Name Partners Date

Visual Quantum Mechanics
The Next Generation

The Shape of the Wave Function

Goal

- To gain an understanding of the general solution of Schrödinger's equation.
- To build the correct relationship between the shape of the wave function and the local kinetic/potential energy of a quantum system.

Introduction

In quantum mechanics, we use wave functions to represent and study quantum systems. In this tutorial, we will explore how the shape of the wave function is related to the physical settings of a quantum system and, conversely, how we can determine information about the shape of the wave function from the physical situation.

A. The Structure of Schrödinger's Equation

Schrödinger's equation has the form

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} + U[x]\,\Psi[x] = E\Psi[x] \qquad (1)$$

Let's see what structure it has and how it determines both the wave function and the allowed energies. The equation involves both Ψ and its second derivative. We can solve for the second derivative.

$$\frac{d^2\Psi}{dx^2} = \frac{2m}{\hbar^2}(U[x]-E)\,\Psi[x] \qquad (2)$$

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So the second derivative of Ψ looks like some function of x times Ψ (x) itself:

$$\frac{d^2\Psi}{dx^2} = -F[x]\ \Psi[x] \tag{3}$$

where

$$F[x] = \frac{2m}{\hbar^2}\left(E - U[x]\right) \tag{4}$$

Check the algebraic steps leading from equation (1) to equation (4).

B. Curvature

In this section we will explore how the sign of the function F[x] controls how the function Ψ looks. Assume that the function Ψ [x] is positive. We will explore three pieces of a wave function: an increasing exponential, a decreasing exponential, and a piece of a sine or cosine oscillation. Assume that each of these three functions satisfies equations such as equations (3) and (4).

B-1. Suppose Figure 1 represents a piece of a wave function, Ψ . At four or five points along the curve, indicate the slope of the curve, *d*Ψ */dx*, by drawing a small segment of the tangent to the curve at that point.

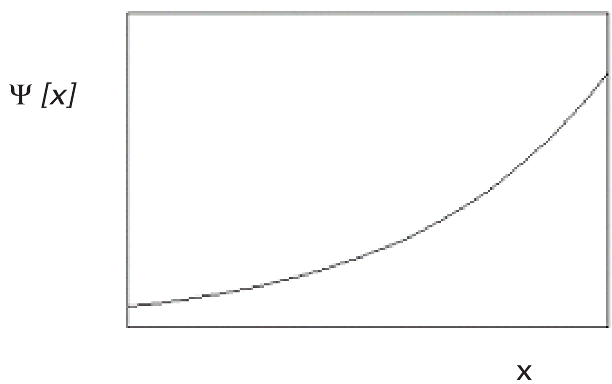


Figure 1: Segment of a wave function in Region 1.

B-2. Plot the approximate values of the slopes that you have obtained. Do it qualitatively, not quantitatively. That is, don't worry about exact numbers. Just graph the signs and relative sizes.

B-3. Use your sketch to answer the questions below.

- Is the derivative of the wave function positive or negative in this region?

- Is the derivative of the wave function increasing or decreasing as x increases?

B-4. Use your points on the plot of the derivative and your answers to the questions above to sketch a graph of $d\Psi/dx$ vs. x. On this graph indicate the slope of $d\Psi/dx$ at 4 to 5 points.

- How are these slopes related to the second derivative of the wave function?

- Use these results to determine if the second derivative of the wave function is positive or negative in this region?

- Use this result to determine the sign of the function F[x]. Describe how you reached your answer.

- In this region, is E greater or less than U[x]? Use Equation (4) to explain your reasoning.

B-5. Figure 2 represents a piece of a wave function, Ψ, in a different region. At four or five points along the curve, indicate the slope of the curve, $d\Psi/dx$, by drawing a small segment of the tangent to the curve at that point.

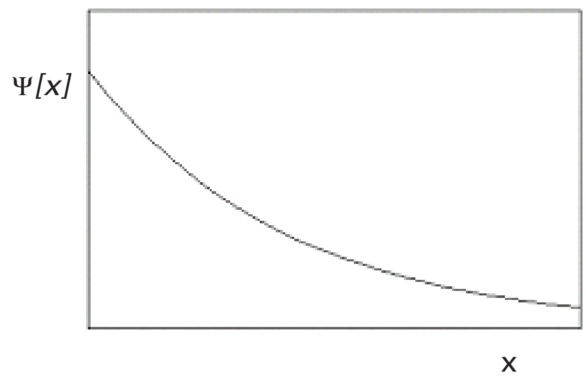
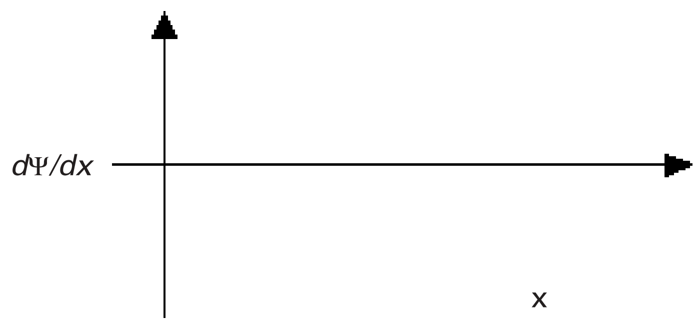


Figure 2: A segment of a wave function in Region 3.

B-6. Qualitatively plot the values of the slopes that you have obtained.



B-7. Use your sketch to determine the sign of the wave function in this region.

- Is the second derivative of the wave function positive or negative in this region? (If you cannot answer this question with high confidence, follow the procedure described in B-4.)

- Is the function F[x] positive or negative in this region? Explain.

- In the region we are looking at, is E greater or less than U[x]? Explain your reasoning.

- How is this result similar to what you found in questions B-3 and B-4?

- How is this result different from the results to B-3 and B-4?

- Describe the conditions on U and E which would result in wave functions such as those shown in Figures 1 and 2. Explain your answers.

B-8. Figure 3 represents a piece of a wave function, Ψ in a third region. Again, at four or five points along the curve, indicate the slope of the curve, $d\Psi/dx$, by drawing a small segment of the tangent to the curve at those points.

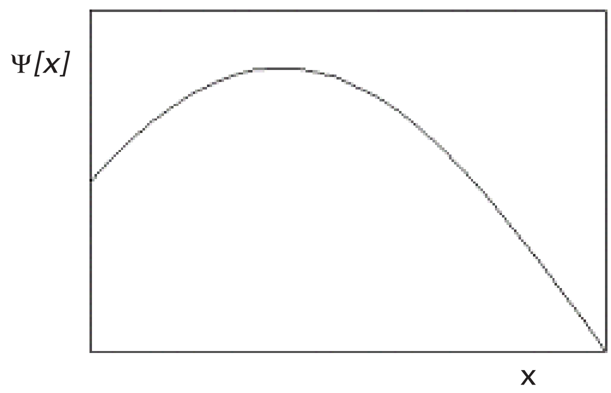
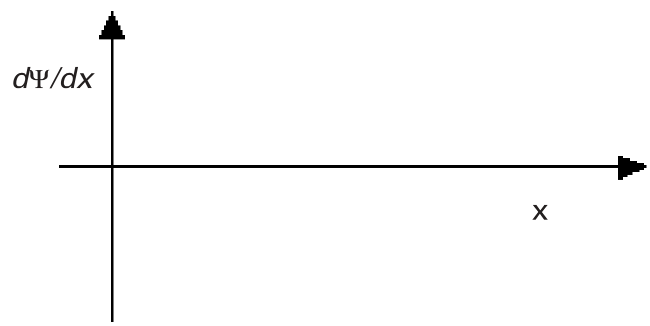


Figure 3: A segment of a wave function in Region 2.

B-9. Qualitatively plot the values of the slopes that you have obtained.



B-10. Use your sketch to answer the questions below.

- What is the sign of the second derivative of the wave function at each of the points in this region?

- Is the function F[x] positive or negative in this region? Use equation (3) to explain your answer.

- In this region, is E greater or less than U[x]? Use equation (4) to explain your answer.

C. Energies, Slopes and Curvatures

So far, we have worked primarily with mathematical functions in Schrödinger's Equation and its solutions. We have simply manipulated the mathematics without any reference to the physical situation. Now, we will take the next step --- connect the mathematics to the energy of the particle represented by the wave function.

C1. Complete the table below by indicating the relation between U(x) and E -- E > U, U > E; U = E -- for each situation.

		$\psi(x)$	
		Positive	Negative
$\frac{d^2\psi}{dx^2}$	positive		
	negative		

Table 1

C-2. Use this result and your answers in part B to describe the relationship between U and E which would result in a wave function such as the one that is shown in Figure 1. Explain your answers.

C-3. For the wavefunction in Figure 2 is the relationship between U and E the same or different from the answer in C1? Explain your answer.

C-4. If the second derivative of Ψ is negative, and Ψ is positive, will the wave function curve towards the x-axis or away from the x-axis? Explain this result in terms of how the slope of the tangent line changes as x increases.

To start we return to Schrödinger's Equation [equation 2] which is repeated here for convenience

$$\frac{d^2\Psi}{dx^2} = \frac{2m}{\hbar^2}(U[x] - E)\,\Psi[x] \qquad (2).$$

The second derivative of a function is called its *curvature*. Paying attention to a wave function's curvature and the way it is controlled by the relative sign of the total energy and the potential energy at a given point will help you understand why a particular wave function looks as it does.

C-5. If (E-U) is positive, and the wave function is positive, is the curvature of the wave function positive or negative? Does this correspond to an exponential-like or a cosine-like wave function?

C-6. What if the E-U is positive and the wave function is negative?

C-7. What if the E-U is negative and the wave function is positive?

C-8. Complete the table below by indicating whether Ψ is exponential-like or cosine-like for each situation.

		wave function	
		+	-
curvature	+		
	-		

Table 2

C-0. Summarize the results by describing how the sign of E-U helps you qualitatively sketch wave functions and how these rules for sketching are related to Schrödinger's Equation.

D. The Structure of the Square Well Wave Functions

As a specific case, let's look at the ground state in the square well potential. In Figure 4 are two graphs:

- a plot showing the potential energy as a function of x and the energy level as a dashed line (the lower part of the figure)
- a graph of the wave function for that energy level (the upper part of the figure).

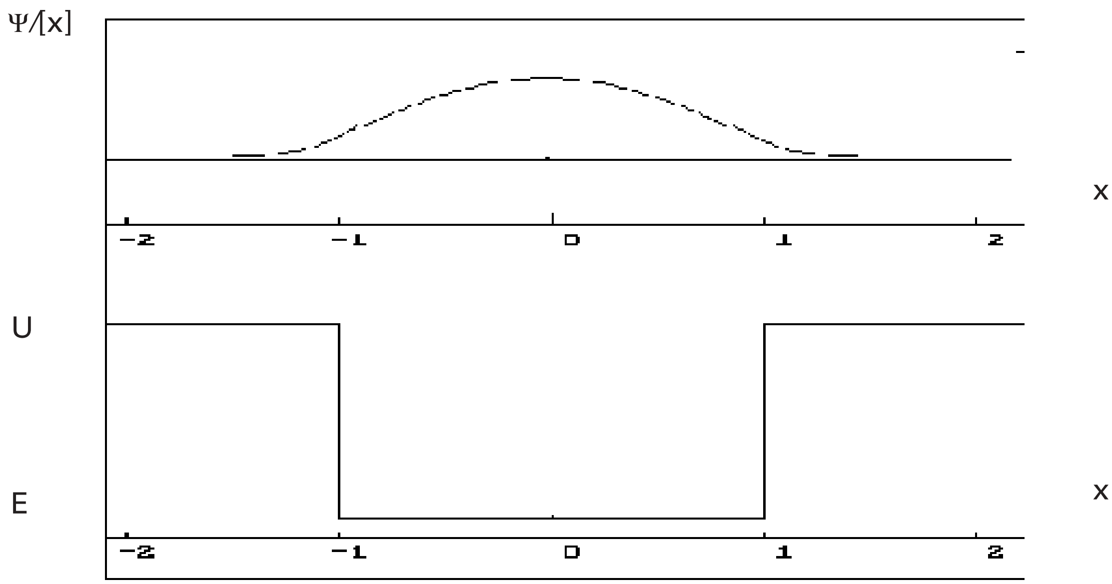


Figure 4: Diagram of a potential well and its corresponding wave function.

D-1. On the figure above use a ruler to draw **vertical** lines through the points x = -1.2, x = -0.5, x = 0, x = +0.5, and x = +1.2

D-2. Complete the table below by indicating +, 0, or - for the first four columns and “exponential” or “cosine” for the last column.

location (x)	sign of Ψ	sign of dΨ/dx	sign of $d^2\Psi/dx^2$	sign of E-U[x]	shape of wave function
-1.2					
-0.5					
0					
+0.5					
+1.2					

Table 3: Data table

D-3. How does the change in (E-U) from negative to positive to negative again control the shape of the wave function? Explain.

In this activity we have focused on the sign of E-U[x] and not the numerical value of this quantity. However, you can see that the numerical value of E-U[x] and the numerical value of $\Psi(x)$ determine, within a known constant, the value of the curvature of $\Psi(x)$.

For a different value of E, the value of (E-U), and thus the curvature in each region, will be different. For most values, the curvatures in each region will be such that the wave functions of given curvatures will not fit together to make a smooth wave function that converges to zero when E-U < 0. Only at the correct energies can you make a smooth match from one region to the other and get aresult that makes sense physically. Thus, the discrete energies for a particle in a well are a result of the functional relationships given in Schrödinger's Equation.