

# Time Development QuILT

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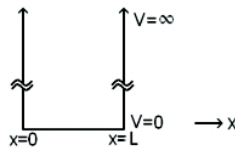
## The Time Evolution of a Wave Function

- A “system” refers to an electron in a potential energy well, e.g., an electron in a one-dimensional infinite square well. The system is specified by a given Hamiltonian.
- Assume all systems are isolated.
- Assume all systems have a time-independent Hamiltonian operator  $\hat{H}$ .
- TISE and TDSE are abbreviations for the time-independent Schrödinger equation and the time-dependent Schrödinger equation, respectively.
- The symbol  $\sum$  in all questions denotes a sum over a complete set of states.

### PART A

#### • Information for questions (I)-(VI)

In the following questions, an electron is in a one-dimensional infinite square well of width  $L$ . (The stationary states are  $\psi_n(x) = \sqrt{\frac{2}{L}} \sin(n\pi x/L)$ , and the allowed energies are  $E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$ , where  $n = 1, 2, 3, \dots$ )



(I) Suppose the wave function for an electron at time  $t = 0$  is given by  $\psi(x, 0) = \sqrt{2/L} \sin(5\pi x/L)$ .

Which one of the following is the wave function at time  $t$ ?

- (a)  $\psi(x, t) = \sqrt{\frac{2}{L}} \sin(5\pi x/L) \cos(E_5 t/\hbar)$
- (b)  $\psi(x, t) = \sqrt{\frac{2}{L}} \sin(5\pi x/L) e^{-iE_5 t/\hbar}$
- (c) Both (a) and (b) above are appropriate ways to write the wave function.
- (d) None of the above.

(II) The wave function for an electron at time  $t = 0$  is given by  $\psi(x, 0) = \sqrt{\frac{2}{L}} \sin(5\pi x/L)$ . Which one of the following is true about the probability density,  $|\psi(x, t)|^2$ , after time  $t$ ?

- (a)  $|\psi(x, t)|^2 = \frac{2}{L} \sin^2(5\pi x/L) \cos^2(E_5 t/\hbar)$ .
- (b)  $|\psi(x, t)|^2 = \frac{2}{L} \sin^2(5\pi x/L) e^{-i2E_5 t/\hbar}$ .
- (c)  $|\psi(x, t)|^2 = \frac{2}{L} \sin^2(5\pi x/L)$  which is time-independent.
- (d) None of the above.

(III) Now suppose that the wave function for an electron at time  $t = 0$  is given by  $\psi(x, 0) = A \sin^5(\pi x/L)$  where  $A$  is a suitable normalization constant. Which one of the following is the wave function at time  $t$ ?

- (a)  $\psi(x, t) = A \sin^5(\pi x/L) \cos(E_5 t/\hbar)$
- (b)  $\psi(x, t) = A \sin^5(\pi x/L) e^{-iE_5 t/\hbar}$
- (c) Both (a) and (b) above are appropriate ways to write the wave function.
- (d) None of the above.

(IV) The wave function for an electron at time  $t = 0$  is given by  $\psi(x, 0) = A \sin^5(\pi x/L)$  where  $A$  is a suitable normalization constant. Which one of the following is true about the probability density  $|\psi(x, t)|^2$  after time  $t$ ?

- (a)  $|\psi(x, t)|^2 = |A|^2 \sin^{10}(\pi x/L) \cos^2(E_5 t/\hbar)$ .
- (b)  $|\psi(x, t)|^2 = |A|^2 \sin^{10}(\pi x/L) e^{-i2E_5 t/\hbar}$ .
- (c)  $|\psi(x, t)|^2 = |A|^2 \sin^{10}(\pi x/L)$  which is time-independent.
- (d) None of the above.

Open the simulation by double-clicking the green arrow associated with this exercise. Shown is the wave function for an electron in the one-dimensional infinite square well at time  $t = 0$  given by  $\psi(x, 0) = \sqrt{\frac{2}{L}} \sin(5\pi x/L)$  for which in the simulation  $\hbar = 2m = L = 1$ . Click on the time-development to evolve the wave function in time.

(V) Does  $|\psi(x, t)|^2$  for a given  $x$  change with time in the simulation?

- (a) Yes.
- (b) No.
- (c) I do not know what I should be looking at in the simulation.

Next, choose the simulation that shows the wave function for an electron in the one-dimensional infinite square well at time  $t = 0$  given by  $\psi(x, 0) = A \sin^5(\pi x/L)$ .

Click on the time-development to evolve the wave function in time.

(VI) Does  $|\psi(x, t)|^2$  for a given  $x$  change with time in the simulation?

(a) Yes.

(b) No.

(c) I do not know what I should be looking at in the simulation.

Try to reconcile your previous responses with what you observed in the simulation. Remember to begin the simulation by double-clicking the green arrow associated with this exercise.

You watched the time-development simulation for two initial wave functions  $\psi(x, 0) = \sqrt{\frac{2}{L}} \sin(5\pi x/L)$  and  $\psi(x, 0) = A \sin^5(\pi x/L)$  and noted that  $|\psi(x, t)|^2$  for the first initial wave function does not depend on time, whereas it does depend on time for the second wave function.

**PART B**

**Let's think systematically about time evolution of a wave function by working through the following questions.**

(1) Choose all of the following statements that are correct about the time evolution of a general wave function:

- (I) The time evolution of a general wave function is governed by the Hamiltonian operator for that system.
- (II) The time evolution of a general wave function is governed by the time-independent Schrödinger equation (TISE):  $\hat{H}\psi_n(x) = E_n\psi_n(x)$ .
- (III) A general wave function  $\psi(x, 0)$  at time  $t = 0$  will evolve into  $\psi(x, t) = e^{-iEt/\hbar} \psi(x, 0)$  at time  $t$ .

(a) (I) only

(b) (II) only

(c) (III) only

(d) (I) and (II) only

(e) (I) and (III) only

(2) Choose all of the following statements that are correct about the time evolution of a general wave function:

- (I) The time evolution of a wave function is governed by the time-dependent Schrödinger equation (TDSE).
- (II) Given  $\Psi(x, 0)$  and the Hamiltonian,  $\hat{H}$ , for a system, we can determine the wave function at time  $t$  by first calculating the momentum eigenstates.
- (III) Given  $\Psi(x, 0)$  and the Hamiltonian,  $\hat{H}$ , we can determine the wave function at time  $t$  if we first expand  $\Psi(x, 0)$  in terms of the energy eigenstates.

- (a) (I) only
- (b) (II) only
- (c) (III) only
- (d) (I) and (II) only
- (e) (I) and (III) only

(3) Choose all of the following statements that are important steps in evaluating the wave function at time  $t$  given  $\Psi(x, 0)$  at time  $t = 0$ :

- (I) Solve the TISE to obtain the stationary states  $\psi_n(x)$  and the allowed energies  $E_n$ .
- (II) Solve the TDSE to obtain the stationary states  $\psi_n(x)$  and the allowed energies  $E_n$ .
- (III) Write  $\Psi(x, 0)$  as a linear superposition of the eigenstates of *any* operator,  $\hat{A}$ , corresponding to a physical observable:  $\Psi(x, 0) = \sum c_n \psi_n^{(\hat{A})}(x)$ .

- (a) (I) only
- (b) (II) only
- (c) (III) only
- (d) (I) and (III) only
- (e) (II) and (III) only

(4) Choose all of the following statements that are correct:

- (I) The stationary states for a Hamiltonian,  $\hat{H}$ , form a complete set of states.
- (II) Any allowed wave function can be written as a linear superposition of stationary states:  $\Psi(x) = \sum c_n \psi_n(x)$
- (III)  $c_n$  in (II) above can be evaluated using orthogonality of wave functions.

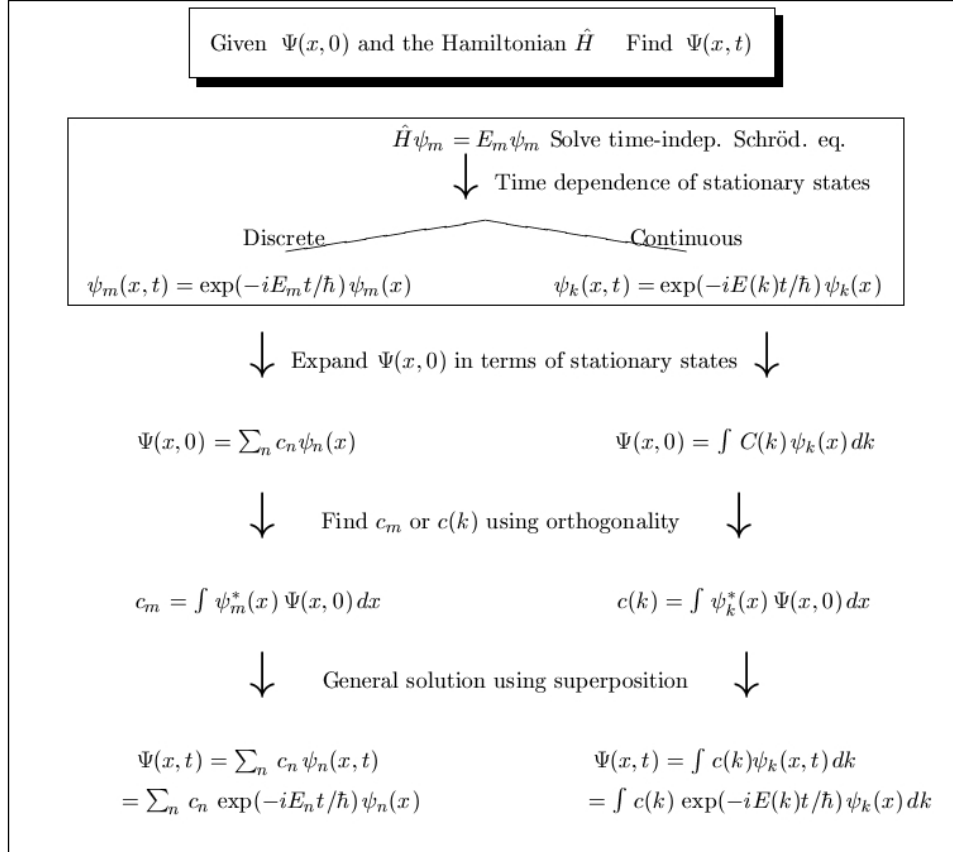
Choose all of the above statements that are correct.

- (a) (I) only
- (b) (II) only
- (c) (III) only
- (d) (I) and (II) only
- (e) All of the above.

Summary: The following procedure can be used to calculate the wave function  $\Psi(x, t)$  at time  $t$  given the wave function  $\Psi(x, 0)$  at time  $t = 0$  for an electron in a system with a given Hamiltonian  $\hat{H}$ .

- FIRST: Solve the TISE for that system to find the stationary states  $\psi_n(x)$  and allowed energies  $E_n$ .
- SECOND: Write the given initial wave function as a linear superposition of the stationary states:  $\Psi(x, 0) = \sum_{n=1}^{\infty} c_n \psi_n(x)$ .
- THIRD: To find  $c_n$ 's for each  $\psi_n(x)$ , multiply both sides of  $\Psi(x, 0) = \sum c_n \psi_n(x)$  by  $\psi_m^*(x)$ , integrate over all space, and use orthogonality of stationary states:  $\int \psi_m^*(x) \psi_n(x) dx = \delta_{mn}$
- FOURTH: Tack on the time dependence with each stationary state component to obtain the time dependence of the general state:  $\Psi(x, t) = \sum_{n=1}^{\infty} c_n e^{-iE_n t/\hbar} \psi_n(x)$ .

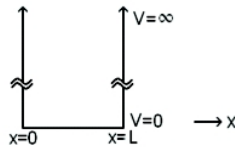
**Flow chart for computing the time evolution of a state**



**PART C**

• **Information for the next four questions**

In the following four questions, an electron is in a one-dimensional infinite square well of width  $L$ . (The stationary states are  $\psi_n(x) = \sqrt{\frac{2}{L}} \sin(n\pi x/L)$ , and the allowed energies are  $E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$ , where  $n = 1, 2, 3, \dots$ )



(1.1) The wave function of the electron at time  $t = 0$  is given by  $\Psi(x, 0) = \sqrt{\frac{2}{7}}\psi_1(x) + \sqrt{\frac{5}{7}}\psi_2(x)$  where  $\psi_1(x)$  and  $\psi_2(x)$  are the ground state and first excited state. Which one of the following is the wave function  $\Psi(x, t)$  at time  $t$ ?

- (a)  $e^{-iEt/\hbar} \Psi(x, 0)$
- (b)  $e^{-Et/\hbar} \Psi(x, 0)$
- (c)  $e^{-ixt/\hbar} \Psi(x, 0)$
- (d)  $\sqrt{\frac{2}{7}}\psi_1(x + \omega t) + \sqrt{\frac{5}{7}}\psi_2(x + \omega t)$  where  $E = \hbar\omega$
- (e) None of the above.

(1.2) Calculate  $|\Psi(x, t)|^2$  for the above wave function. Does it depend on time? Explain your reasoning.

Now open the simulation (remember to double-click the green arrow) and choose the initial wave function  $\Psi(x, 0) = \sqrt{\frac{2}{7}}\psi_1(x) + \sqrt{\frac{5}{7}}\psi_2(x)$ . Watch the time evolution of  $|\Psi(x, t)|^2$ . Is the time evolution of this wave function consistent with what you predicted earlier? Explain.

(2) An electron is confined in a one-dimensional infinite square well. Choose one of the following statements that is correct about whether  $\psi(x) = A \sin^2(\pi x/L)$  is an allowed wave function for the electron.

( $A$  is a suitable normalization constant):

- (a) It is an allowed wave function.
- (b) It is not allowed because it does not satisfy  $\hat{H}\psi = E\psi$  where  $\hat{H}$  is the Hamiltonian operator.
- (c) It is not allowed because it is not a linear function but the Schrödinger equation is linear.
- (d) It is not allowed because it is not an energy eigenfunction nor is it a linear superposition of energy eigenfunctions.
- (e)  $A \sin^2(\pi x/L)$  is an allowed wave function for two electrons but not for one electron.

(3) The initial wave function for an electron in a one-dimensional infinite square well at  $t = 0$  is given by  $\Psi(x, 0) = A \sin^2(\pi x/L)$ . Choose all of the following statements related to  $\Psi(x, t)$  at time  $t$  that are correct.

(I)  $\Psi(x, t) = A e^{-iE_n t/\hbar} \sin^2(\pi x/L)$

(II)  $\Psi(x, t) = \sum c_n e^{-iE_n t/\hbar} \psi_n(x)$  where the expansion coefficients

$$c_n = \int \psi_n^*(x) A \sin^2(\pi x/L) dx.$$

(III)  $\Psi(x, t) = \sum c_n \sin^2(\pi x/L) e^{-iE_n t/\hbar} \psi_n(x)$  where the expansion coefficients

$$c_n = \int \psi_n^*(x) A \sin^2(\pi x/L) dx.$$

- (a) (I) only
- (b) (II) only
- (c) (III) only
- (d) (I) and (II) only
- (e) (I) and (III) only

(4) An electron is confined in a one-dimensional infinite square well. The wave function at time  $t = 0$  is denoted by  $\Psi(x, 0)$ .  $|\Psi(x_0, t)|^2 dx$  is the probability of finding the electron in the narrow range between  $x_0$  and  $x_0 + dx$  at time  $t$ . Choose all of the following statements that are correct:

(I) If  $\Psi(x, 0)$  is a stationary state,  $|\Psi(x_0, t)|^2 dx$  will not depend on time.

(II) If  $\Psi(x, 0)$  is localized in space around a position  $x_0$ ,  $|\Psi(x_0, t)|^2 dx$  will not depend on time.

(III) If  $\Psi(x, 0)$  is in an energy eigenstate,  $|\Psi(x_0, t)|^2 dx$  will not depend on time.

- (a) (I) only
- (b) (II) only
- (c) (III) only
- (d) (I) and (III) only
- (e) All of the above.

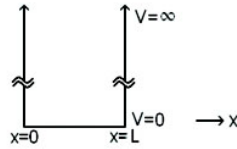
### Practice Worksheet for the Time Evolution of a Wave Function

Given the wave function at time  $t = 0$ , use the above flow chart to obtain the wave function at time  $t$ ,  $\Psi(x, t)$ , for the following cases. In all problems,  $A$  is a suitable normalization constant. All final answers can be written in terms of the normalization constant  $A$ , the stationary state wave functions  $\psi_n(x)$ , and the allowed energies  $E_n$ .

You NEED NOT evaluate  $A$ ,  $\psi_n(x)$  and  $E_n$ . You may also use the flow chart given earlier as needed.



(I) In the following questions, an electron is in a one-dimensional infinite square well of width  $L$ .



1. The initial wave function at  $t = 0$  is given by  $\Psi(x, 0) = \sqrt{\frac{1}{8}}\psi_1(x) + \sqrt{\frac{7}{8}}\psi_2(x)$  where  $\psi_1(x)$  and  $\psi_2(x)$  are the ground state and the first excited state wave functions. Find  $\Psi(x, t)$ .
2. Calculate  $|\Psi(x, t)|^2$  for the above wave function. Does it depend on time? Explain why it should or should not depend on time.
3. Now open the simulation (double-click the green arrow) and choose the initial wave function  $\Psi(x, 0) = \sqrt{\frac{1}{8}}\psi_1(x) + \sqrt{\frac{7}{8}}\psi_2(x)$ . Watch the time evolution of  $|\Psi(x, t)|^2$ . Is the time evolution of this wave function consistent with what you predicted earlier? Explain.
4. Now consider an initial wave function at  $t = 0$  given by  $\Psi(x, 0) = Ax(L - x)$ . Find  $\Psi(x, t)$ . You need not evaluate the integrals involved but you must set them up (write all the unknown quantities in terms of  $A$ ,  $L$ ,  $\psi_n(x)$ , and  $E_n$ ). You need NOT evaluate  $\psi_n(x)$  and  $E_n$ .
5. Calculate  $|\Psi(x, t)|^2$  for the above wave function. Does it depend on time? Explain why it should or should not depend on time.
6. Now open the simulation (double-click the green arrow) which shows the initial wave function  $\Psi(x, 0) = Ax(L - x)$ . Watch the time evolution of  $|\Psi(x, t)|^2$ . Is the time evolution of this wave function consistent with what you predicted earlier? Explain.

7. The initial wave function at  $t = 0$  is given by  $\Psi(x, 0) = A \sin^3(\pi x/L)$ . Find  $\Psi(x, t)$ . You need not evaluate the integrals involved but you must set them up (write all the unknown quantities in terms of  $A$ ,  $L$ ,  $\psi_n(x)$ , and  $E_n$ ). You need NOT evaluate  $\psi_n(x)$  and  $E_n$ .

8. Calculate  $|\Psi(x, t)|^2$  for the above wave function. Does it depend on time? Explain why it should or should not depend on time.

9. Now open the simulation (double-click the green arrow) which shows the initial wave function  $\Psi(x, 0) = A \sin^3(\pi x/L)$ . Watch the time evolution of  $|\Psi(x, t)|^2$ . Is the time evolution of this wave function consistent with what you predicted earlier? Explain.

(II) In the following problems, an electron is in a one-dimensional harmonic oscillator well with potential energy  $V(x) = m\omega^2 x^2/2$  and with  $E_n = (n + \frac{1}{2})\hbar\omega$  for  $n = 0, 1, 2, \dots$

1. The electron is in the ground state at  $t = 0$ . The ground state wave function is given by  $\Psi(x, 0) = Ae^{-\alpha x^2}$  where  $\alpha = \frac{m\omega}{2\hbar}$ . Find  $\Psi(x, t)$ .

2. Calculate  $|\Psi(x, t)|^2$  for the above wave function. Does it depend on time? Explain why it should or should not depend on time.

3. Now open the simulation which shows the initial wave function to be  $\Psi(x, 0) = Ae^{-\alpha x^2}$ . Watch the time evolution of  $|\Psi(x, t)|^2$ . Is the time evolution of this wave function consistent with what you predicted earlier? Explain.

4. The initial wave function at time  $t = 0$  is given by  $\Psi(x, 0) = \sqrt{\frac{1}{3}}\psi_1(x) + e^{i\theta}\sqrt{\frac{2}{3}}\psi_2(x)$  where  $\psi_1(x)$  and  $\psi_2(x)$  are the ground state and first excited state wave functions for the one-dimensional harmonic oscillator well.  $\theta$  is a real constant. Find  $\Psi(x, t)$ .

5. Calculate  $|\Psi(x, t)|^2$  for the above wave function. Does it depend on time? Explain why it should or should not depend on time.

6. Now open a simulation by double-click, selecting an angle,  $\theta$ , which shows the initial wave function to be  $\Psi(x,0) = \sqrt{\frac{1}{3}}\psi_1(x) + e^{i\theta}\sqrt{\frac{2}{3}}\psi_2(x)$ . Watch the time evolution of  $|\Psi(x,t)|^2$ . Is the time evolution of this wave function consistent with what you predicted earlier? Explain.

(III) Consider an electron which is free to move in a one-dimensional space (free particle). Solutions to the TISE for this problem are of the form  $e^{ikx}$ , where  $k = \sqrt{2mE}/\hbar$  is a continuous variable (and so is  $E$ ).

1. The initial wave function at  $t = 0$  is given by  $\Psi(x,0) = Ae^{-\alpha x^2}$  ( $\alpha$  is a positive real constant with the dimension of inverse square length). Find  $\Psi(x,t)$ . You need not evaluate the integrals involved but you must set them up (write all the unknown quantities in terms of  $A$ ,  $\alpha$ ,  $\psi_n(x)$ , and  $E_n$ ). You need NOT evaluate  $\psi_n(x)$  and  $E_n$ .
2. Calculate  $|\Psi(x,t)|^2$  for the above wave function. Does it depend on time? Explain why it should or should not depend on time.
3. Now open the simulation which shows the initial wave function to be  $\Psi(x,0) = Ae^{-\alpha x^2}$ . Watch the time evolution of  $|\Psi(x,t)|^2$ . Is the time evolution of this wave function consistent with what you predicted earlier? Explain.