# Qualitative Questions

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| 1 | For the following four topics include a sketch the potential and the wavefunctions with your description in words |
| 2 | The transmission and reflection coefficients for a potential step up |
| 3 | The transmission and reflection coefficients for a potential step down |
| 4 | The transmission and reflection coefficients for a potential well (down) |
| 5 | The transmission and reflection coefficients for a potential barrier (up) |
| | |
| 6 | Why study the square well? |
| 7 | Sketch the first four energy eigenfunctions for the square well in x-space |
| 8 | Sketch the corresponding first four probability densities for the square well in x-space |
| 9 | Sketch the first four energy eigenfunctions for the square well in p-space |
| 10 | Sketch the first four energy eigenfunctions for the square well in E-space |
| 11 | Obtaining the eigenfunctions for the square well |
| 12 | Obtaining the eigenenergies for the square well |
| | |
| 13 | The past, present, and future time evolution of a 1d free-particle Gaussian wave packet |
| 14 | The spreading of a Gaussian wave packet and the dispersion of empty space for matter waves |
| 15 | The eigenstates of momentum for the one-dimensional free particle |
| 16 | The phase velocity and the group velocity for the one-dimensional free particle |
| 17 | The minimum uncertainty state for the free particle |
| | |
| 18 | Why study the harmonic oscillator? |
| 19 | Sketch the first four energy eigenfunctions for the harmonic oscillator in x-space |
| 20 | Sketch the corresponding first four probability densities for the harmonic oscillator in x-space |
| 21 | Sketch the first four energy eigenfunctions for the harmonic oscillator in p-space |
| 22 | Sketch the first four energy eigenfunctions for the harmonic oscillator in E-space |
| 23 | Obtaining the eigenenergies for the harmonic oscillator via the separation of variables |
| 24 | Obtaining the eigenfunctions for the harmonic oscillator via the separation of variables |
| 25 | Charles Hermite, the Hermite equation, and the Hermite polynomials |
| 26 | Factoring the Hamiltonian for the harmonic oscillator |
| 27 | The ladder operators for the harmonic oscillator in Hilbert space |
| 28 | The ladder operators for the harmonic oscillator in position space |
| 29 | Obtaining the eigenenergies for the simple harmonic oscillator using the ladder operators |
| 30 | Obtaining the eigenfunctions for the simple harmonic oscillator using the ladder operators |
| 31 | The minimum uncertainty state for the harmonic oscillator |
| 32 | The zero-point energy and the zero-point motion of the harmonic oscillator |

# Superposition States in the Square Well

Consider a particle moving in the infinitely deep square well.

The initial state vector is a superposition of the first excited state $\mid 2 >$ and the second excited state $\mid 3 >$

$$|\psi(0) >= N \left[ \, | \, 2 > + | \, 3 > \right].$$

(a) Calculate the normalization constant N.

(b) Express the normalized time-dependent state vector $|\psi(t) >$ in terms of the energy eigenkets.

(c) Express the normalized time-dependent position-space wavefunction $\psi(x,t) =< x|\psi(t) >$ in terms of the energy eigenfunctions in position space.

(d) Sketch the first-excited-state wavefunction $\psi_2(x,0)$ and the corresponding probability density $|\psi_2(x,0)|^2$ inside the well.

(e) Sketch the second-excited-state wavefunction $\psi_3(x,0)$ and the corresponding probability density $|\psi_3(x,0)|^2$ inside the well.

(f) Sketch the interference-cross-term $\psi_2(x,0)\ \psi_3(x,0)\cos(\omega_{32}t)$ inside the well.

(g) Explain how the sum of these three functions (d, e, and f) produces the time-dependent motion of the particle in the well.

(h) Using the applet at http://falstad.com/qm1d or your own software, make some sketches of the position-space probability density versus time. Your sketches should show the position-space probability density when $< x >$ is maximum, zero, and minimum.

(i) Use the applet at http://falstad.com/qm1d or your own software, to show that the oscillation frequency of the position-space probability density is $\omega_{32} = \omega_3 - \omega_2$.

(j) If the position is measured at time t, what results can be found, and with what probabilities will these results be found?

(k) If the energy is measured at time t, what results can be found, and with what probabilities will these results be found?

(l) Calculate the expectation value of the energy $< E(t) >$ and the uncertainty in the energy $\Delta E(t)$

(*ii*) We see that, for large $n$, although the absolute value of the momentum is well-defined, its sign is not. This is why $\Delta P_n$ is large: for probability distributions with two maxima like that of figure 3, the root-mean-square deviation reflects the distance between the two peaks; it is no longer related to their widths.

## 2. Evolution of the particle's wave function

Each of the states $| \varphi_n \rangle$, with its wave function $\varphi_n(x)$, describes a stationary state, which leads to time-independent physical predictions. Time evolution appears only when the state vector is a linear combination of several kets $| \varphi_n \rangle$. We shall consider here a very simple case, for which at time $t = 0$ the state vector $| \psi(0) \rangle$ is:

$$| \psi(0) \rangle = \frac{1}{\sqrt{2}} [\, | \varphi_1 \rangle + | \varphi_2 \rangle ] \tag{14}$$

### a. WAVE FUNCTION AT THE INSTANT $t$

Apply formula (D-54) of chapter III; we immediately obtain:

$$| \psi(t) \rangle = \frac{1}{\sqrt{2}} [ e^{-i \frac{\pi^2 \hbar}{2ma^2} t} | \varphi_1 \rangle + e^{-2i \frac{\pi^2 \hbar}{ma^2} t} | \varphi_2 \rangle ] \tag{15}$$

or, omitting a *global* phase factor of $| \psi(t) \rangle$:

$$| \psi(t) \rangle \propto \frac{1}{\sqrt{2}} [\, | \varphi_1 \rangle + e^{-i\omega_{21}t} | \varphi_2 \rangle ] \tag{16}$$

with:

$$\omega_{21} = \frac{E_2 - E_1}{\hbar} = \frac{3\pi^2 \hbar}{2ma^2} \tag{17}$$

### b. EVOLUTION OF THE SHAPE OF THE WAVE PACKET

The shape of the wave packet is given by the probability density:

$$|\psi(x, t)|^2 = \frac{1}{2} \varphi_1^2(x) + \frac{1}{2} \varphi_2^2(x) + \varphi_1(x)\, \varphi_2(x) \cos \omega_{21} t \tag{18}$$

We see that the time variation of the probability density is due to the interference term in $\varphi_1 \varphi_2$. Only one Bohr frequency appears, $\nu_{21} = (E_2 - E_1)/h$, since the initial state (14) is composed only of the two states $| \varphi_1 \rangle$ and $| \varphi_2 \rangle$. The curves corresponding to the variation of the functions $\varphi_1^2$, $\varphi_2^2$ and $\varphi_1 \varphi_2$ are traced in figures 4-a, b and c.

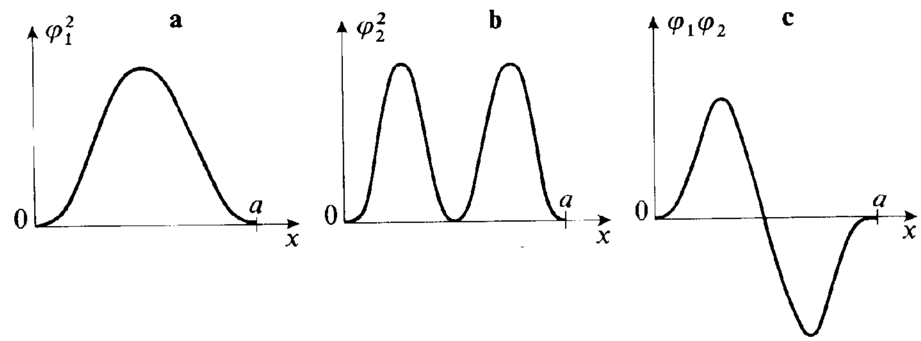



FIGURE 4

**Graphical representation of the functions $\varphi_1^2$ (the probability density of the particle in the ground state), $\varphi_2^2$ (the probability density of the particle in the first excited state) and $\varphi_1\varphi_2$ (the cross term responsible for the evolution of the shape of the wave packet).**

Using these figures and relation (18), it is not difficult to represent graphically the variation in time of the shape of the wave packet (*cf.* fig. 5): we see that the wave packet oscillates between the two walls of the well.

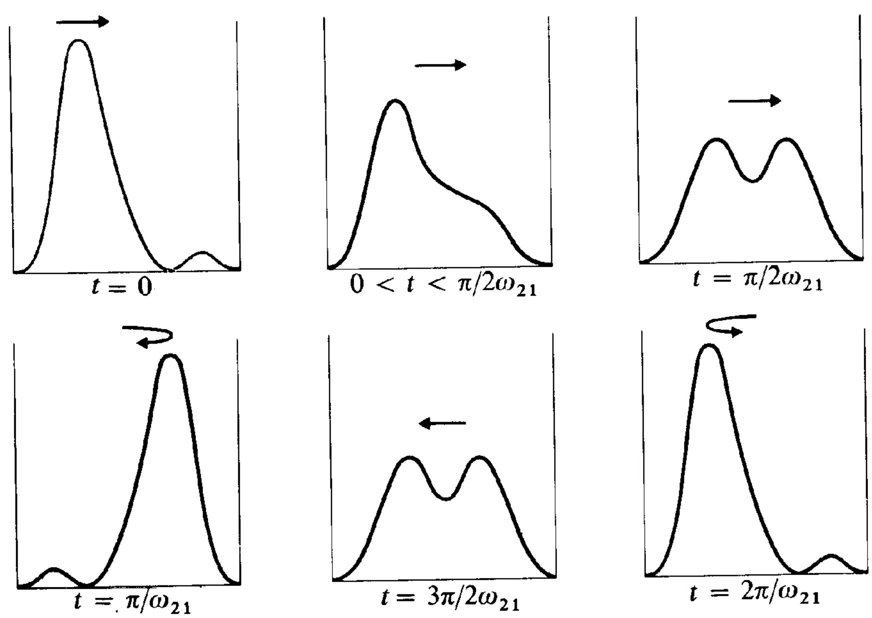



FIGURE 5

**Periodic motion of a wave packet obtained by superposing the ground state and the first excited state of a particle in an infinite well. The frequency of the motion is the Bohr frequency $\omega_{21}/2\pi$.**

### c. MOTION OF THE CENTER OF THE WAVE PACKET

Let us calculate the mean value $\langle X \rangle(t)$ of the position of the particle at time $t$. It is convenient to take:

$$X' = X - a/2 \tag{19}$$

since, by symmetry, the diagonal matrix elements of $X'$ are zero:

$$\begin{aligned} \langle \varphi_1 | X' | \varphi_1 \rangle &\propto \int_0^a \left(x - \frac{a}{2}\right) \sin^2\left(\frac{\pi x}{a}\right) dx = 0 \\ \langle \varphi_2 | X' | \varphi_2 \rangle &\propto \int_0^a \left(x - \frac{a}{2}\right) \sin^2\left(\frac{2\pi x}{a}\right) dx = 0 \end{aligned} \tag{20}$$

We then have:

$$\langle X' \rangle(t) = \text{Re}\,\{ e^{-i\omega_{21}t} \langle \varphi_1 | X' | \varphi_2 \rangle \} \tag{21}$$

with:

$$\begin{aligned} \langle \varphi_1 | X' | \varphi_2 \rangle &= \langle \varphi_1 | X | \varphi_2 \rangle - \frac{a}{2} \langle \varphi_1 | \varphi_2 \rangle \\ &= \frac{2}{a} \int_0^a x \sin\frac{\pi x}{a} \sin\frac{2\pi x}{a} dx \\ &= -\frac{16a}{9\pi^2} \end{aligned} \tag{22}$$

Therefore:

$$\langle X \rangle(t) = \frac{a}{2} - \frac{16a}{9\pi^2} \cos \omega_{21} t \tag{23}$$

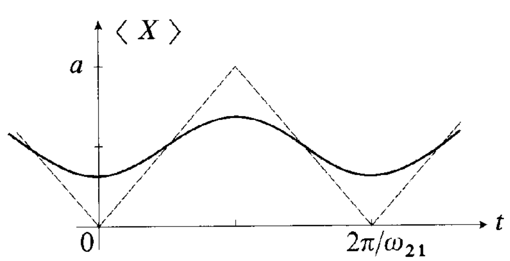



FIGURE 6

**Time variation of the mean value $\langle X \rangle$ corresponding to the wave packet of figure 5. The dashed line represents the position of a classical particle moving with the same period. Quantum mechanics predicts that the center of the wave packet will turn back before reaching the wall, as explained by the action of the potential on the "edges" of the wave packet.**

The variation of $\langle X \rangle(t)$ is represented in figure 6. In dashed lines, the variation of the position of a classical particle has been traced, for a particle moving to and fro in the well with an angular frequency of $\omega_{21}$ (since it is not subjected to any force except at the walls, its position varies linearly with $t$ between 0 and $a$ during each half-period).

We immediately notice a very clear difference between these two types of motion, classical and quantum mechanical. The center of the quantum wave packet, instead of turning back at the walls of the well, executes a movement of smaller amplitude and retraces its steps before reaching the regions where the potential is not zero. We see again here a result of §D-2 of chapter I: since the potential varies infinitely quickly at $x = 0$ and $x = a$, its variation within a domain of the order of the dimension of the wave packet is not negligible, and the motion of the center of the wave packet does not obey the laws of classical mechanics (see also chapter III, § D-1-d-γ). The physical explanation of this phenomenon is the following: before the center of the wave packet has touched the wall, the action of the potential on the "edges" of this packet is sufficient to make it turn back.

COMMENT:

The mean value of the energy of the particle in the state $|\psi(t)\rangle$ calculated in (15) is easy to obtain:

$$\langle H \rangle = \frac{1}{2} E_1 + \frac{1}{2} E_2 = \frac{5}{2} E_1 \tag{24}$$

as is:

$$\langle H^2 \rangle = \frac{1}{2} E_1^2 + \frac{1}{2} E_2^2 = \frac{17}{2} E_1^2 \tag{25}$$

which gives:

$$\Delta H = \frac{3}{2} E_1 \tag{26}$$

Note in particular that $\langle H \rangle$, $\langle H^2 \rangle$ and $\Delta H$ are not time-dependent; since $H$ is a constant of the motion, this could have been foreseen. In addition, we see from the preceding discussion that the wave packet evolves appreciably over a time of the order of:

$$\Delta t \simeq \frac{1}{\omega_{21}} \tag{27}$$

Using (26) and (27), we find:

$$\Delta H \,.\, \Delta t \simeq \frac{3}{2} E_1 \times \frac{\hbar}{3E_1} = \frac{\hbar}{2} \tag{28}$$

We again find the time-energy uncertainty relation.

# Transmission and Reflection

Consider the transmission and reflection coefficients for a potential with two steps down as shown in the attached figure.

(a) Sketch the components of the wavefunctions in each region.

(b) Write down the functional form of the wavefunction in the three regions.

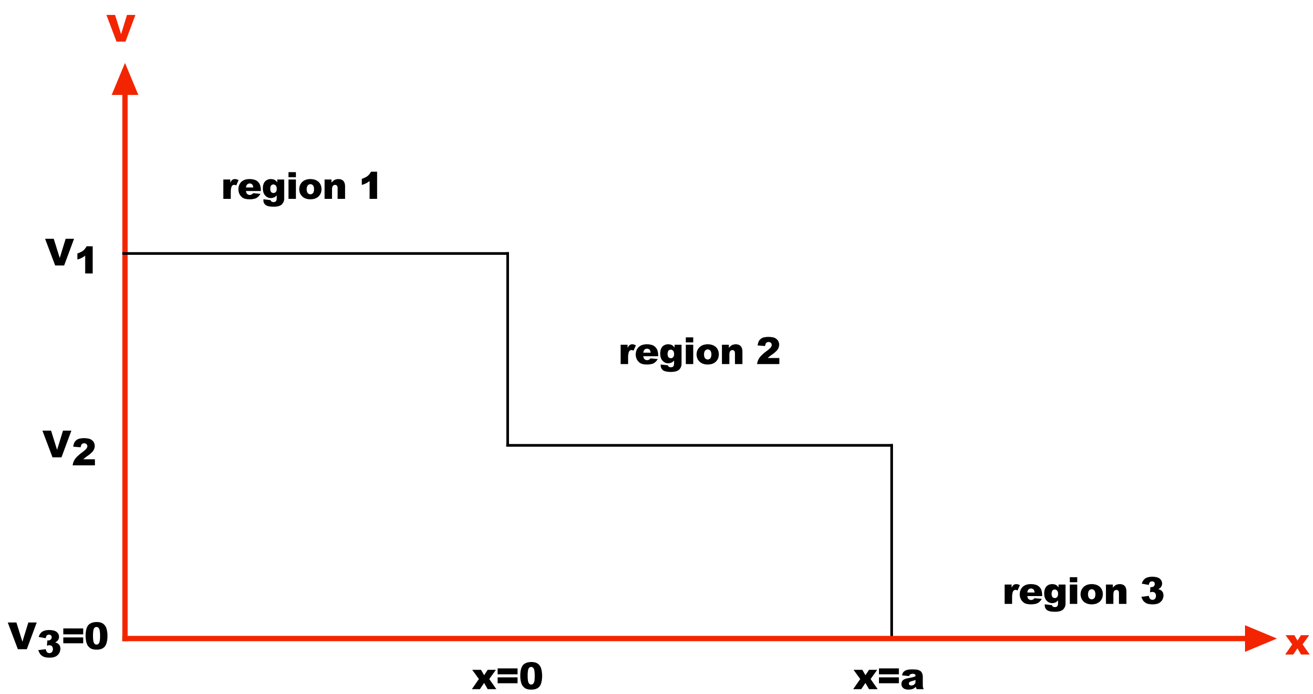
(c) Match the boundary conditions on the wavefunctions at each step to obtain the corresponding set of two equations relating the amplitudes.

(d) Match the boundary conditions on the derivatives of the wavefunctions at each step to obtain the corresponding set of two equations relating the amplitudes.

(e) Naively, there are six unknowns, but only four equations. Explain how we use these four equations to solve the problem.

Now consider the transmission and reflection coefficients for the single step up potential that we discussed in class.

(f) Use the applet at http://phet.colorado.edu/simulations, or your own program, to compute reflection and transmission $R(E)$ and $T(E)$ values versus $E$. Plot your computed $R(E)$ and $T(E)$ curves and compare them with the plot shown in class.



V
region 1
V1
region 2
V2
region 3
V3=0
x=0
x=a
x