Lecture 11

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Contents

1 The Infinite Square Well

In our last lecture we examined the quantum wavefunction of a particle moving in a circle. Here we introduce another instructive toy model, the **infinite square well potential**. This forces a particle to live on an interval of the real line, the interval conventionally chosen to be $x \in [0, a]$. At the ends 0 and a of the interval there are hard walls that prevent the particle from going to $x > a$ and $x < 0$. The potential is defined as follows and shown in figure 1.

$$V(x) \;=\; \begin{cases} 0\,, & 0 < x < a\,, \\ \infty & x \leq 0\,,\, x \geq 0 \end{cases} \tag{1.1}$$

It is reasonable to assume that the wavefunction must vanish in the region where the potential is

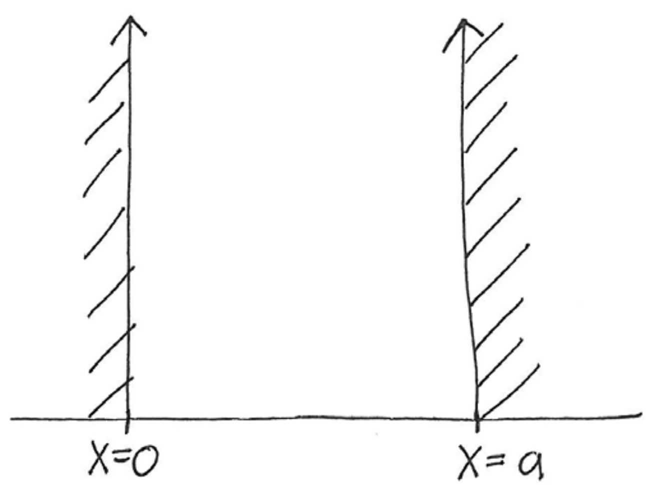

Figure 1: The infinite square well potential

infinite. Classically any region where the potential exceeds the energy of the particle is forbidden. Not so in quantum mechanics. But even in quantum mechanics a particle can't be in a region of *infinite* potential. We will be able to justify these claims by studying the more complicated *finite* square well in the limit as the height of the potential goes to infinity. But for the meantime we simply state the fact:

$$\psi(x) = 0 \quad \text{for } \; x < 0 \text{ and for } \; x > a\,. \tag{1.2}$$

Since the wavefunction must be continuous we must have that it should vanish at $x = 0$ and at $x = a$:

1. $\psi(x = 0) = 0$.

2. $\psi(x = a) = 0$.

These are our boundary conditions. You may wonder about the continuity of the first derivative $\psi'(x)$. This derivative vanishes outside the interval and continuity would say that ψ' should vanish at 0 and at a. But this is impossible. A solution of Schrödinger's equation (a second order differential equation) for which *both* the wavefunction and its derivative vanishes at a point is identically zero! If a solution exist we must accept that ψ' can have discontinuities at an infinite wall. Therefore we do not impose any boundary condition on ψ'. The two conditions above will suffice to find a solution. In that solution ψ' is discontinuous at the endpoints.

In the region $x \in [0, a]$ the potential vanishes and the Schrödinger equation takes the form

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi\,, \tag{1.3}$$

and as we did before, one can show that the energy E must be positive (do it!). This allows us to define, as usual, a real quantity k such that

$$k^2 \equiv \frac{2mE}{\hbar^2} \quad \rightarrow \quad E = \frac{\hbar^2 k^2}{2m}\,. \tag{1.4}$$

The differential equation is then

$$\frac{d^2\psi}{dx^2} = -k^2\psi\,, \tag{1.5}$$

and the general solution can be written as

$$\psi(x) = c_1 \cos kx + c_2 \sin kx\,, \tag{1.6}$$

with constants c_1 and c_2 to be determined. For this we use our boundary conditions.

The condition $\psi(x = 0) = 0$ implies that c_1 in Eq 1.6 must be zero. The coefficient of $\sin kx$ need not be, since this function vanishes automatically for $x = 0$. Therefore the solution so far reads

$$\psi(x) = c_2 \sin kx\,. \tag{1.7}$$

Note that if we demanded continuity of ψ' we would have to ask for $\psi'(x = 0) = 0$ and that would make c_2 equal to zero, and thus ψ identically zero. That **is not** a solution. There is no particle if $\psi = 0$.

At this point we must impose the vanishing of ψ at $x = a$.

$$c_2 \sin ka = 0 \quad \rightarrow \quad ka = n\pi \quad \rightarrow \quad k_n = \frac{n\pi}{a}\,. \tag{1.8}$$

Here n must be an integer and the solution would be

$$\psi_n(x) = N \sin\Big(\frac{n\pi x}{a}\Big)\,, \tag{1.9}$$

with N a normalization constant. Which integers n are acceptable here? Well, $n = 0$ is not acceptable, because it would make the wavefunction zero. Moreover, n and $-n$ give the same wavefunction, up to a sign. Since the sign of a wavefunction is irrelevant, it would thus be double counting to include both positive and negative n's. We restrict ourselves to n being positive integers.

To solve for the coefficient, we utilize the normalization condition; every $\psi_n(x)$ must be normalized.

$$1 = N^2 \int_0^a \sin^2\left(\frac{n\pi x}{a}\right) dx \;=\; N^2 \,\tfrac{1}{2}\cdot a \quad\rightarrow\quad N \;=\; \sqrt{\frac{2}{a}}\,. \tag{1.10}$$

Therefore, all in all, our solutions are:

$$\boxed{\psi_n = \sqrt{\frac{2}{a}}\sin\Big(\frac{n\pi x}{a}\Big)\,, \quad E_n \;=\; \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2\pi^2 n^2}{2ma^2}\,, \quad n = 1, 2, \cdots .} \tag{1.11}$$

Each value of n gives a different energy, implying that in the one-dimensional infinite square well there are no degeneracies in the energy spectrum! The ground state –the lowest energy state– corresponds to $n = 1$ and has nonzero energy.

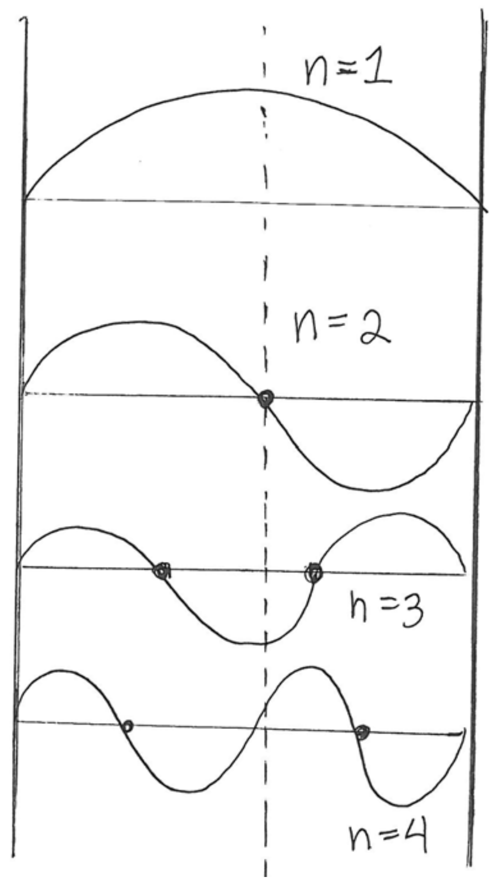

Figure 2: The four lowest energy eigenstates for the infinite square well potential. The n^{th} wavefunction solution ψ_n has $n-1$ nodes. The solutions are alternately symmetric and antisymmetric about the midpoint $x = a$.

Figure 2 shows the first four solutions to the 1-d infinite square well, labeled from $n = 1$ to $n = 4$. We note a few features:

1. The ground state $n = 1$ has no nodes. A node is a zero of the wavefunction that is not at the ends of the domain of the wavefunction. The zeroes at $x = 0$ and $x = a$ do not count as nodes. Clearly $\psi_1(x)$ does not vanish anywhere in the interior of $[0, a]$ and therefore it has no nodes. It

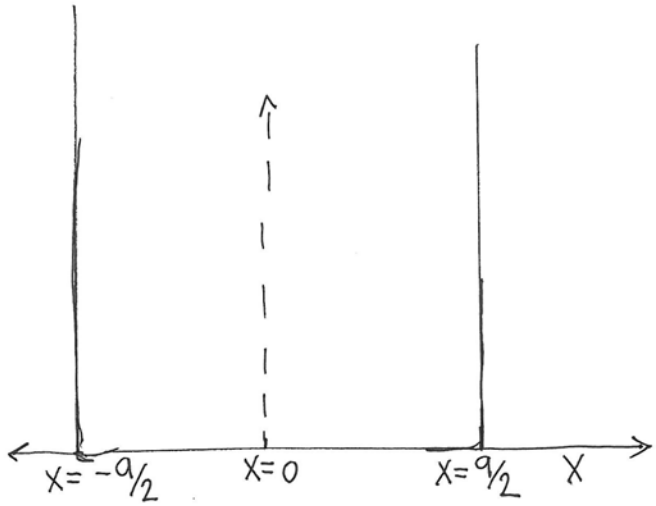

Figure 3: The infinite square well shifted to the left to make it symmetric about the origin.

is in fact true that any normalizable ground state of a one-dimensional potential does not have nodes.

2. The first excited state, $n = 2$ has one node. It is at $x = a$, the midpoint of the interval. The second excited state, $n = 3$ has two nodes. The pattern in fact continues. The n-th excited state will have n nodes.

3. In the figure the dotted vertical line marks the interval midpoint $x = \frac{a}{2}$. We note that the ground state is symmetric under reflection about $x = \frac{a}{2}$. The first excited state is antisymmetric, indeed its node is at $x = \frac{a}{2}$. The second excited state is again symmetric. Symmetry and antisymmetry alternate forever.

4. The symmetry just noted is not accidental. It holds, in general for potentials $V(x)$ that are even functions of x: $V(-x) = V(x)$. Our potential, does not satisfy this equation, but this could have been changed easily and with no consequence. We could shift the well over so that rather than having $V(x) = 0$ from $0 \leq x \leq a$, it extends from $-\frac{a}{2} \leq x \leq \frac{a}{2}$ and then it would be symmetric about the origin $x = 0$ (see figure 3). We will later prove that the bound states of a one-dimensional even potential are either even or odd! Here we are just seeing an example of such result.

5. The wavefunctions $\psi_n(x)$ with $n = 1, 2, \ldots$ form a complete set that can be used to expand any function in the interval $x \in [0, a]$ that vanishes at the endpoints. If the function does not vanish at the endpoints, the convergence of the expansion is delicate, and physically such wavefunction would be problematic as one can verify that the expectation value of the energy is infinite.

2 The Finite Square Well

We now examine the finite square well, defined as follows and shown in figure 4.

$$V(x) = \begin{cases} -V_0\,, & \text{for} \quad |x| \leq a\,, \quad V_0 > 0\,, \\ \;\;0\,, & \text{for} \quad |x| \geq a\,. \end{cases} \tag{2.12}$$

Note that the potential energy is zero for $|x| > a$. The potential energy is negative and equal to $-V_0$ in the well, because we defined V_0 to be a positive number. The width of the well is $2a$. Note

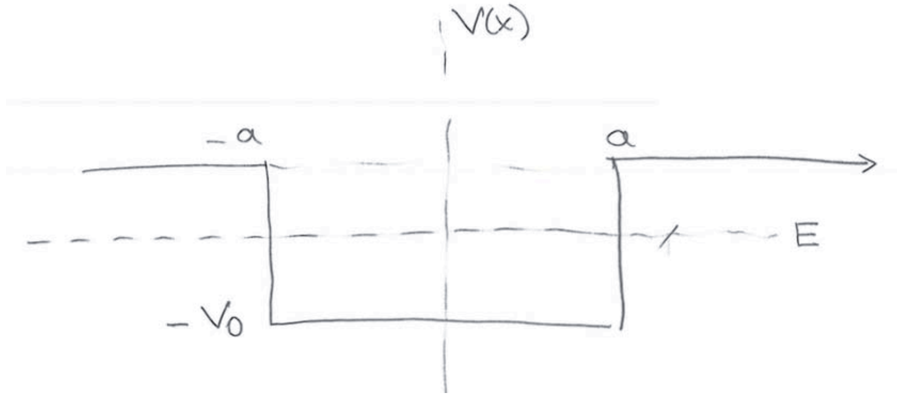

Figure 4: The finite square well potential

also that we have placed the bottom of the well differently than in the case of the infinite square well. The bottom of the infinite square well was at zero potential energy. If we wanted to obtain the infinite square well as a limit of the finite square well we would have to take V_0 to infinity, but care is needed to compare energies. The ones in the infinite square well are measured with respect to a bottom at zero energy. The ones in the finite square well are measure with respect to a bottom at $-V_0$.

We will be interested in **bound states** namely, energy eigenstates that are normalizable. For this the energy E of the states must be negative. This is readily understood. If $E > 0$, any solutions in the region $x > a$ where the potential vanishes would be a plane wave, extending all the way to infinity. Such a solution would not be normalizable. The energy E is shown as a dashed line in the figure. We have

$$-V_0 < E < 0 \,. \tag{2.13}$$

Note that since E is negative we have $E = -|E|$. For a bound state of energy E, the energy $\tilde{E}$ measured with respect to the bottom of the potential is

$$\tilde{E} \;=\; E - (-V_0) = V_0 - |E| > 0 \,. \tag{2.14}$$

Those $\tilde{E}$ are the ones that can be compared with the energies of the infinite square well in the limit as $V_0 \to \infty$.

What are the bound state solutions to the Schrödinger equation with this potential? We have to examine how the equation looks in the various regions where the potential is constant and then use boundary conditions to match the solutions across the points where the potential is discontinuous. We have the equation Let's examine the regions, where, for simplicity, we define $A(x)$ by

$$\frac{d^2\psi}{dx^2} \;=\; -\frac{2m}{\hbar^2}(E - V(x))\,\psi = \alpha(x)\psi \,, \tag{2.15}$$

where we have defined the factor $\alpha(x)$ that multiplies the wavefunction on the right-hand side of the Schrödinger equation. We then consider the two regions

- region $|x| > a$: $\alpha(x)$ is a positive constant. The wavefunction in this region constructed with real exponentials.

- region $|x| < a$: $\alpha(x)$ is a negative constant. The wavefunction in this region is constructed with trigonometric functions.

The potential $V(x)$ for the finite square well is an even function of x: $V(-x) = V(x)$ We can therefore use the theorem cited earlier (and proven later!) that for an even potential the bound states are either symmetric or antisymmetric. We begin by looking for even solutions, that is, solutions ψ for which $\psi(-x) = \psi(x)$.

Even solutions. Since the potential is piecewise continuous we must study the differential equation in two regions:

- $|x| < a$

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}(E - (-V_0))\psi = -\frac{2m}{\hbar^2}(V_0 - |E|)\psi \tag{2.16}$$

$V_0 - |E|$ is a positive constant thus define a real $k > 0$ by

$$\boxed{k^2 \equiv \frac{2m}{\hbar^2}(V_0 - |E|) > 0\,, \quad k > 0\,.} \tag{2.17}$$

It is interesting to note that this equation is not too different from the free-particle equation $k^2 = \frac{2mE}{\hbar^2}$. Indeed, $V_0 - |E|$ is the kinetic energy of the particle and thus k has the usual interpretation. The differential equation to be solved now reads

$$\psi'' = -k^2\psi\,, \tag{2.18}$$

for which the only possible even solution is

$$\boxed{\psi(x) = \cos kx\,, \quad |x| < a\,.} \tag{2.19}$$

We are not including a normalization constant because, at this state we do not aim for normalized eigenstates. We will get an eigenstate and while it will not be normalized, it will be *normalizable*, and that's all that is essential. We are after is the possible energies. Normalized wavefunctions would be useful to compute expectation values.

- $|x| > a$

$$\psi'' = -\frac{2m}{\hbar^2}(E - 0)\,\psi = \frac{2m|E|}{\hbar^2}\,\psi \tag{2.20}$$

This time we define a real positive constant κ with the relation

$$\boxed{\kappa^2 = \frac{2m|E|}{\hbar^2}\,, \quad \kappa > 0\,.} \tag{2.21}$$

The differential equation to be solved now reads

$$\psi'' = \kappa^2\psi\,, \tag{2.22}$$

and the solutions are exponentials. In fact we need exponentials that decay as $x \to \pm\infty$, otherwise the wavefunction will not be normalizable. This should be physically intuitive, in a classically forbidden region the probability to be far away from the well must be vanishingly small. For $x > a$ we choose the decaying exponential

$$\boxed{\psi(x) = A\, e^{-\kappa x}, \quad x > a\,,} \tag{2.23}$$

where A is a normalization constant to be determined by the boundary conditions. More generally, given that the solution is even, we have

$$\psi(x) \;=\; A\, e^{-\kappa|x|},\ |x| > a\,. \tag{2.24}$$

It is now useful to note that κ^2 and k^2 satisfy a simple relation. Using their definitions above we see that the energy $|E|$ drops out of their sum and we have

$$k^2 + \kappa^2 = \frac{2mV_0}{\hbar^2} \tag{2.25}$$

At this point we make progress by introducing **unit free** constants ξ, η, and z_0 as follows:

$$\begin{aligned} \eta \;&\equiv\; ka > 0\,, \\ \xi \;&\equiv\; \kappa a > 0\,, \\ z_0^2 \;&\equiv\; \frac{2mV_0a^2}{\hbar^2}\,. \end{aligned} \tag{2.26}$$

Clearly ξ is a proxy for κ and η is a proxy for k. Both depend on the energy of the bound state. The parameter z_0, unit-free, just depends on the data associated with the potential (the depth V_0 and the width $2a$) and the mass m of the particle. If you are given a potential, you know the number z_0. A very deep and/or wide potential has very large z_0, while a very shallow and/or narrow potential has small z_0. As we will see the value of z_0 tells us how many bound states the square well has.

Multiplying (2.25) by a^2 and using our definitions above we get

$$\boxed{\eta^2 + \xi^2 \;=\; z_0^2\,.} \tag{2.27}$$

Let us make clear that solving for ξ is actually like solving for the energy. From Eq. (2.21), we can see

$$\xi^2 \;=\; \kappa^2 a^2 \;=\; \frac{2m|E|a^2}{\hbar^2} \;=\; \frac{2mV_0a^2}{\hbar^2}\frac{|E|}{V_0} \;=\; z_0^2\,\frac{|E|}{V_0}\,, \tag{2.28}$$

and from this we get

$$\frac{|E|}{V_0} \;=\; \Big(\frac{\xi}{z_0}\Big)^2. \tag{2.29}$$

This is a nice equation, the left hand side gives the energy as a fraction of the depth V_0 of the well and the right-hand side involves ξ and the constant z_0 of the potential. The quantity η also encodes the energy in a slightly different way. From (2.17) we have

$$\eta^2 \;=\; k^2a^2 \;\equiv\; \frac{2ma^2}{\hbar^2}(V_0 - |E|)\,, \tag{2.30}$$

and using (2.14) we see that this provides the energy $\tilde{E}$, measured relative to the bottom of the potential

$$\tilde{E} \;=\; V_0 - |E| \;=\; \eta^2 \frac{\hbar^2}{2ma^2}\,. \tag{2.31}$$

This formula is convenient to understand how the infinite square energy levels appear in the limit as the depth of the finite well goes to infinity. Note that the above answer for the energies is given by the unit free number η multiplied by the characteristic energy of an infinite well of width a.

Let us finally complete the construction. We must impose the continuity of the wavefunction and the continuity of ψ' at $x = a$. Using the expressions for ψ for $x < a$ and for $x > a$ these conditions give

$$\begin{aligned} \psi \text{ continuous at } x = a \implies & \qquad \cos(ka) \;=\; Ae^{-\kappa a} \\ \psi' \text{ continuous at } x = a \implies & \quad -k\sin(ka) \;=\; -\,\kappa A e^{-\kappa a}\,, \end{aligned} \tag{2.32}$$

Dividing the second equation by the first we eliminate the constant A and find a second relation between k and κ! This is exactly what is needed. The result is

$$k\tan ka \;= \kappa \quad \to \quad ka\tan ka \;= \kappa a \quad \to \quad \xi = \eta\tan\eta\,. \tag{2.33}$$

Our task of finding the bound states is now reduced to finding solutions to the simultaneous equations

$$\boxed{\text{Even solutions: } \;\eta^2 + \xi^2 \;=\; z_0^2\,, \qquad \xi = \eta\tan\eta\,, \qquad \xi\,,\eta > 0\,.} \tag{2.34}$$

These equations can be solved numerically to find all solutions that exist for a given fixed value of z_0. Each solution represents one bound state. We can understand the solution space by plotting these two equations in the *first quadrant* of an (η, ξ) plane, as shown in figure 5.

The first equation in (2.34) is a piece of a circle of radius z_0. The second equation, $\xi = \eta\tan\eta$, gives infinitely many curves as η grows from zero to infinity. The value of ξ goes to infinity for η approaches each odd multiple of $\pi/2$. The bound states are represented by the intersections in the plot (heavy dots).

In the figure we see two intersections, which means two bound states. The first intersection takes place near $\eta = \pi/2$ and with large $\xi \sim z_0$. This is the ground state, or the most deeply bound bound-state. This can be seen from (2.29). Alternatively, it can be seen from equation (2.31), noting that this is the solution with smallest η. The second solution occurs for η near $3\pi/2$. As the radius of the circle becomes bigger we get more and more intersections; z_0 controls the number of even bound states. Finally, note that there is always an even solution, no matter how small z_0 is, because the arc of the circle will always intersect the first curve of the $\xi = \eta\tan\eta$ plot. Thus, at least one bound state exists however shallow the finite well is.

Odd solutions. For odd solutions all of our definitions $(k, \kappa, z_0, \eta, \xi)$ remain the same. The wavefunction now is of the form

$$\psi(x) \;=\; \begin{cases} \sin kx\,, & |x| < a \\ Ae^{-k|x|}\,, & |x| > a \end{cases} \tag{2.35}$$

Matching ψ and ψ' at $x = a$ now gives $\xi = -\eta\cot\eta$ (do it!). As a result the relevant simultaneous equations are now

$$\boxed{\text{Odd solutions: } \;\eta^2 + \xi^2 \;= z_0^2\,, \qquad \xi = -\eta\cot\eta\,, \qquad \xi\,,\eta > 0\,.} \tag{2.36}$$

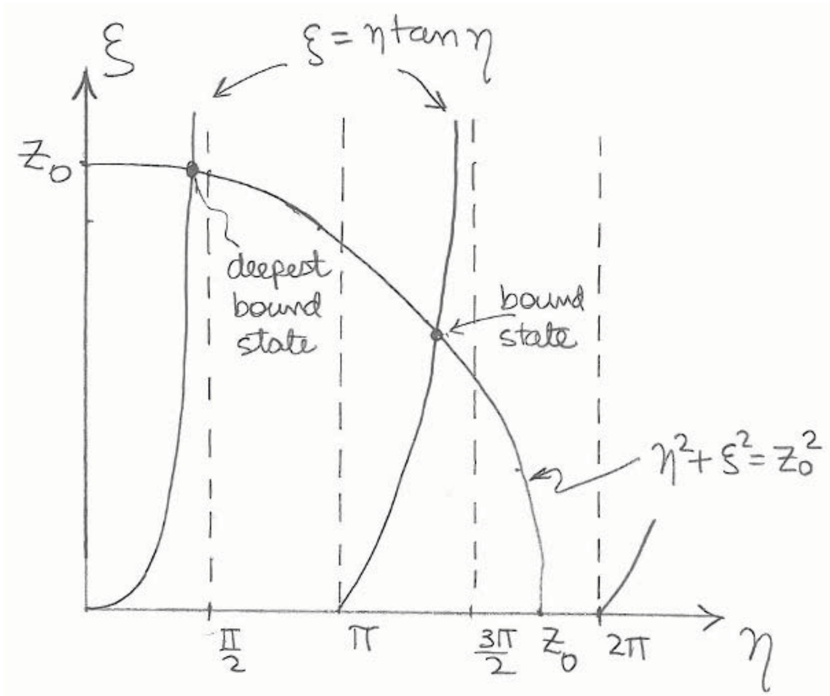

Figure 5: Graphical representation of the simultaneous equations (2.34). The intersections of the circle with the $\eta \tan \eta$ function represent even bound state solutions in the finite square well potential. The deepest bound state is the one with lowest η.

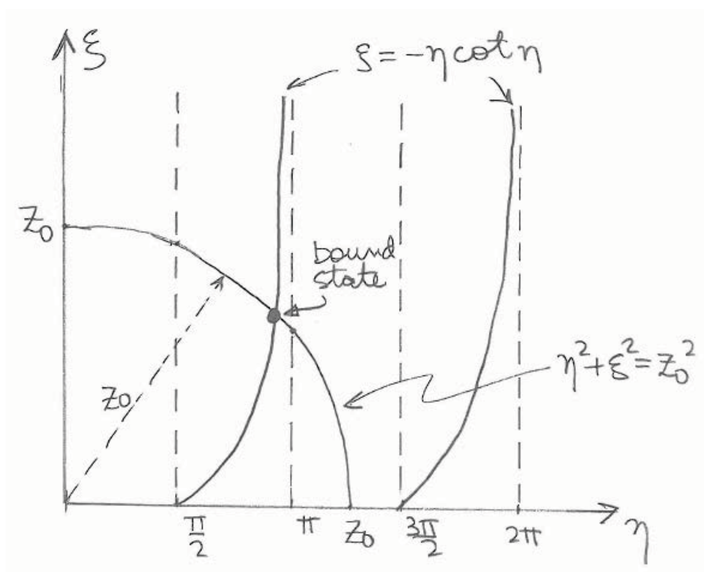

Figure 6: Graphical representation of (2.36). The intersections of the circle with the curves $\xi = -\eta \cot \eta$ are odd bound-state solutions in the finite square-well potential. In the case displayed there is just one bound state.

In figure 6 the curve $\xi = -\eta \cot \eta$ does not appear for $\eta < \pi/2$ because ξ is then negative. For $z_0 < \frac{\pi}{2}$ there are no odd bound-state solutions, but we still have the even bound state.

We could have anticipated the quantization of the energy by the following argument. Suppose you

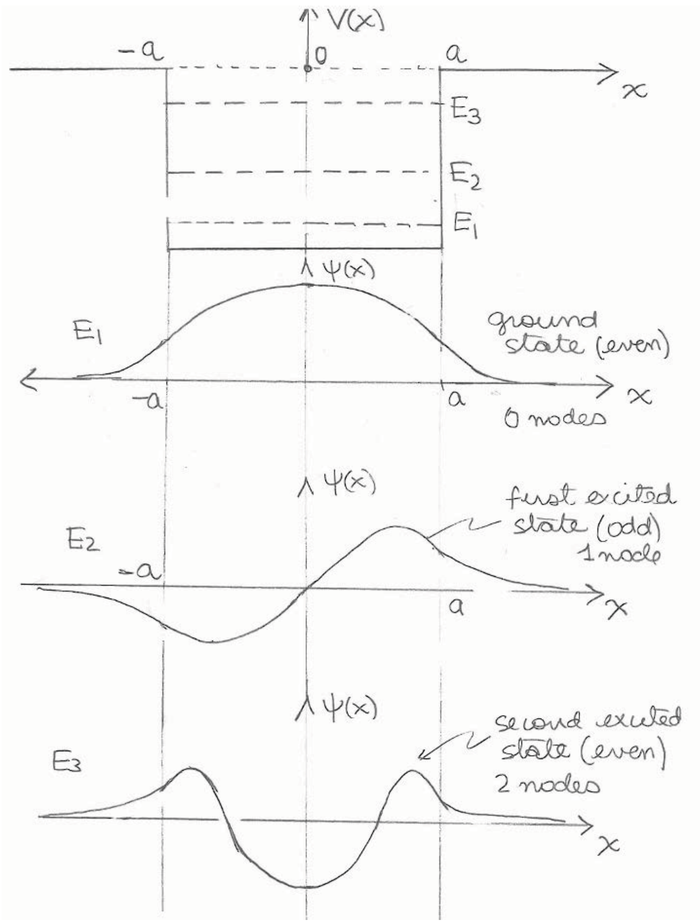

Figure 7: Sketching eigenstates of a finite square well potential. The energies are $E_1 < E_2 < E_3$.

try to calculate energy eigenstates which, as far as solving the Schrödinger equation, are determined up to an overall normalization. Suppose you don't know the energy is quantized and you fix some arbitrary fixed energy and calculate. Both in the even and in the odd case, we can set the coefficient of the $\sin kx$ or $\cos kx$ function inside the well equal to one. The coefficient of the decaying exponential outside the well was undetermined, we called it A. Therefore we just have one unknown, A. But we have two equations, because we impose continuity of ψ and of ψ' at $x = a$. If we have one unknown and two equations, we have no reason to believe there is a solution. Indeed, generally there is none. But then, if we think of the energy E as an unknown, that energy appears at various places in the equations (in k and κ) and therefore having two unknowns A and E and two equations, we should expect a single solution! This is indeed what happened.

In figure 7 we sketch the energy eigenstates of a square-well potential with three bound states of energies $E_1 < E_2 < E_3$. A few features of the wavefunctions are manifest: they alternate as even, odd, and even. They have zero, one, and two nodes, respectively. The second derivative of ψ is negative for $|x| < a$ and positive for $|x| > a$ (it is in fact discontinuous at $x = \pm a$). The exponential decay in the region $|x| > a$ is fastest for the ground state and slowest for the least bound state.

Sarah Geller transcribed Zwiebach's notes to create the first LaTeX version of this document.

8.04 Quantum Physics I
Spring 2016