

## Warm-up: Drawing Bound and Scattering State Wave Functions

- Bound states and scattering states refer to energy eigenstates. They are solutions to the TISE  $H\Psi = E\Psi$ . They are states of definite (fixed) energy.
- The particles are not launched from one side in any question. One direction is not preferred over the other.
- Please draw only the real part of the wave functions in all the questions.
- The zero of the energy is chosen such that the potential energy is zero very far away from the region where the particle is interacting

1. An electron with energy  $E$  is interacting with the finite square well shown in Figure 1. In which regions, if any, is the energy  $E$  of the electron less than the potential energy  $V(x)$ ?

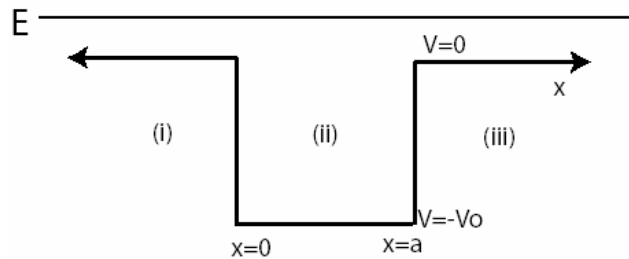


Figure 1

- (I) Region (i)  
 (II) Region (ii)  
 (III) Region (iii)

- (a) (I) only  
 (b) (II) only  
 (c) (III) only  
 (d) (I) and (III) only  
 (e) None of the above.

2. An electron with energy  $E$  is in the finite potential well shown in Figure 1. Which regions, if any, are classically forbidden regions (classically, a particle will never be found in the classically forbidden regions)?

- (I) Region (i)  
 (II) Region (ii)  
 (III) Region (iii)

- (a) (I) only  
 (b) (II) only  
 (c) (III) only  
 (d) (I) and (III) only  
 (e) None of the above.

3. Choose all of the following statements that are correct about the wave function of the electron in question 1?

- (a) It will be rapidly decaying in region (ii) and oscillatory elsewhere.
- (b) It will be oscillatory in region (ii) and exponentially decaying elsewhere.
- (c) It will be oscillatory in all three regions.
- (d) The exact total energy and potential energy needs to be known to determine the shape of the wave function.
- (e) None of the above.

4.  $E$  is the total energy of the particle. Choose all of the following that are correct.

- (I)  $K = E - V(x)$ , where  $K$  is the kinetic energy of the electron at a particular location.
- (II)  $K=E$  in regions (i) and (iii) because  $V=0$ .
- (III)  $K = E - (-V_0) = E + V_0$  in region (ii).

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

**Note:** The wave function of the electron is delocalized and the probability of finding the electron upon measurement of its position can be nonzero in several regions simultaneously. However, for the purposes of sketching the high  $n$  (principle quantum number) bound state wave functions and scattering wave functions, we can use a semi-classical approximation. In this approximation we think of the electron as a particle and we use  $E=K+V(x)$  to find the kinetic energy and the momentum of the particle for different positions  $x$ . Then we use the de Broglie relation to find the particle's wavelength in different regions.

5. Semi-classically, the momenta of the electron in regions (i), (ii) and (iii) are  $p_1, p_2$  and  $p_3$  respectively. Which ordering of their magnitudes is correct?

- (a)  $p_1 < p_2 < p_3$ .
- (b)  $p_1 > p_2 > p_3$ .
- (c)  $p_1 = p_3 < p_2$ .
- (d)  $p_1 < p_3 < p_2$ .
- (e)  $p_1 = p_2 = p_3$ .

6. The de Broglie relation that relates the wavelength of a particle to its momentum is given by,

(a)  $p = \frac{h}{\lambda}$ .

(b)  $p = \frac{\lambda}{h}$ .

(c)  $p = h\lambda$ .

(d)  $p = \frac{\lambda}{\omega}$ .

(e)  $p = \hbar\omega$ .

7. The de Broglie wavelengths of the electron in regions (i), (ii) and (iii) are  $\lambda_1, \lambda_2$  and  $\lambda_3$  respectively. Which ordering of their magnitudes is correct?

(a)  $\lambda_1 < \lambda_2 < \lambda_3$ .

(b)  $\lambda_1 > \lambda_2 > \lambda_3$ .

(c)  $\lambda_2 < \lambda_1 = \lambda_3$ .

(d)  $\lambda_1 < \lambda_3 < \lambda_2$ .

(e)  $\lambda_1 = \lambda_2 = \lambda_3$ .

**Summary:**

So far, we know that a “classical particle” with the energy shown in Figure 1 will be allowed in all regions, so the wave function of the quantum mechanical particle with that energy will be oscillatory in all regions. Momentum and kinetic energy are directly related,  $K = \frac{p^2}{2m}$ ; de Broglie wavelength and momentum are inversely proportional,

$p = \frac{h}{\lambda}$ . This information is enough to determine the relative wavelengths of the wave function of the electron in different regions.

There is one last thing that needs to be determined before the wave function of the electron can be drawn qualitatively. That is the relative amplitude of the wave function in different regions.

8. Consider the following conversation between Peter and Mary Jane.

**Peter:** The greater the momentum of a particle, the greater is its speed.

**MJ:** Right.

**Peter:** The faster the particle, the less time it spends at a given position.

**MJ:** I'm still with you.

**Peter:** We can think of it as it is moving forward faster, so the probability of finding it at any one location is smaller. The probability density is related to square of the amplitude of the wave function,  $|\Psi(x)|^2$ . Thus, the faster is the particle in a region, the smaller is the amplitude of the wave function in that region. You're still following?

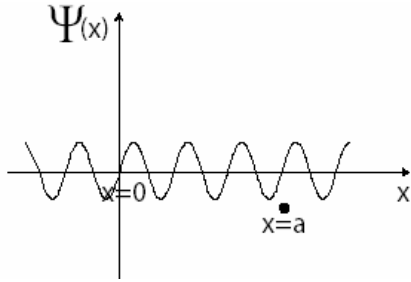
**MJ:** Yes.

**Peter:** Then, knowing the relative momenta of the particle in different regions, we know the wavelength and the amplitude. We can draw the wave function.

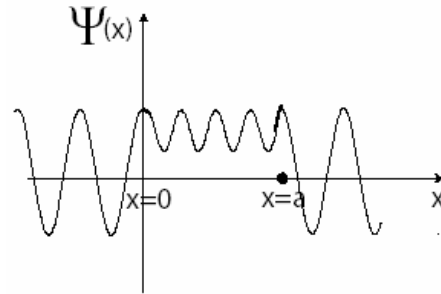
**MJ:** OK, leave the drawing to me, and see if I got it.

Do you agree with Peter's reasoning? Explain

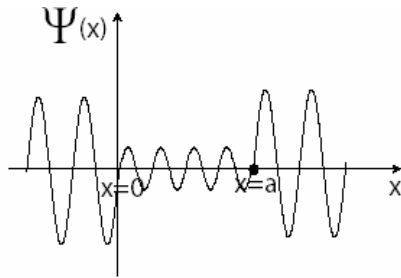
9. Which of the following figures that MJ drew is qualitatively correct?



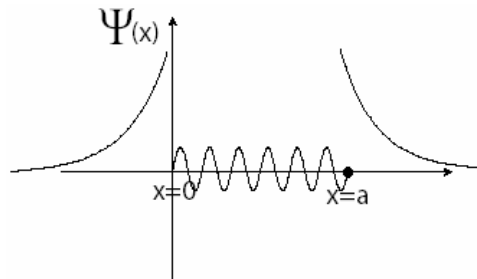
(a)



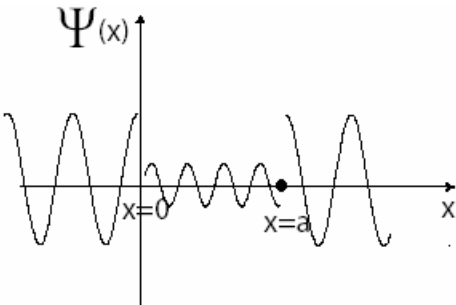
(d)



(b)



(e)



(c)

10. Consider the following conversation between Mary Jane and Peter.

**Mary Jane:** I don't understand what is wrong with my drawing in choice (c). To me it looks like it is the same as (b) as far as what we learned so far is concerned.

**Peter:** It does seem that way, but look at the boundaries of the well. The wave function should be continuous everywhere including at the boundaries of the well.

**Mary Jane:** What about the drawing in choice (d)? That is continuous.

**Peter:** Right, but the wave function does not go to zero in the middle region. In the middle region it does not cross the  $x$ -axis at any point, but it should, similar to the sine function in the other regions.

Do you agree with Peter's reasoning for both cases? Explain why or why not.

11. An electron with energy  $E$  is in the finite square well shown in Figure 2. In which regions, if any, is the energy  $E$  of the electron less than the potential energy  $V(x)$ ?

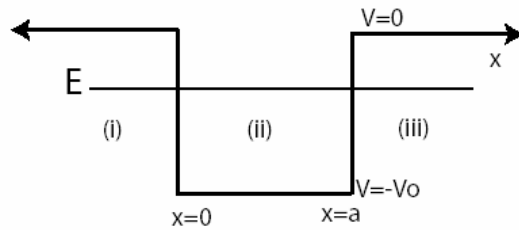


Figure 2

- (I) Region (i)
- (II) Region (ii)
- (III) Region (iii)

- (a) (I) only
- (b) (II) only
- (c) (III) only
- (d) (I) and (III) only
- (e) None of the above.

12. An electron with energy  $E$  is in the finite potential well shown in Figure 2. Which regions, if any, are classically forbidden regions?

- (I) Region (i)
- (II) Region (ii)
- (III) Region (iii)

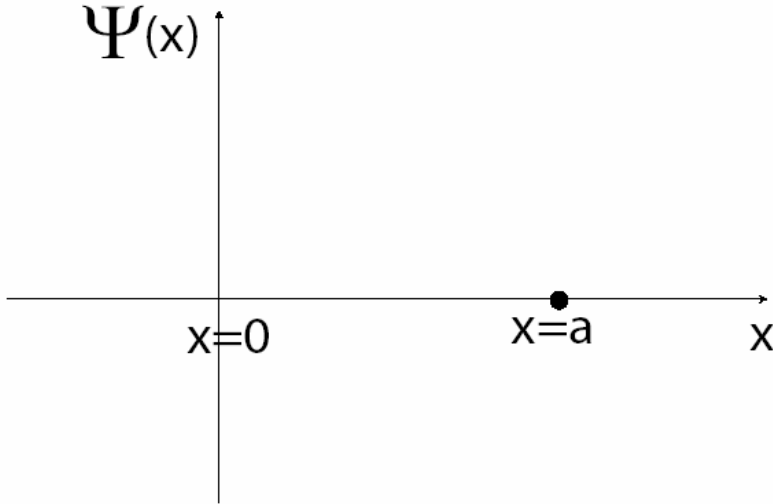
- (a) (I) only
- (b) (II) only
- (c) (III) only
- (d) (I) and (III) only
- (e) None of the above.

13. Choose all of the following statements that are correct about the wave function of the electron in question 11?

- (I) It will be rapidly decaying in region (i).
- (II) It will be oscillatory in region (ii).
- (III) It will be oscillatory in region (iii).

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

14. Are the answers to questions 11-13 sufficient information to draw a qualitative rough sketch of the wave function of the electron in the finite square well in Figure 2? If yes, draw the wave function below. If no, explain why not, and what other information is required.



## Summary:

- In quantum mechanics, particles can be found in classically forbidden regions with a finite probability. The wave function of a particle in the classically forbidden regions may be nonzero, but it will be rapidly decaying.
- The classically allowed regions are where the particle has oscillatory wave functions. The amplitude and wavelength of the oscillatory wave function depend on the energy  $E$  of the particle, relative to the potential energy  $V(x)$ .
- If there is more than one classically allowed region, the relative amplitude and wavelength of the wave function must be determined, to be able to draw a qualitative picture.
- The relative amplitude and wavelength of a wave between two regions is determined by the semi-classical approximation.

## The Semi-Classical Approximation:

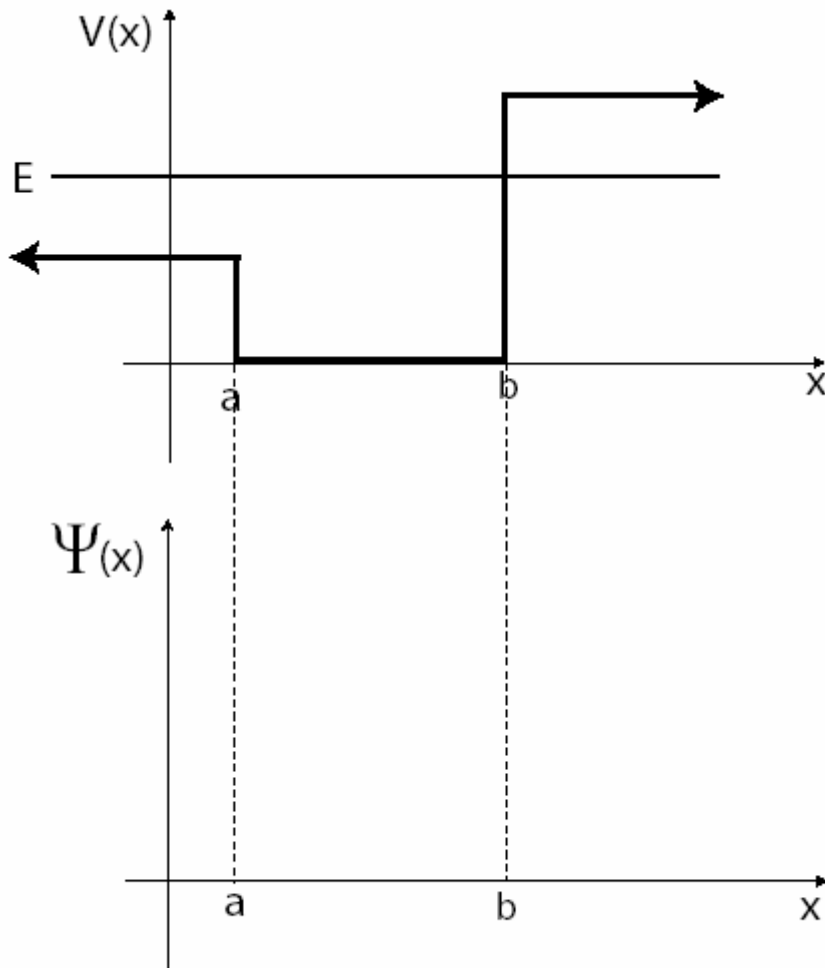
- Particles are waves, with wavelengths that are related to their momenta by the de Broglie relation,  $p = \frac{h}{\lambda}$ , where  $p$  is the particle's momentum,  $h$  is the Planck constant, and  $\lambda$  is the wavelength.
- For a fixed energy, we can say that the higher the potential energy, the lower the kinetic energy, since  $E=K+V(x)$ , where  $E$  is the total energy of the particle,  $K$  is the kinetic energy, and  $V$  is the potential energy. Given  $E$  and  $V(x)$  we can determine the kinetic energy,  $K$  (if  $K \geq 0$ ).
- The higher the kinetic energy, the higher the momentum, because classically we know that  $K = \frac{p^2}{2m}$ . That is why this method is called semi-classical.
- From the de Broglie relation, one can see that momentum and wavelength are inversely proportional. That means, the greater the momentum, the shorter will be the wavelength.
- One also has to employ the semi-classical approximation to determine how the amplitude will be affected by the momentum. The greater the momentum, the greater the speed. If a particle is moving fast, it will spend less time at every position. This means it has to have smaller amplitude. So, the larger the momentum, the smaller the amplitude.
- With this approach, it is easy to draw qualitative sketches of wave functions of particles in any potential.

*Please go back and check that your answers and figures agree with the above summary.*

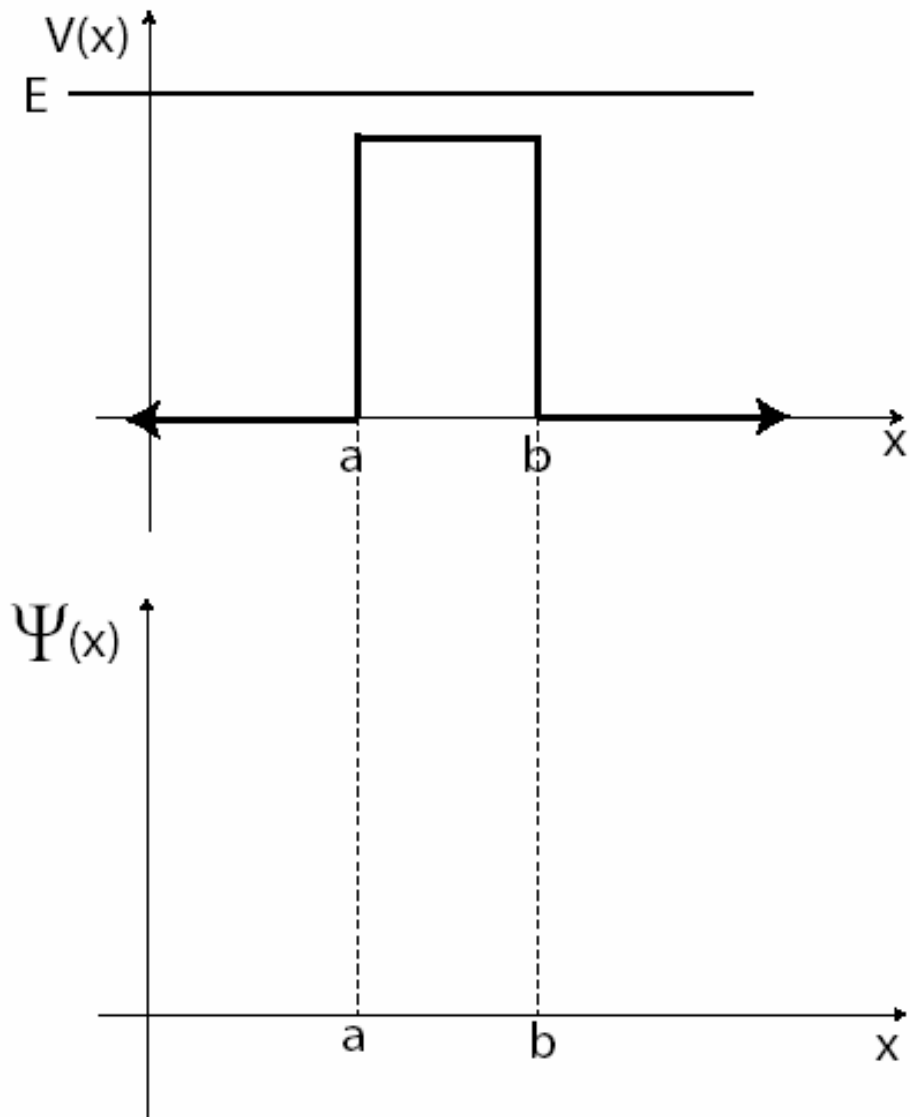
### Pretest: Drawing Bound and Scattering State Wave Functions

- Bound states and scattering states refer to energy eigenstates. They are solutions to the TISE  $H\Psi = E\Psi$ . The energy will be fixed in all cases.
- The particles are not launched from one side in the questions. One direction is not preferred over the other.
- Please draw only the real part of the wave functions in all the questions.

1. Draw the wave function for an electron in the following finite square well with energy  $E$ . Explain.



2. Draw the wave function for an electron interacting with the following finite barrier with energy  $E$ . Explain.



## Tutorial: Drawing Bound and Scattering State Wave Functions

1. An electron with energy  $E$  is interacting with the potential barrier shown in Figure 3 below. Choose all of the following statements that are correct about the electron.

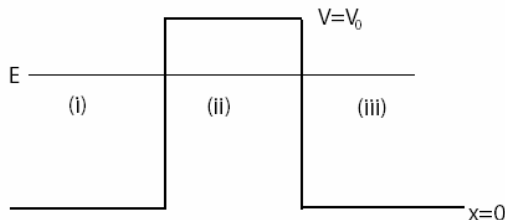


Figure 3

- (I) Region (ii) is classically forbidden to the electron.
- (II) Its wave function will be oscillatory in region (i) and (iii).
- (III) Its wave function will be oscillatory in region (ii).

- (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 that are correct about the electron in Figure 3.

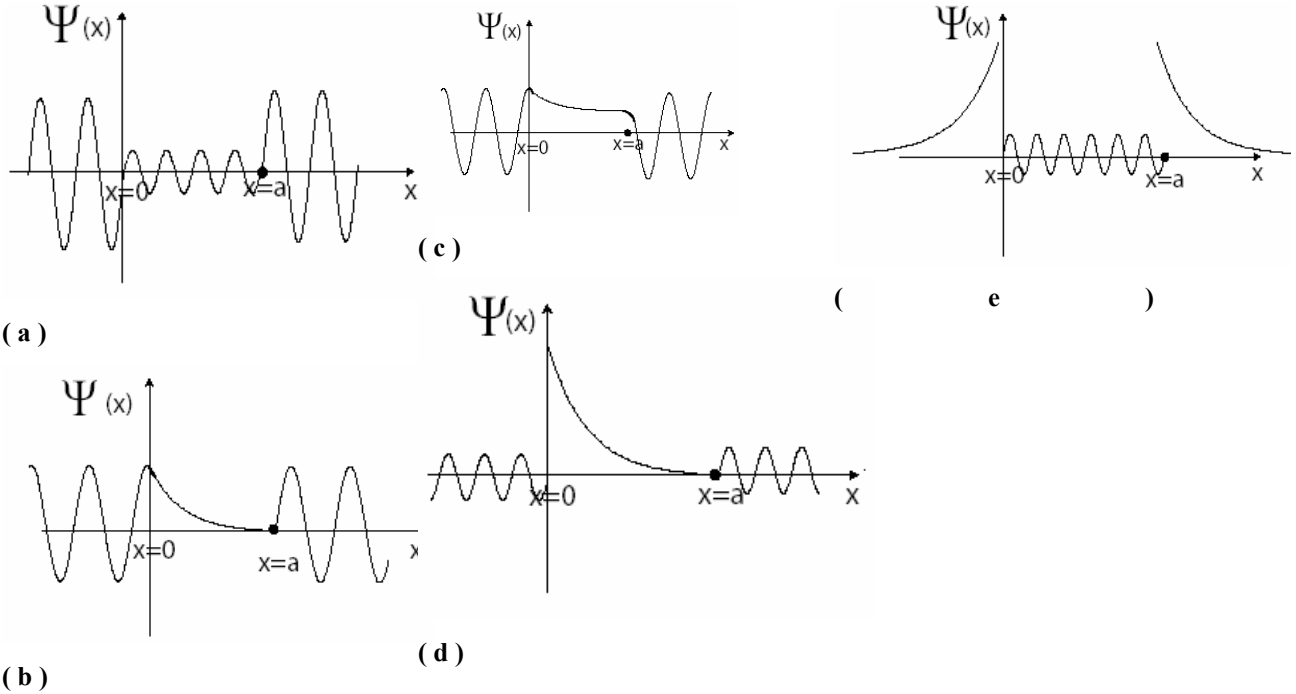
- (I) Its kinetic energies  $K_1$  and  $K_3$  in regions (i) and (iii) are the same.
- (II) Its momenta  $p_1$  and  $p_3$  in regions (i) and (iii) are the same.
- (III) Its wavelengths  $\lambda_1$  and  $\lambda_3$  in regions (i) and (iii) are the same.

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

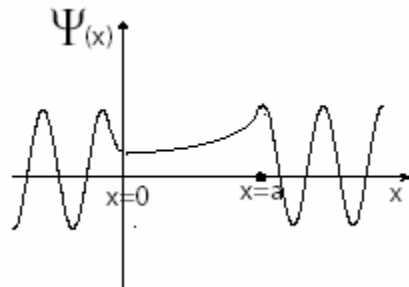
3. What can be said about the amplitudes  $A_1$  and  $A_3$  of the electron in regions (i) and (iii) in Figure 3?

- (a)  $A_1 = A_3$
- (b)  $A_1 < A_3$
- (c)  $A_1 > A_3$
- (d) The wave function is decaying rapidly. Amplitude makes sense only for the oscillatory part of the wave function.
- (e) There is not enough information. The total energy and potential energy need to be known exactly.

4. Choose the figure that best represents the wave function of the electron in Figure 3.



5. Jim drew the following wave function for the electron in Figure 3. Consider the following conversation between Jim and Tina about his drawing.



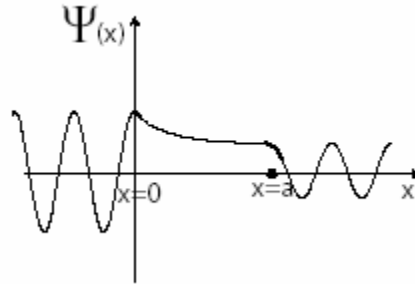
**Jim:** Can't the wave function also look like this, since we are not launching particles from one side or the other? Rather, these are energy eigenstates and the wave function represents the probability amplitude of finding the particle at a position. There is no reason why the left side should be preferred over the right.

**Tina:** I disagree. A particle approaches from the left, because it is moving in the positive  $x$  direction. The direction of the  $x$ -axis is by convention, and we have to draw the wave function accordingly.

**Jim:** The direction does not mean anything here because this is not a wave packet being sent from one side. The wave function I drew is as valid a solution to the TISE as the wave function in choice (c) of the previous question.

With whom do you agree? Explain why.

6. Alex drew the following wave function for the electron in Figure 3. Consider the following conversation between Alex and Alice about his drawing.



**Alex:** I think the wave function in question 4 must look like this. I remember this to be the wave function for the finite barrier from my quantum mechanics class.

**Alice:** This would be the wave function for a beam of particles approaching the barrier from the left. Then, the probability of finding the particles would be smaller to the right of the barrier. The smaller probability would mean that the amplitude of the wave function would have to be smaller.

**Alex:** Exactly. So this should be the wave function for the electron in Figure 3.

**Alice:** No. I said this *would* be the case for a beam coming from the left side, we are not launching particles from the left side (or the right). What we are doing is plotting the solution of the TISE when neither side is preferred. This solution to the TISE should not differentiate between the two sides unless we specifically add something to the problem about the particle coming from one side. So the amplitude will be the same. We are drawing energy eigenfunctions (which are solutions to the TISE) for a problem where neither side is preferred.

With whom do you agree? Explain why.

7. Choose all of the statements that are correct about an electron with energy  $E$  in the infinite square well shown in Figure 4.

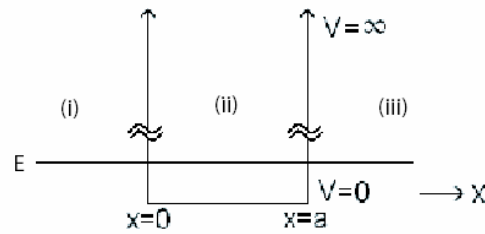
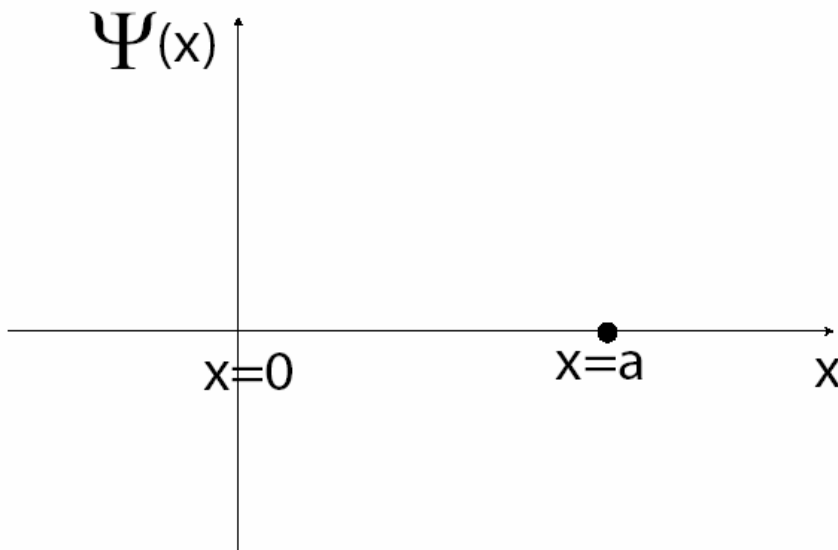


Figure 4

- (I) The regions (i) and (iii) are classically forbidden.  
 (II) The electron cannot be found in the regions (i) and (iii).  
 (III) There is a finite probability that the electron will be found in regions (i) and (iii), but the wave function will be rapidly decaying.
- (a) (I) only  
 (b) (II) only  
 (c) (III) only  
 (d) (I) and (II) only  
 (e) (I) and (III) only
8. On the set of axes below, draw a wave function for the electron in the infinite square well in Figure 4.



9. Is the derivative of the wave function continuous at the boundaries  $x=0$  and  $x=a$ ? Explain why or why not.

10. Consider the following conversation below, between Lisa and Debbie.

**Lisa:** I thought in quantum mechanics, particles could be found in the classically forbidden regions, and the wave function was rapidly decaying in that region. Why is the infinite square well different? Why must the wave function go to zero in the classically forbidden region?

**Debbie:** The potential goes to infinity abruptly at the boundaries. The potential is infinite everywhere outside the well. Even in quantum mechanics, if the potential energy is infinite somewhere, the particle cannot be found there.

**Lisa:** But the simple harmonic oscillator potential energy also goes to infinity. How can the particle be found outside the well then?

**Debbie:** It is equal to infinity only as  $x \rightarrow \pm\infty$ , and the particle cannot be found as  $x \rightarrow \pm\infty$ . Therefore the harmonic oscillator only allows bound states in which the wave function is normalizable and goes to zero as  $x \rightarrow \pm\infty$ .

**Lisa:** I understand. For the infinite square well, because the potential energy is infinite everywhere outside the well, the wave function goes to zero outside instead of decaying rapidly.

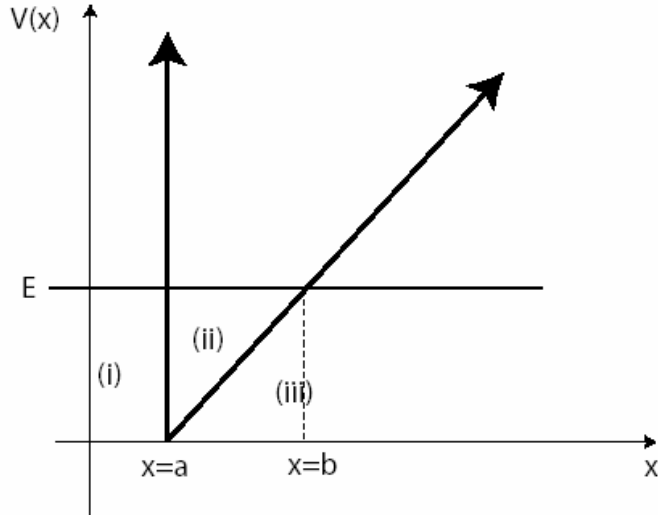
**Debbie:** Yes. The infinite square well is a good model for cases where the probability of finding the particle outside a region is very small. For example, the probability of free electrons in a metal leaking out into the air is negligible, so we can approximate it with an infinite potential outside the boundaries of the metal.

**Lisa:**  $V(x) = \infty$  outside the metal is an approximation for a very large repulsive potential, which makes the wave function have a discontinuous slope (first derivative) at the boundary.

Do you agree with Debbie's explanation? Why or why not?

An electron with energy  $E$  is in the potential energy well shown in Figure 5 below. Answer the following questions that will lead you through drawing the wave function.

$$V(x) = \infty \text{ for all } x < a$$



**Figure 5**

**11.** Write down the range of  $x$  for all of the regions that are classically forbidden for this electron. (*Hint: Think of classical turning points.*)

**12.** Can the electron be found in region (i)? Explain why or why not.

**13.** Can the electron be found in region (ii)? Explain why or why not.

**14.** Can the electron be found in region (iii)? Explain why or why not.

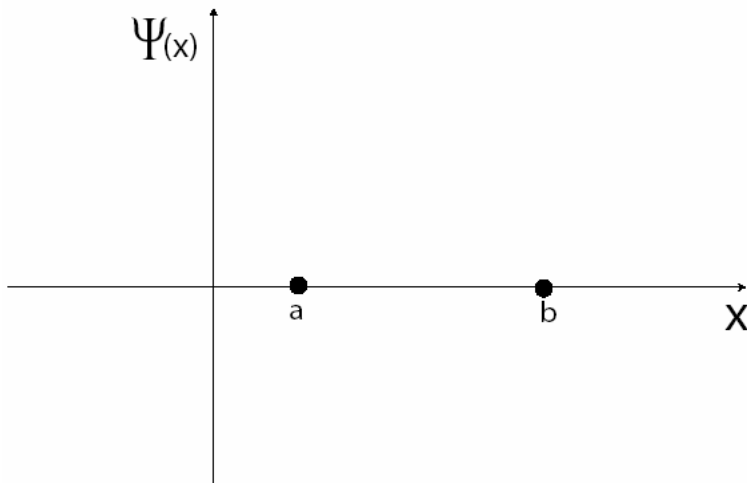
**15.** The kinetic energy  $K=E-V(x)$  is positive (greater than zero) in the region \_\_\_\_\_.

**16.** Is there a region where the wave function is always zero? Explain why or why not.

**17.** Is there a region where the wave function is rapidly decaying? Explain why or why not.

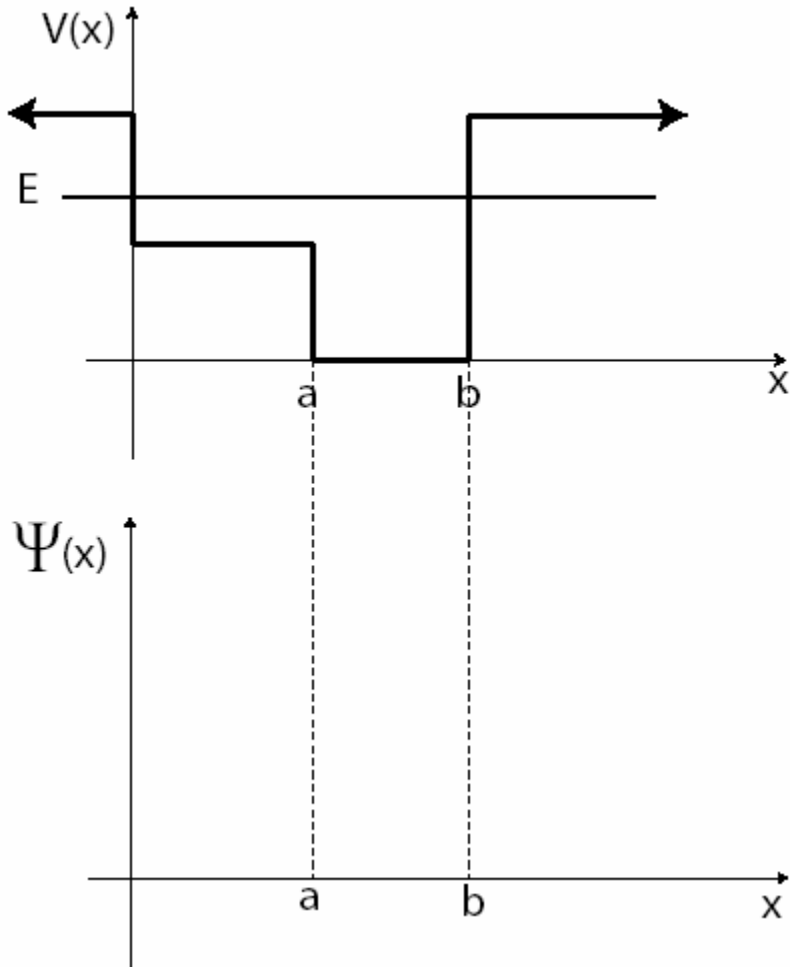
**18.** Is there a region where the wave function is oscillatory? Explain why or why not.

19. In the region that the wave function is oscillatory, is the kinetic energy  $K=E-V(x)$  constant, increasing, or decreasing, as position increases?
20. Based on your answer to the previous question, in the region that the wave function is oscillatory, is the momentum  $p$  constant, increasing, or decreasing as position increases?
21. Write down the de Broglie relation that relates the momentum of a particle to its de Broglie wavelength.
22. Using your answers to the previous two questions, what can you say about the wave length of the oscillatory wave function? Is it constant, increasing or decreasing with increasing position?
23. We had shown earlier that the amplitude can be related to the momentum also. How is the amplitude of the oscillatory wave function changing? Increasing or decreasing with increasing position?
24. Draw the wave function of the electron on the figure below.

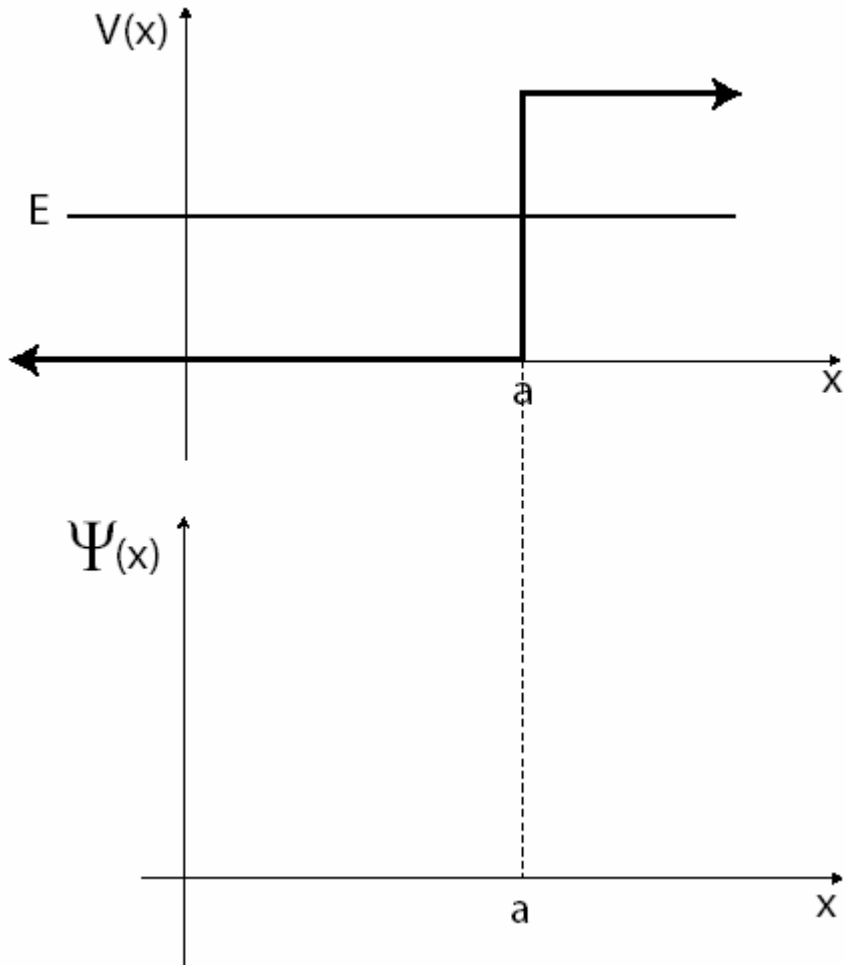


25. Is the wave function you drew continuous everywhere? If not, go back and fix it.
26. Is the first derivative of the wave function you drew continuous everywhere except at  $x=a$ ? If not, go back and fix it.

27. An electron with energy  $E$  is in the potential energy well shown below. Draw the wave function. Feel free to go back and study the examples and summaries to help your drawing. Explain your drawing, comment on different regions.



28. An electron with energy  $E$  is interacting with the potential energy step function shown below. Draw the wave function. Feel free to go back and study the examples and summaries to help your drawing. Explain your drawing, comment on the different regions.

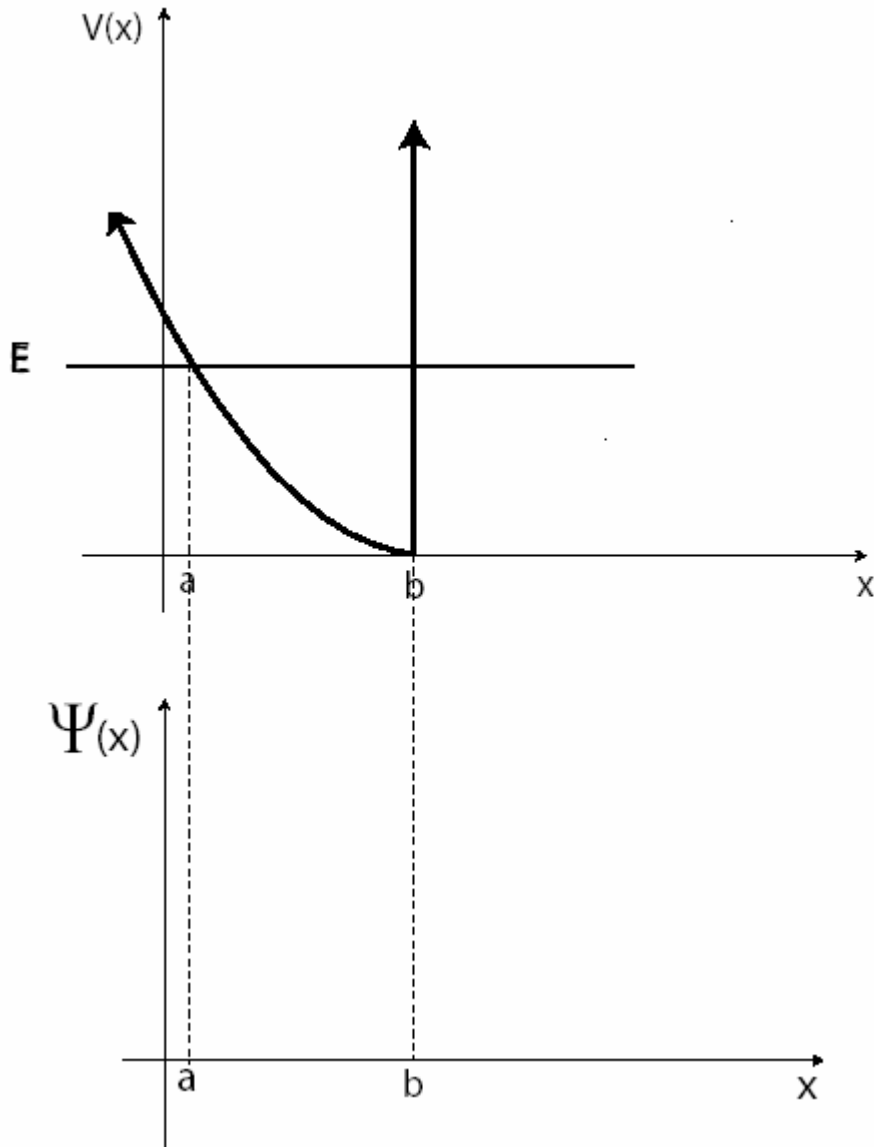


29. Check that the wave functions you drew in the previous two questions are continuous everywhere. Also check that the first derivatives (slope) of the wave functions are continuous where necessary. If they are not, go back and fix your figures.

### Posttest: Drawing Bound and Scattering State Wave Functions

- Bound states and scattering states refer to energy eigenstates. They are solutions to the TISE  $H\Psi = E\Psi$ . The energy will be fixed in all cases.
- The particles are not launched from one side in the questions. One direction is not preferred over the other.
- Please draw only the real part of the wave functions in all the questions.

1. Draw the wave function for an electron in the following half harmonic oscillator with energy  $E$ . Explain.



2. Draw the wave functions for two different electrons in the following finite square wells with energy  $E$ . Explain.

