Quantum I Review – Solutions

This is a series of questions to help you review QMI. Work with your peers and feel free to use your book!

Notes for these problems

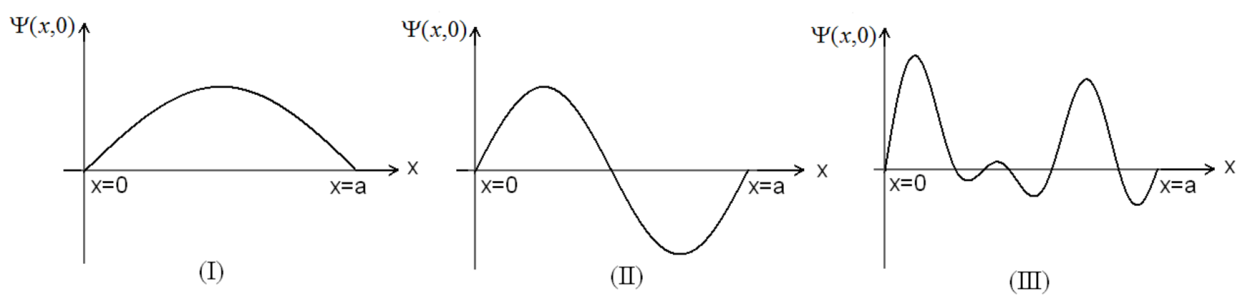
- $\hat{x}$, $\hat{p}$, and $\hat{H}$ correspond to the position, momentum and Hamiltonian operators respectively for a given quantum system.
- A physical observable is "well-defined" when it has a definite value for a given wave function.
- "1-D" is an abbreviation for one-dimensional. All questions refer to systems with one spatial dimension.
- $\psi(x)$ is a time-independent wave function. $\Psi(x,t)$ is a function at time t.

1-D Infinite Square Well

A particle sits inside a 1-D infinite square well of width a:

$$V(x) = \begin{cases} 0, & 0 \le x \le a \\ \infty, & \text{otherwise} \end{cases}$$

1. Choose all the possible wave functions $\Psi(x, t = 0)$ for this system (all graphs are continuous and differentiable for $0 \le x \le a$.



All are possible

2. Suppose at $t = 0$ the particle is in the first excited state. Which of the following expectation values depend on time $\langle\hat{x}\rangle$, $\langle\hat{p}\rangle$, $\langle\hat{H}\rangle$?
None

3. If the particle is in the $n = 5$ state, what is the probability density as a function of time?
$|\boldsymbol{\Psi}(x,t)|^2 = \frac{2}{a}\sin^2\left(\frac{5\pi x}{a}\right)$ **which is time independent.**

4. The wave function at some time is

$$\Psi(x, t=0) = \sqrt{\frac{2}{7}}\psi_1(x) + i\sqrt{\frac{5}{7}}\psi_2(x)$$

a. What are the possible values for the energy (a list of E_n is sufficient)?
E_1 and E_2

b. What is the expectation value of the energy as a function of E_n?
$\langle E\rangle = \frac{2}{7}E_1 + \frac{5}{7}E_2$ (note the time independence)

c. If a measurement is made and the resulting energy is $\frac{4\pi^2\hbar^2}{2ma^2}$ what is the spatial wavefunction?
$\psi_2(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{2\pi x}{a}\right)$

5. A particle is in the state

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

a. which of the following expectation values are independent of time $\langle\hat{x}\rangle$, $\langle\hat{p}\rangle$, $\langle\hat{H}\rangle$?
Only $\langle\hat{H}\rangle$, see the appended pdf for derivations.

b. If we make a position measurement and get $x = a/2$ and then *immediately* measure the energy, what values might we get?
E_1. In general, we can only get the odd energies!

c. Same question, but this time, we measured $x = a/4$ instead.
Either E_1 or E_2. In general, we can get any energy where $\mathrm{mod}(n, 4) = 0$

Quantum Mechanical Harmonic Oscillator

A particle sits in $V(x) = -\frac{1}{2}kx^2 = m\omega^2x^2$ such that $\omega \equiv \sqrt{\frac{k}{m}}$. The eigenstates ψ_n can be represented in bra-ket notation as $|n\rangle$

6. Write the position $\hat{x}$ and momentum $\hat{p}$ operators in terms of the raising and lowering operators $\hat{a}_+$ and $\hat{a}_-$.

$$x = \sqrt{\frac{\hbar}{2m\omega}}\,(a_- + a_+), \qquad p = i\sqrt{\frac{m\hbar\omega}{2}}(a_+ - a_-)$$

7. Using these representations determine the following
   a. $\langle n|x|m\rangle$
   b. $\langle n|p|m\rangle$
   c. $\langle x^2\rangle$
   d. $\langle p^2\rangle$

8. Use the above to prove the quantum analog of the viral theorem $\langle V\rangle = \langle T\rangle = \frac{\langle H\rangle}{2}$

Derivation of the expectation values for a particle in a superposition of the first two states of an infinite square well

B. Toggerson
Physics 564
University of Massachusetts Amherst

Spring 2025

1 $\langle \hat{H} \rangle$

In an infinite square well, the energy eigenstates $\psi_n(x)$ satisfy

$$H\psi_n(x) = E_n\psi_n(x),$$

with the corresponding eigenenergies

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}, \quad n = 1, 2, 3, \ldots$$

For the ground state ($n = 1$) and the first excited state ($n = 2$), we have:

$$E_1 = \frac{\pi^2\hbar^2}{2ma^2}, \quad E_2 = \frac{4\pi^2\hbar^2}{2ma^2}.$$

At time $t = 0$, the particle is in the state

$$\psi(x, 0) = \frac{1}{\sqrt{2}}\Big(\psi_1(x) + \psi_2(x)\Big).$$

Since the Hamiltonian is time-independent, the time evolution of each energy eigenstate is given by a phase factor:

$$\psi_n(x, t) = \psi_n(x)e^{-iE_nt/\hbar}.$$

Thus, the state at time t is

$$\psi(x,t) = \frac{1}{\sqrt{2}}\Big(\psi_1(x)e^{-iE_1t/\hbar} + \psi_2(x)e^{-iE_2t/\hbar}\Big).$$

The expectation value of the Hamiltonian in the state $\psi(x,t)$ is given by

$$\langle H\rangle = \int_0^a \psi^*(x,t)\, H\, \psi(x,t)\, dx.$$

Since $\psi_1(x)$ and $\psi_2(x)$ are eigenstates of H and are orthogonal (i.e., $\langle\psi_1|\psi_2\rangle = 0$), we can simplify the calculation.

Writing out the state explicitly:

$$\psi(x,t) = \frac{1}{\sqrt{2}}\left[\psi_1(x)e^{-iE_1t/\hbar} + \psi_2(x)e^{-iE_2t/\hbar}\right],$$

the complex conjugate is

$$\psi^*(x,t) = \frac{1}{\sqrt{2}}\left[\psi_1^*(x)e^{iE_1t/\hbar} + \psi_2^*(x)e^{iE_2t/\hbar}\right].$$

When you compute the expectation value, you get cross terms such as:

$$\frac{1}{2}\left(e^{iE_1t/\hbar}e^{-iE_2t/\hbar}\langle\psi_1|H|\psi_2\rangle + \text{c.c.}\right).$$

However, because

$$H\psi_2 = E_2\psi_2 \quad \text{and} \quad \langle\psi_1|\psi_2\rangle = 0,$$

these cross terms vanish. Thus, we are left with:

$$\langle H\rangle = \frac{1}{2}\langle\psi_1|H|\psi_1\rangle + \frac{1}{2}\langle\psi_2|H|\psi_2\rangle = \frac{1}{2}E_1 + \frac{1}{2}E_2.$$

Notice that there is no time dependence in the result:

$$\langle H\rangle = \frac{1}{2}(E_1 + E_2).$$

Since the Hamiltonian is time-independent, and the state is a superposition of its eigenstates, the expectation value of the energy (the Hamiltonian) remains constant in time.

Substitute the values for E_1 and E_2:

$$\langle H \rangle = \frac{1}{2}\left(\frac{\pi^2\hbar^2}{2ma^2} + \frac{4\pi^2\hbar^2}{2ma^2}\right) = \frac{1}{2}\left(\frac{5\pi^2\hbar^2}{2ma^2}\right) = \frac{5\pi^2\hbar^2}{4ma^2}.$$

The expectation value of the Hamiltonian does not evolve with time; it remains constant:

$$\langle H \rangle(t) = \frac{E_1 + E_2}{2} = \frac{5\pi^2\hbar^2}{4ma^2}.$$

This result reflects the conservation of energy in a time-independent quantum system.

2 $\langle \hat{x} \rangle$

Expectation Value of Position in Quantum Mechanics

We start with the state at time $t = 0$ given by

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

where for an infinite square well of width a (with $0 \leq x \leq a$) the normalized eigenfunctions are

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\Big(\frac{n\pi x}{a}\Big), \quad n = 1, 2, \ldots$$

and the corresponding energies are

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}.$$

Because the Hamiltonian is time independent, the time evolution of each eigenstate is simply

$$\psi_n(x,t) = \psi_n(x)e^{-iE_nt/\hbar}.$$

Thus, the full time-dependent state is

$$\psi(x,t) = \frac{1}{\sqrt{2}}\Big[\psi_1(x)e^{-iE_1t/\hbar} + \psi_2(x)e^{-iE_2t/\hbar}\Big].$$

Our goal is to compute the expectation value of the position operator x,

$$\langle x\rangle(t) = \int_0^a \psi^*(x,t)\, x\, \psi(x,t)\, dx.$$

Writing out the state explicitly, we have

$$\psi(x,t) = \frac{1}{\sqrt{2}}\Big[\psi_1(x)e^{-iE_1t/\hbar} + \psi_2(x)e^{-iE_2t/\hbar}\Big],$$

and its complex conjugate

$$\psi^*(x,t) = \frac{1}{\sqrt{2}}\Big[\psi_1(x)e^{iE_1t/\hbar} + \psi_2(x)e^{iE_2t/\hbar}\Big],$$

(where we may take the $\psi_n(x)$ to be real). Then

$$\langle x\rangle(t) = \frac{1}{2}\int_0^a \Big\{\psi_1(x)^2+\psi_2(x)^2+e^{i(E_1-E_2)t/\hbar}\psi_1(x)\psi_2(x)+e^{i(E_2-E_1)t/\hbar}\psi_2(x)\psi_1(x)\Big\}x\, dx.$$

This splits into two types of terms:

- Diagonal terms:
$$\frac{1}{2}\Big[\langle\psi_1|x|\psi_1\rangle + \langle\psi_2|x|\psi_2\rangle\Big].$$
- Off-diagonal (interference) terms:
$$\frac{1}{2}\Big[e^{i(E_1-E_2)t/\hbar}\langle\psi_1|x|\psi_2\rangle + e^{i(E_2-E_1)t/\hbar}\langle\psi_2|x|\psi_1\rangle\Big].$$

It is a standard result that for the infinite square well (from 0 to a)

$$\langle\psi_n|x|\psi_n\rangle = \frac{a}{2} \quad \text{for any} n.$$

Thus,

$$\frac{1}{2}\Big[\langle\psi_1|x|\psi_1\rangle + \langle\psi_2|x|\psi_2\rangle\Big] = \frac{1}{2}\Big[\frac{a}{2}+\frac{a}{2}\Big] = \frac{a}{2}.$$

We compute the matrix element

$$\langle\psi_1|x|\psi_2\rangle = \int_0^a \psi_1(x)\, x\, \psi_2(x)\, dx.$$

Using the product-to-sum identity and integration techniques, we obtain

$$\langle \psi_1 | x | \psi_2 \rangle = -\frac{16a}{9\pi^2}.$$

Since the wavefunctions are real, we also have

$$\langle \psi_2 | x | \psi_1 \rangle = \langle \psi_1 | x | \psi_2 \rangle = -\frac{16a}{9\pi^2}.$$

Thus, the off-diagonal contribution to $\langle x \rangle(t)$ is

$$-\frac{16a}{9\pi^2} \cos\Big(\frac{(E_2 - E_1)t}{\hbar}\Big).$$

Adding the diagonal and off-diagonal contributions, we obtain

$$\langle x \rangle(t) = \frac{a}{2} - \frac{16a}{9\pi^2} \cos\Big(\frac{3\pi^2\hbar}{2ma^2} t\Big).$$

- Time Dependence: Unlike the expectation value of the energy, $\langle x \rangle$ is time-dependent because the state is a superposition of two different energy eigenstates. Their relative phase produces the cosine oscillation.
- Oscillation: The center of the oscillation is at $a/2$, and the amplitude is $\frac{16a}{9\pi^2}$.
- Frequency: The oscillation frequency is $\omega = (E_2 - E_1)/\hbar = \frac{3\pi^2\hbar}{2ma^2}$.

3 $\langle \hat{p} \rangle$

We begin with the time-dependent wave function for the infinite square well (with $0 \leq x \leq a$) when the system is in the superposition

$$\psi(x,t) = \frac{1}{\sqrt{2}}\Big[\psi_1(x) e^{-iE_1 t/\hbar} + \psi_2(x) e^{-iE_2 t/\hbar}\Big],$$

with

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\Big(\frac{n\pi x}{a}\Big)$$

and

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \quad (n = 1, 2).$$

Our goal is to calculate the expectation value of the momentum operator,

$$\langle p\rangle(t) = \int_0^a \psi^*(x,t)\,\hat{p}\,\psi(x,t)\,dx,$$

with

$$\hat{p} = -i\hbar\frac{\partial}{\partial x}\,.$$

Because the energy eigenfunctions $\psi_1(x)$ and $\psi_2(x)$ are real, the only time dependence comes from the phase factors.

The state is

$$\psi(x,t) = \frac{1}{\sqrt{2}}\Big[\psi_1(x)e^{-iE_1t/\hbar} + \psi_2(x)e^{-iE_2t/\hbar}\Big],$$

so its complex conjugate is

$$\psi^*(x,t) = \frac{1}{\sqrt{2}}\Big[\psi_1(x)e^{iE_1t/\hbar} + \psi_2(x)e^{iE_2t/\hbar}\Big].$$

Thus,

$$\langle p\rangle(t) = -i\hbar\int_0^a \psi^*(x,t)\frac{\partial}{\partial x}\psi(x,t)\,dx.$$

Plugging in the expressions we have

$$\langle p\rangle(t) = -\frac{i\hbar}{2}\int_0^a\Big\{\psi_1(x)e^{iE_1t/\hbar}+\psi_2(x)e^{iE_2t/\hbar}\Big\}\frac{\partial}{\partial x}\Big[\psi_1(x)e^{-iE_1t/\hbar}+\psi_2(x)e^{-iE_2t/\hbar}\Big]dx.$$

When you expand the derivative, you get four terms. However, the terms in which the same eigenstate appears (the "diagonal" terms) vanish because for a normalized eigenstate with $\psi_n(0) = \psi_n(a) = 0$ one finds

$$\int_0^a \psi_n(x)\psi_n'(x)\,dx = \frac{1}{2}\Big[\psi_n(x)^2\Big]_0^a = 0.$$

Thus only the off-diagonal (interference) terms contribute.

The off-diagonal contributions come from the cross terms:

$$\langle p\rangle(t) = -\frac{i\hbar}{2}\left\{e^{-i\Delta E\,t/\hbar}\int_0^a \psi_1(x)\,\psi_2'(x)\,dx + e^{i\Delta E\,t/\hbar}\int_0^a \psi_2(x)\,\psi_1'(x)\,dx\right\},$$

where we have defined

$$\Delta E = E_2 - E_1.$$

It is useful to denote

$$I \equiv \int_0^a \psi_1(x)\, \psi_2'(x)\, dx.$$

A short integration-by-parts shows that

$$\int_0^a \psi_2(x)\, \psi_1'(x)\, dx = -I,$$

since the boundary terms vanish.

Thus, we can write:

$$\langle p\rangle(t) = -\frac{i\hbar}{2}\Big[e^{-i\Delta E\, t/\hbar} I - e^{i\Delta E\, t/\hbar} I\Big] = -\frac{i\hbar I}{2}\Big[e^{-i\Delta E\, t/\hbar} - e^{i\Delta E\, t/\hbar}\Big].$$

Noting that

$$e^{-i\Delta E\, t/\hbar} - e^{i\Delta E\, t/\hbar} = -2i\, \sin\Big(\frac{\Delta E\, t}{\hbar}\Big),$$

we obtain

$$\langle p\rangle(t) = -\frac{i\hbar I}{2}\Big[-2i\, \sin\Big(\frac{\Delta E\, t}{\hbar}\Big)\Big] = \hbar\, I\, \sin\Big(\frac{\Delta E\, t}{\hbar}\Big).$$

Since our I came with a minus sign later in our calculation (see below), let us carefully compute it.

Thus, the expectation value of the momentum for the state

$$\psi(x,t) = \frac{1}{\sqrt{2}}\Big[\psi_1(x)e^{-iE_1 t/\hbar} + \psi_2(x)e^{-iE_2 t/\hbar}\Big]$$

in the infinite square well (from $x = 0$ to $x = a$) is

$$\langle p\rangle(t) = \frac{8\hbar}{3a}\sin\Big(\frac{3\pi^2\hbar}{2ma^2}\, t\Big).$$