

Lecture 10: Finite Wells and the Structure of Bound States

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Lecture 9 introduced the infinite square well and the general structure of one-dimensional bound states. We now replace the infinite walls by finite barriers. This gives a model in which the wave function can extend into a classically forbidden region, while the allowed energies remain discrete.

Questions.

- Why does a finite well have an exponential tail outside the well?
- Why can the eigenfunctions of a symmetric well be chosen to be even or odd?
- How do continuity conditions determine the allowed energies?
- What does the infinite-well limit tell us about the finite-well solutions?

Lecture roadmap. We review the infinite square well and its nodes, solve the finite square well in three regions, use parity to simplify the solutions, and obtain the allowed energies from matching conditions and graphical intersections.

Review from Lecture 9

For a time-independent Hamiltonian, an energy eigenstate evolves as

$$\hat{H}\phi_n = E_n\phi_n, \quad \psi_n(x, t) = \phi_n(x)e^{-iE_nt/\hbar}. \quad (1)$$

Its probability density is stationary:

$$|\psi_n(x, t)|^2 = |\phi_n(x)|^2. \quad (2)$$

A general state can contain several energies:

$$\psi(x, t) = \sum_n c_n \phi_n(x) e^{-iE_nt/\hbar}. \quad (3)$$

Different energy components acquire different phases, so interference can make the probability density time-dependent.

1 The infinite square well

1.1 Setup and boundary conditions

Consider

$$V(x) = \begin{cases} 0, & 0 < x < a, \\ \infty, & \text{elsewhere.} \end{cases} \quad (4)$$

The infinite walls confine the particle to $0 < x < a$, so

$$\boxed{\phi(0) = 0, \quad \phi(a) = 0.} \quad (5)$$

1.2 Stationary solutions

Inside the well, $V = 0$, and the time-independent Schrödinger equation becomes

$$-\frac{\hbar^2}{2m} \frac{d^2\phi}{dx^2} = E\phi, \quad (6)$$

or

$$\phi'' + k^2\phi = 0, \quad k^2 = \frac{2mE}{\hbar^2}. \quad (7)$$

The general solution is

$$\phi(x) = A \sin(kx) + B \cos(kx). \quad (8)$$

Applying the two boundary conditions gives

$$\phi(0) = 0 \implies B = 0, \quad (9)$$

$$\phi(a) = 0 \implies \sin(ka) = 0 \implies k_n = \frac{n\pi}{a}, \quad n = 1, 2, 3, \dots \quad (10)$$

After normalization,

$$\phi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right), \quad 0 < x < a, \quad (11)$$

and

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}, \quad n = 1, 2, 3, \dots \quad (12)$$

The boundary conditions and normalizability select only discrete values of k and E .

1.3 Nodes

An interior node is a zero strictly between the walls:

$$\phi(x_0) = 0, \quad 0 < x_0 < a. \quad (13)$$

The boundary zeros $\phi(0) = \phi(a) = 0$ are not counted as interior nodes. For the infinite well,

$$\phi_n \text{ has } n - 1 \text{ interior nodes,} \quad E_n = n^2 E_1. \quad (14)$$

For example,

$$\phi_2(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right) \quad (15)$$

has one interior node at $x = a/2$.

The Schrödinger equation is second order. If a solution satisfies

$$\phi(x_0) = 0, \quad \phi'(x_0) = 0 \quad (16)$$

at an interior point, these initial data force

$$\phi(x) = 0 \quad \text{for all } x. \quad (17)$$

Therefore a nonzero eigenfunction crosses the axis at an interior node:

$$\phi(x_0) = 0 \text{ at an interior node} \implies \phi'(x_0) \neq 0. \quad (18)$$

Questions.

Question 1. Which statement is correct for a time-independent Hamiltonian?

- A) Every valid state is stationary.
- B) A single energy eigenstate is stationary; a superposition of different energies generally is not.
- C) A superposition of different energies has one common time phase.

Answer and explanation. The answer is **B**. A single energy eigenstate changes only by an overall phase. Different components of a superposition acquire different phases, which can change the interference pattern.

Questions.

Question 2. For the infinite square well, which statement is correct?

- A) The ground state is $n = 0$ and has one interior node.
- B) The state $n = 3$ has two interior nodes and higher energy than $n = 1$.
- C) All states have the same energy because the potential is zero inside.

Answer and explanation. The answer is **B**. The quantum number begins at $n = 1$, the n -th state has $n - 1$ interior nodes, and $E_n = n^2 E_1$.

Questions.

Question 3. How many interior nodes does ϕ_4 have?

- A) 2
- B) 3
- C) 4
- D) 5

Answer and explanation. The answer is **B**. The nodes are

$$x = \frac{a}{4}, \quad \frac{a}{2}, \quad \frac{3a}{4}.$$

Questions.

Question 4. Can a nonzero energy eigenfunction satisfy

$$\phi(x_0) = 0, \quad \phi'(x_0) = 0$$

at an interior point?

- A) Yes, for an excited state.
- B) No, because these conditions give the identically zero solution.

Answer and explanation. The answer is **B**. A second-order differential equation with both the value and derivative fixed to zero has only the trivial solution.

2 The finite square well

2.1 Setup

Consider the symmetric finite square well

$$V(x) = \begin{cases} 0, & |x| < a/2, \\ V_0, & |x| \geq a/2, \end{cases} \quad 0 < E < V_0. \quad (19)$$

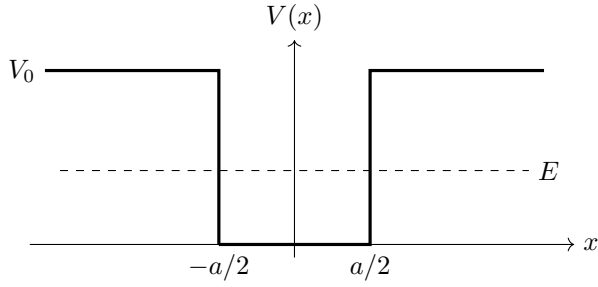


Figure 1: A finite square well with $0 < E < V_0$.

The three regions are

Region I	Region II	Region III
$x \leq -a/2$	$ x < a/2$	$x \geq a/2$
$E < V_0$	$E > 0$	$E < V_0$
forbidden	allowed	forbidden

Define

$$k = \frac{\sqrt{2mE}}{\hbar}, \quad \beta = \frac{\sqrt{2m(V_0 - E)}}{\hbar}. \quad (20)$$

The wave function oscillates where $E > V$ and decays exponentially where $E < V$.

2.2 Solutions in the three regions

Region I: $x \leq -a/2$

The Schrödinger equation is

$$\phi_I'' - \beta^2 \phi_I = 0, \quad (21)$$

with general solution

$$\phi_I = C_1 e^{\beta x} + C_2 e^{-\beta x}. \quad (22)$$

As $x \rightarrow -\infty$, $e^{-\beta x}$ diverges, so normalizability requires

$$\phi_I(x) = C_1 e^{\beta x}. \quad (23)$$

It is convenient to absorb a constant into the coefficient:

$$\phi_I(x) = C e^{\beta(x+a/2)}, \quad C = \phi_I(-a/2). \quad (24)$$

Region II: $|x| < a/2$

Inside the well,

$$\phi_{II}'' + k^2 \phi_{II} = 0, \quad (25)$$

so

$$\boxed{\phi_{II}(x) = A \cos(kx) + B \sin(kx).} \quad (26)$$

Region III: $x \geq a/2$

The equation is again

$$\phi_{III}'' - \beta^2 \phi_{III} = 0.$$

Normalizability excludes the growing exponential as $x \rightarrow +\infty$, giving

$$\boxed{\phi_{III}(x) = D e^{-\beta(x-a/2)}, \quad D = \phi_{III}(a/2).} \quad (27)$$

3 Parity in a symmetric well

The potential is symmetric:

$$\boxed{V(-x) = V(x).} \quad (28)$$

If

$$\hat{H}\phi(x) = E\phi(x),$$

then replacing x by $-x$ gives

$$\hat{H}\phi(-x) = E\phi(-x).$$

Thus $\phi(x)$ and $\phi(-x)$ have the same energy. Their sum and difference are also energy eigenfunctions:

$$\phi_+(x) = \phi(x) + \phi(-x), \quad \phi_+(-x) = \phi_+(x), \quad (29)$$

$$\phi_-(x) = \phi(x) - \phi(-x), \quad \phi_-(-x) = -\phi_-(x). \quad (30)$$

At least one of these functions is nonzero. Therefore eigenfunctions of a symmetric potential can be chosen to have definite parity:

$$\boxed{\text{even: } \phi(-x) = \phi(x), \quad \text{odd: } \phi(-x) = -\phi(x).} \quad (31)$$

For ordinary one-dimensional bound states, the energy is nondegenerate, so each energy eigenfunction itself has one definite parity.

Since $\cos(kx)$ is even and $\sin(kx)$ is odd, the inside solution becomes

	inside solution	condition at $x = 0$	
even	$\phi_{II}(x) = A \cos(kx)$	$\phi'(0) = 0$	(32)
odd	$\phi_{II}(x) = B \sin(kx)$	$\phi(0) = 0$	

4 Matching at the finite walls

For a finite jump in the potential, both the wave function and its first derivative are continuous:

$$\boxed{\phi\left(\frac{a^-}{2}\right) = \phi\left(\frac{a^+}{2}\right), \quad \phi'\left(\frac{a^-}{2}\right) = \phi'\left(\frac{a^+}{2}\right).} \quad (33)$$

It is efficient to divide the derivative condition by the value condition, thereby matching the logarithmic derivative ϕ'/ϕ .

4.1 Even states

For an even state,

$$\phi_{II} = A \cos(kx), \quad \phi_{III} = D e^{-\beta(x-a/2)}.$$

At $x = a/2$,

$$\left. \frac{\phi'}{\phi} \right|_{a/2^-} = -k \tan\left(\frac{ka}{2}\right), \quad (34)$$

$$\left. \frac{\phi'}{\phi} \right|_{a/2^+} = -\beta. \quad (35)$$

Therefore

$$\boxed{k \tan\left(\frac{ka}{2}\right) = \beta \quad (\text{even states}).} \quad (36)$$

4.2 Odd states

For an odd state,

$$\phi_{II} = B \sin(kx), \quad \phi_{III} = D e^{-\beta(x-a/2)}.$$

At $x = a/2$,

$$\left. \frac{\phi'}{\phi} \right|_{a/2^-} = k \cot\left(\frac{ka}{2}\right), \quad (37)$$

$$\left. \frac{\phi'}{\phi} \right|_{a/2^+} = -\beta. \quad (38)$$

Thus

$$\boxed{-k \cot\left(\frac{ka}{2}\right) = \beta \quad (\text{odd states}).} \quad (39)$$

Both matching conditions must be satisfied together with

$$\boxed{k^2 + \beta^2 = \frac{2mV_0}{\hbar^2}.} \quad (40)$$

The last relation follows directly from the definitions of k and β :

$$k^2 + \beta^2 = \frac{2mE}{\hbar^2} + \frac{2m(V_0 - E)}{\hbar^2}.$$

5 Dimensionless form and graphical solutions

Define

$$\xi = \frac{ka}{2}, \quad \eta = \frac{\beta a}{2}. \quad (41)$$

The matching equations become

$$\boxed{\xi \tan \xi = \eta} \quad (\text{even}), \quad (42)$$

$$\boxed{-\xi \cot \xi = \eta} \quad (\text{odd}). \quad (43)$$

The relation between ξ and η is

$$\xi^2 + \eta^2 = \frac{a^2}{4}(k^2 + \beta^2) \quad (44)$$

$$= \frac{mV_0 a^2}{2\hbar^2} \equiv \rho^2. \quad (45)$$

Thus, for fixed V_0 , a , and m ,

$$\boxed{\eta = \sqrt{\rho^2 - \xi^2}} \quad (46)$$

is one fixed quarter circle in the (ξ, η) -plane. The energy is determined by ξ :

$$\boxed{E = \frac{\hbar^2 k^2}{2m} = \frac{2\hbar^2 \xi^2}{ma^2}}. \quad (47)$$

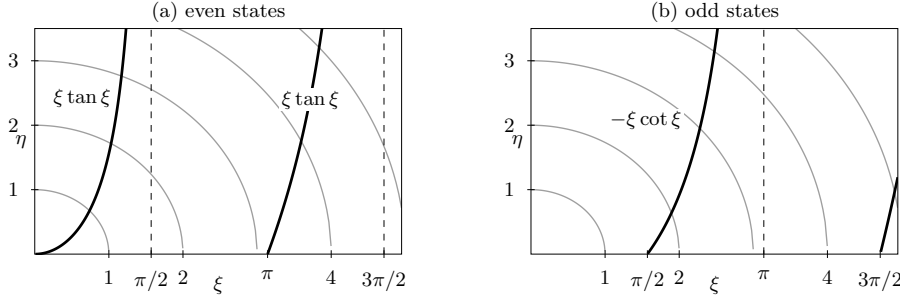


Figure 2: Graphical solutions for the even and odd matching equations. The quarter circles represent different values of ρ ; for one fixed physical well, only its corresponding circle is used. Each intersection gives one allowed bound-state energy.

The matching equations are transcendental equations. Their solutions are the intersections of the appropriate curve with the single quarter circle determined by V_0 , a , and m :

$$\boxed{\text{one intersection} \iff \text{one allowed energy.}} \quad (48)$$

There is always at least one even bound state. The first odd state appears only when the well is sufficiently strong. Its threshold is

$$\rho = \frac{\pi}{2} \iff \boxed{V_0 a^2 = \frac{\pi^2 \hbar^2}{2m}}. \quad (49)$$

The equality corresponds to $E = V_0$, which is not yet a normalizable bound state. Therefore

$$\rho > \frac{\pi}{2} \implies \text{at least one odd bound state.} \quad (50)$$

Increasing $V_0 a^2$ increases ρ , produces more intersections, and therefore supports more bound states.

6 Physical interpretation

Inside the well, $E > V$, so the wave function oscillates:

$$\phi_{II}(x) = A \cos(kx) + B \sin(kx). \quad (51)$$

Outside the well, $E < V$, so normalizability selects exponential decay:

$$\phi_{\text{out}}(x) \propto e^{-\beta|x|}. \quad (52)$$

For example, to the right of the well,

$$|\phi_{III}(x)|^2 = |D|^2 e^{-2\beta(x-a/2)}. \quad (53)$$

The penetration length is

$$\ell = \frac{1}{\beta} = \frac{\hbar}{\sqrt{2m(V_0 - E)}}. \quad (54)$$

Thus

$$V_0 - E \text{ larger} \implies \beta \text{ larger} \implies \text{faster decay and shorter penetration length.} \quad (55)$$

The finite barrier permits a nonzero probability of finding the particle outside the classically allowed region.

6.1 Infinite-well limit

As $V_0 \rightarrow \infty$,

$$\beta \rightarrow \infty, \quad \ell = \frac{1}{\beta} \rightarrow 0. \quad (56)$$

The matching equations then require the trigonometric factors to approach their zeros or poles:

$$\text{even:} \quad \frac{ka}{2} \longrightarrow \left(n + \frac{1}{2}\right)\pi, \quad n = 0, 1, 2, \dots, \quad (57)$$

$$\text{odd:} \quad \frac{ka}{2} \longrightarrow n\pi, \quad n = 1, 2, 3, \dots \quad (58)$$

The even and odd families combine into

$$k_n = \frac{n\pi}{a}, \quad E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}. \quad (59)$$

The exponential tails disappear, and the finite-well spectrum approaches the infinite-well spectrum.

Lecture 10 summary

- An infinite square well has $\phi(0) = \phi(a) = 0$, which gives

$$\phi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right), \quad E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}.$$

- The n -th infinite-well state has $n - 1$ interior nodes. Boundary zeros are not counted as interior nodes.
- In a symmetric potential, energy eigenfunctions can be chosen to have definite parity. For a nondegenerate one-dimensional bound state, the eigenfunction itself is either even or odd.
- In a finite well, the wave function oscillates where $E > V$ and decays exponentially where $E < V$.
- Continuity of ϕ and ϕ' gives

$$k \tan(ka/2) = \beta \quad (\text{even}), \quad -k \cot(ka/2) = \beta \quad (\text{odd}).$$

- With $\xi = ka/2$, $\eta = \beta a/2$, and

$$\rho^2 = \frac{mV_0 a^2}{2\hbar^2},$$

the allowed energies are the intersections of the matching curves with one fixed quarter circle.

- A finite barrier gives a nonzero tail outside the well. Its penetration length is

$$\ell = \frac{\hbar}{\sqrt{2m(V_0 - E)}}.$$

- As $V_0 \rightarrow \infty$, the tails vanish and the finite-well spectrum approaches the infinite-well spectrum.

Suggested reading. Griffiths and Schroeter, *Introduction to Quantum Mechanics*, 3rd ed., sections on one-dimensional bound states and the finite square well. Review Lecture 9 on the infinite square well, nodes, and the distinction between classically allowed and forbidden regions.