(10) Bound States of Finite Wells

1 Last Time

- Qualitative shape of Energy Eigenstates in 1D potentials

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2 This Time

- Finite steps, barriers and wells

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3 Piecewise Constant Potentials

- Sh 5.(3,4), Sc 4.1

Last time we rearranged the Schrödinger equation into the form of a simple 2$^{\text{nd}}$ oder PDE.

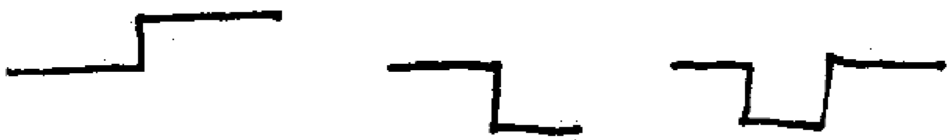
1D Energy ES

$$\begin{aligned}
\frac{-\hbar^2}{2m}\partial_x^2 \ \phi_E(x) &= (E - V(x)) \ \phi_E(x) \\
\partial_x^2 \ \phi_E(x) &= -k^2(x) \, \phi_E(x) \\
\text{where} \qquad & k^2(x) = \frac{2m}{\hbar^2} \, (E - V(x))
\end{aligned}$$

and noted that for a slowly changing $V(x)$ we could expect oscillatory solutions in classically allowed regions where $E > V(x)$, and exponential solutions in classically forbidden regions where $E < V(x)$.

To ensure that the criterion of a slowly changing potential is met, we will start by studying potentials that are piecewise constant.

Piecewise Constant Potentials



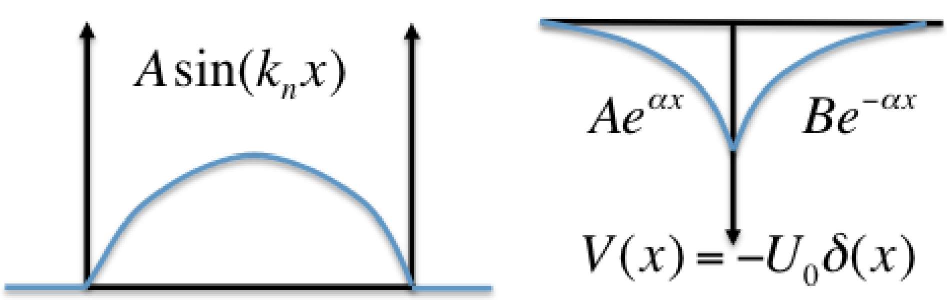
In each constant region we know the energy eigenstates which solve the Schrödinger equation are

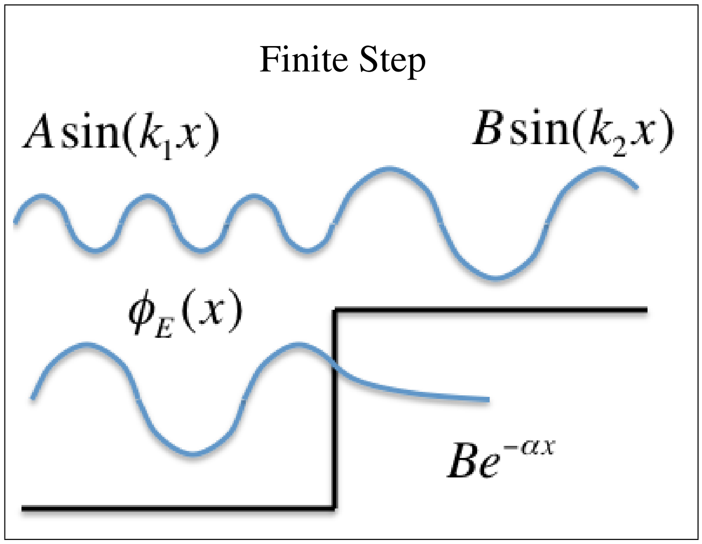
$$
\begin{aligned}
E > V \quad &\Rightarrow \quad \phi_E(x) = Ae^{ikx} + Be^{-ikx} \\
\text{or} \quad & \quad \phi_E(x) = C\sin(kx) + D\cos(kx) \\
E < V \quad &\Rightarrow \quad \phi_E(x) = Ae^{\alpha x} + Be^{-\alpha x} \\
\text{where} \quad & \quad\; k^2 = \frac{2m}{\hbar^2}(E - V) \;\; \text{and} \;\; \alpha^2 = -k^2
\end{aligned}
$$

At the boundaries between piecewise regions, we need to patch our solutions together. There are some rules about how to do this which derive from the PDE we are solving.

$V(x)$	$\partial_x^2 \phi_E(x)$	$\partial_x \phi_E(x)$	$\phi_E(x)$
finite step	finite step	continuous	continuous
infinite step	infinite step	finite step	continuous

Infinite Steps





For piecewise constant $V(x)$, finding $\phi_E(x)$ reduces to matching known solutions at the boundaries between regions of constant potential.

*At each boundary, you must match the **value** and **first derivative** of the wavefunction.*

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4 Bound State of the Delta Function Potential

Because the delta function potential is an interesting one, let's look quickly at how we would find its energy eigenstates.

We will restrict our solutions to bound states (i.e., $E < 0$), but the same arguments apply to unbound states.

Solutions should solve

$$\begin{aligned} V(x) &= -U_0\delta(x) \\ \Rightarrow \partial_x^2\ \phi_E(x) &= -\frac{2m}{\hbar^2}\left(E + U_0\delta(x)\right)\ \phi_E(x) \end{aligned}$$

We know that away from $x = 0$ we will have exponential solutions since $E < V$. Since they must be normalizable we are left with

$$\phi_E(x) = \begin{cases} Ae^{\alpha x} & x < 0 \\ Be^{-\alpha x} & x > 0 \end{cases}$$

The challenge then is just to find the conditions for matching the $x > 0$ solution to the $x < 0$ solution.

By continuity, we know that $A = B$.

And we can find the value of A by normalizing the state

$$\begin{aligned} 1 &= 2\int_0^\infty |\phi_E(x)|^2 \, dx = 2\int_0^\infty |A|^2 e^{-2\alpha x} \, dx \\ &= \frac{-|A|^2}{\alpha} e^{-2\alpha x}\Big|_0^\infty = \frac{|A|^2}{\alpha} \\ \Rightarrow |A|^2 &= \alpha = \sqrt{\frac{-2mE}{\hbar^2}} \quad \because \quad E < 0 \end{aligned}$$

We now know A in terms of the energy, but we have no idea what E should be for our bound state.

This leaves the derivative which, while not continuous (since the delta function is infinite), does have a matching condition. Since the integral of the delta function is finite, the discontinuity in the derivative of $\phi_E(x)$ is also finite.

Integrate both sides of our PDE once...

$$\begin{aligned} \int_{-\epsilon}^{\epsilon} \partial_x^2 \, \phi_E(x) \, dx &= \int_{-\epsilon}^{\epsilon} -\frac{2m}{\hbar^2} \left(E + U_0 \delta(x)\right) \, \phi_E(x) \, dx \\ \partial_x \, \phi_E(x)\Big|_{-\epsilon}^{\epsilon} &= -\frac{2m}{\hbar^2} \left(U_0 \, \phi_E(0) + E \int_{-\epsilon}^{\epsilon} \phi_E(x) \, dx \right) \\ A\partial_x \left(e^{-\alpha x} - e^{\alpha x}\right)\Big|_{x=0} &= -\frac{2m}{\hbar^2} U_0 \, A \end{aligned}$$

where the last step comes from taking the limit as $\epsilon \to 0$, uses the solutions to the left and right of $x = 0$, and expresses the fact that there is a finite discontinuity in $\partial_x \phi_E(x)$ at $x = 0$. We can satisfy this matching condition with an appropriate choice of E such that

$$\begin{aligned} -2\alpha &= -\frac{2m}{\hbar^2}U_0 \\ \text{sub in } \alpha \text{ ...} \quad \frac{\sqrt{-2mE}}{\hbar} &= \frac{m}{\hbar^2}U_0 \\ \Rightarrow -2mE &= \frac{m^2}{\hbar^2}U_0^2 \\ \Rightarrow E &= -\frac{m}{2\hbar^2}U_0^2 \end{aligned}$$

But wait! I hear you cry... your units are wrong!
Well, the units of U_0 are tricky.

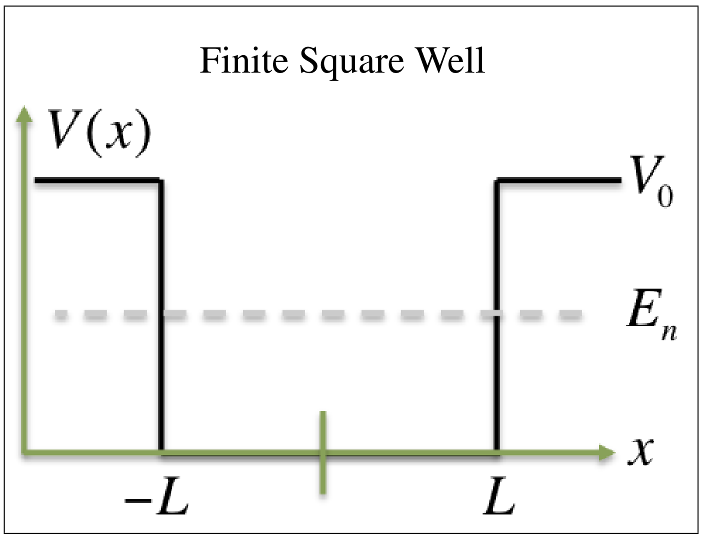
$$[U_0\delta(x)] = [\text{J}] \Rightarrow [U_0] = [\text{J m}]$$

$$\Rightarrow [\frac{m}{2\hbar^2}U_0^2] = [\frac{\text{kg}}{\text{J}^2\ \text{s}^2}\text{J}^2\ \text{m}^2] = [\frac{\text{kg m}^2}{\text{s}^2}] = \text{J}$$

So, the result of all of this is that the delta function potential has a single bound state, with an energy determined by the "amplitude" of the delta function U_0.

5 Bound States of the Finite Square Well

Moving on to the cousin of our first 1D potential, the finite square well, we will see how energy eigenstates are found when the potential has a finite discontinuity in it. Let's start by writing the potential and seeing what we can say about the solutions. (As before, we will focus on the bound states.)



$$V(x) = \begin{cases} 0 & -L < x < L \\ V_0 & \text{elsewhere} \end{cases}$$

$$\phi_E(x) = \begin{cases} A\cos(kx) + B\sin(kx) & -L < x < L \\ Ce^{\alpha x} + De^{-\alpha x} & x < -L \\ Fe^{\alpha x} + Ge^{-\alpha x} & x > L \end{cases}$$

where

$$k^2 = \frac{2m}{\hbar^2}E \ \text{ and } \ \alpha^2 = \frac{2m}{\hbar^2}(V_0 - E)$$

Normalizablility implies $D = 0$ and $F = 0$.
Symmetry implies $\mathbb{P}(x) = \mathbb{P}(-x)$, so either $A = 0$ or $B = 0$.

Which leaves us with

$$\phi_{even}(x) = \begin{cases} A\cos(kx) & -L < x < L \\ Ce^{\alpha x} & x < -L \\ Ce^{-\alpha x} & x > L \end{cases}$$

$$\phi_{odd}(x) = \begin{cases} B\sin(kx) & -L < x < L \\ Ce^{\alpha x} & x < -L \\ -Ce^{-\alpha x} & x > L \end{cases}$$

We'll work out the even solutions here, and leave the odd ones as an exercise for later.

Thus far we have lined up the known solutions and made sure that they can be physical, but we still need to impose the continuity requirements at $x = \pm L$.

Continuity of

$$\begin{aligned} \phi(x) &\Rightarrow A\cos(kL) = Ce^{-\alpha L} \\ \partial_x \phi(x) &\Rightarrow -kA\sin(kL) = -\alpha Ce^{-\alpha L} \\ &\Rightarrow k\tan(kL) = \alpha \end{aligned}$$

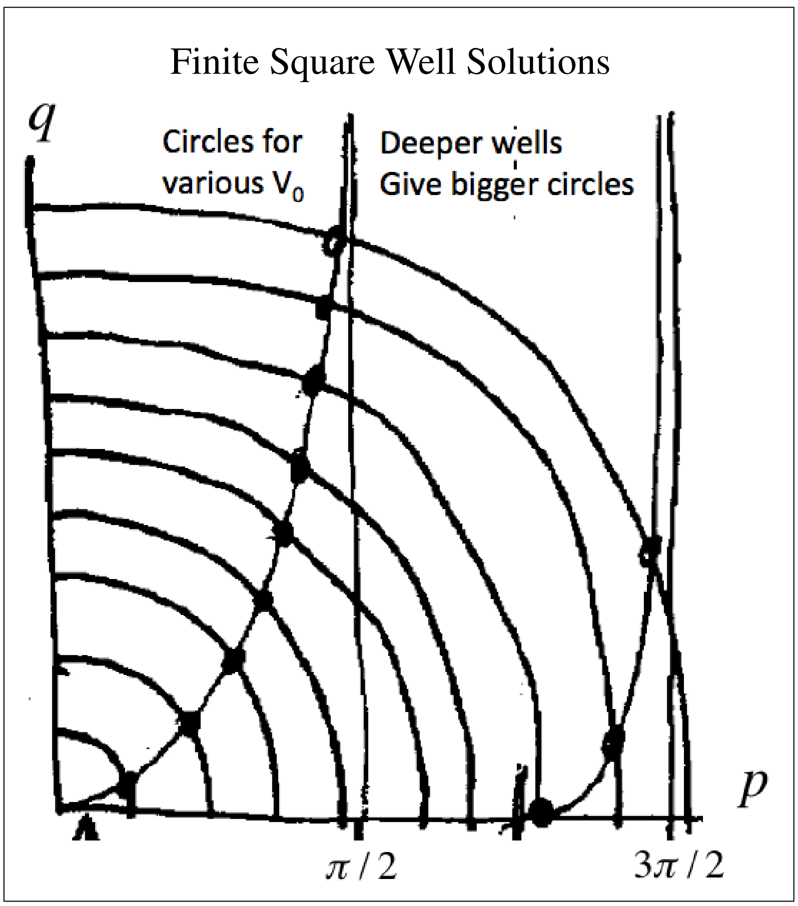
We know k and α in terms of E and V_0, so now all we have to do is solve to find the values of E which correspond to bound states.

But these are nasty transcendental equations, so solving them is not so easy.

Our approach to the solution will be to draw the left and right side of the equations vs. some dimensionless variables, and take the intersections as our solutions. We start by defining

Variables for graphical solution:

$$p = kL \quad \text{and} \quad q = \alpha L$$
$$\Rightarrow q = p \tan p \quad \text{and} \quad p^2 + q^2 = g_0^2$$
$$\text{where} \quad g_0^2 = L^2 \frac{2m}{\hbar^2} V_0$$
$$\text{since} \quad k^2 L^2 = L^2 \frac{2m}{\hbar^2} E \quad \text{and} \quad \alpha^2 L^2 = L^2 \frac{2m}{\hbar^2}(V_0 - E)$$

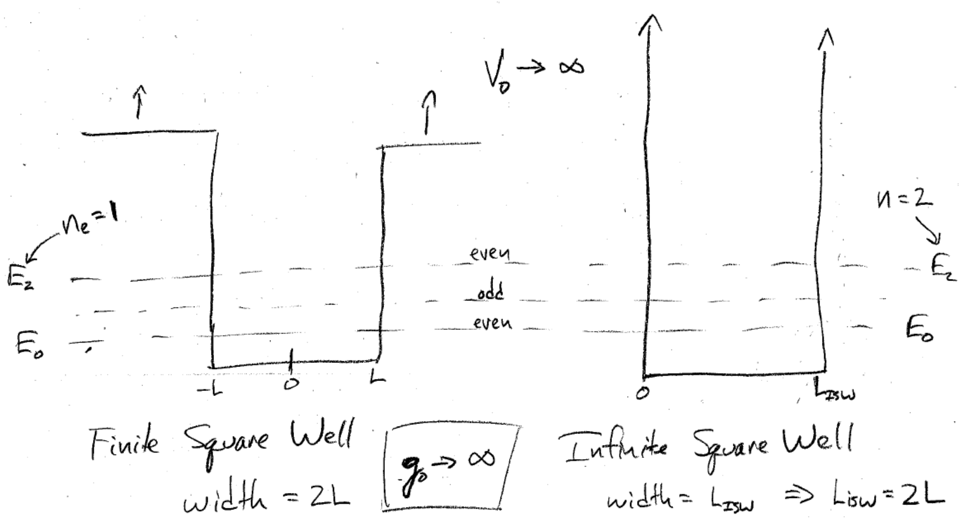


Because this is a transcendental equation, we can't really do better than that for a solution, and yet this already tells us a lot. For instance, there is always at least one bound state, and the number of bound states increases as

$$N_{bound} = \left\lceil \frac{g_0}{\pi} \right\rceil$$

We can also check these solutions agains the infinite square well by taking the limit as $V_0 \to \infty$. (Keep in mind that we have only found the *even* solutions here, so half of the solutions are missing.)

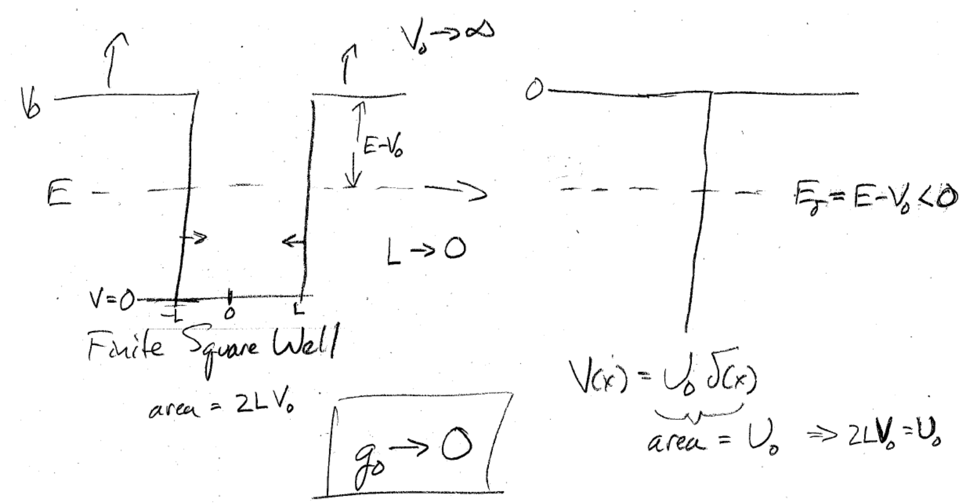
Finite vs. Infinite Well



$$\begin{aligned}
V_0 \to \infty \quad &\Rightarrow \quad g_0 \to \infty \\
\Rightarrow p_{n_e} \quad &= \quad \left(n_e + \tfrac{1}{2}\right)\pi \\
\Rightarrow L^2 \frac{2m}{\hbar^2} E_{n_e} \quad &= \quad \left(n_e + \tfrac{1}{2}\right)^2 \pi^2 \\
\Rightarrow E_{n_e} \quad &= \quad \frac{\hbar^2}{2mL^2}\left(n_e + \tfrac{1}{2}\right)^2 \pi^2 \\
\text{note} \quad & \quad\;\; n = 2n_e \;\; \text{and} \;\; L_{\text{ISW}} = 2L \\
\Rightarrow E_n \quad &= \quad \frac{\hbar^2 (n+1)^2 \pi^2}{2m(2L)^2} \qquad \text{Right!}
\end{aligned}$$

And finally, we can check against our delta function solution. Let's make the delta function with a very deep, very narrow well. (Here, recall that the energy in that exercise was measured down from the top of the well, not up from the bottom.)

Finite vs. Delta Well



$$
\begin{array}{rcl}
V_0 \to \infty & \text{and} & L \to 0 \\
\text{finite "area" of the well} & \Rightarrow & 2LV_0 = U_0 \\
\text{use } \; E_\delta = E - V_0 & \text{recall} & E_\delta < 0 \\
g_0^2 = L^2 \dfrac{2m}{\hbar^2} V_0 \to 0 & & \text{since } L^2 \text{ beats } V_0
\end{array}
$$

First, note that g_0 goes to zero, so the finite square well solution already tells us to expect just one bound state of the δ well.

$$
\begin{array}{rcl}
\text{Finite Square Well} & & \text{Delta Well} \\
k^2 = \dfrac{2m}{\hbar^2} E & \to & k^2 = \dfrac{2m}{\hbar^2}(V_0 + E_\delta) \\
\alpha^2 = -\dfrac{2m}{\hbar^2}(E - V_0) & \to & \alpha^2 = -\dfrac{2m}{\hbar^2} E_\delta \\
\alpha = k \tan(kL) & \to & \alpha = k^2 L \quad \text{(small angle approx)}
\end{array}
$$

Putting these equations together, we find the energy of the single bound state.

$$
\begin{aligned}
\alpha^2 = k^4 L^2 \quad &\Rightarrow \quad -\frac{2m}{\hbar^2} E_\delta = \left(\frac{2m}{\hbar^2} \left(V_0 + E_\delta \right) L \right)^2 \\
\text{since } V_0 \to \infty \text{ we can say} \quad & \quad V_0 + E_\delta \approx V_0 \\
-\frac{2m}{\hbar^2} E_\delta \quad &= \quad \left(\frac{2m}{\hbar^2} \right)^2 (LV_0)^2 \\
\text{recall from area match} \quad & \quad LV_0 = U_0/2 \\
\Rightarrow E_\delta \quad &= \quad -\frac{m}{2\hbar^2} U_0^2
\end{aligned}
$$

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6 Next Time

- Particle scattering
- Probability current
- The S-matrix and how you can know EVERYTHING