^2} \quad \text{for n even}$$

$$= 0 \quad \text{for n } odd$$

Hence, the first-order correction to the wavefunction becomes

$$\left|\phi_1^{(1)}\right\rangle = -\frac{8eFL_z}{\pi^2}\frac{2m_0L_z^2}{\hbar^2\pi^2}\sum_{n=2}^{\infty}\left[\frac{n}{(1-n)^2(n-1)^2(n+1)^2}\right]|\psi_n\rangle$$

$$= \frac{16em_0FL_z^3}{\pi^4\hbar^2}\sum_{n=2}^{\infty}\left[\frac{n}{(n-1)^3(n+1)^3}\right]|\psi_n\rangle$$

For $n = 2$, the term in the square brackets in the sum is

$$[...] = \frac{2}{27}$$

For $n = 4$ (which is the next non-zero term in the summation), we similarly have

$$[...] = \frac{4}{27\times125}$$

This second term is therefore smaller than the first term by a factor

$$\frac{4}{27\times125}\times\frac{27}{2} = \frac{2}{125}$$

which is a relatively quite small number. Therefore, we will neglect all but the first term in the summation, so we have

$$\left|\phi_1^{(1)}\right\rangle \simeq \frac{32em_0}{27\pi^4\hbar^2}FL_z^3|\psi_2\rangle$$

Now that we have a new approximate wavefunction

$$|\psi_n\rangle \simeq |\psi_1\rangle + \left|\phi_1^{(1)}\right\rangle$$

we can evaluate the expectation value of position to lowest order in F.

We have

$$\langle z\rangle = \left(\langle\psi_1| + \left\langle\phi_1^{(1)}\right|\right) z \left(|\psi_1\rangle + \left|\phi_1^{(1)}\right\rangle\right)$$

$$= \langle\psi_1|z|\psi_1\rangle + \left\langle\phi_1^{(1)}\right|z\left|\phi_1^{(1)}\right\rangle$$

$$+ \langle\psi_1|z\left|\phi_1^{(1)}\right\rangle + \left\langle\phi_1^{(1)}\right|z|\psi_1\rangle$$

We have

$$\langle\psi_1|z|\psi_1\rangle=\frac{L_z}{z}$$

(this can be evaluated directly, though it is obvious by the symmetry of the state).

The second term

$$\langle\phi_1^{(1)}|z|\phi_1^{(1)}\rangle$$

can be neglected because it would be a term in F^2.

We next note that, as previously evaluated,

$$\begin{aligned}\langle\psi_1|z|\psi_2\rangle&=\langle\psi_2|z|\psi_1\rangle\\&=\frac{z}{L_z}\left(\frac{L_z}{\pi}\right)^2\int_0^\pi x\sin(2x)\sin(x)dx\\&=-\frac{16L_z}{9\pi^2}\end{aligned}$$

so

$$\begin{aligned}\langle z\rangle&=\frac{L_z}{2}-\frac{2\times16L_z}{9\pi^2}\frac{32}{27}\frac{em_0}{\pi^4\hbar^2}FL_z^3\\&=\frac{L_z}{2}-\frac{1024}{243\pi^6}\frac{em_0FL_z^4}{\hbar^2}\end{aligned}$$