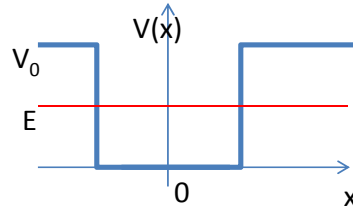


Recap



1. Ansatz

2. Boundary conditions at infinity

$$\Psi_E(x) = \begin{cases} A_+ e^{\kappa x} + A_- e^{-\kappa x} & x \leq -a \\ B_+ e^{ikx} + B_- e^{-ikx} & |x| < a \\ C_+ e^{\kappa x} + C_- e^{-\kappa x} & x \geq a \end{cases} \quad \begin{aligned} \kappa &= \frac{1}{\hbar} \sqrt{2m(V_0 - E)} \\ k &= \frac{1}{\hbar} \sqrt{2mE} \end{aligned}$$

3. Symmetry

symmetric solutions:

$$B_+ = B_- \quad A_+ = C_- \quad \rightarrow B_c := 2 B_+$$

$$\Psi_E(x) = \begin{cases} A_+ e^{\kappa x} & x \leq -a \\ B_c \cos kx & |x| < a \\ A_+ e^{-\kappa x} & x \geq a \end{cases}$$

anti-symmetric solutions:

$$\Psi_E(x) = \begin{cases} A_+ e^{\kappa x} & x \leq -a \\ B_s \sin kx & |x| < a \\ -A_+ e^{-\kappa x} & x \geq a \end{cases}$$

→ for now concentrate on symmetric solutions ...

Matching Conditions

symmetric solutions:

$$\Psi_E(x) = \begin{cases} A_+ e^{\kappa x} & x \leq -a \\ B_c \cos kx & |x| < a \\ A_+ e^{-\kappa x} & x \geq a \end{cases}$$

$$\begin{aligned} \kappa &\equiv \kappa(E) = \frac{1}{\hbar} \sqrt{2m(V_0 - E)} \\ k &\equiv k(E) = \frac{1}{\hbar} \sqrt{2mE} \end{aligned}$$

Continuity of $\Psi(x)$ and $d/dx \Psi(x)$:

$$\begin{aligned} \Psi : \quad A_+ e^{-\kappa a} &= B_c \cos(ka) \\ \frac{d}{dx} \Psi : \quad -\kappa A_+ e^{-\kappa a} &= -B_c k \sin(ka) \end{aligned}$$

$$\begin{pmatrix} e^{-\kappa a} & -\cos(ka) \\ -\kappa e^{-\kappa a} & k \sin(ka) \end{pmatrix} \begin{pmatrix} A_+ \\ B_c \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

Non-trivial solution if and only if conditions for Ψ and $d/dx \Psi$ linear dependent:

→ Condition for energy eigenstates:

$$\kappa = k \frac{\sin(ka)}{\cos(ka)}$$

$$\det \begin{pmatrix} e^{-\kappa(E)a} & -\cos(k(E)a) \\ -\kappa(E)e^{-\kappa(E)a} & k(E) \sin(k(E)a) \end{pmatrix} \stackrel{!}{=} 0$$

solutions $E \rightarrow E_n$:

$$\begin{aligned} \kappa_n &:= \frac{1}{\hbar} \sqrt{2m(V_0 - E_n)} \\ k_n &:= \frac{1}{\hbar} \sqrt{2mE_n} \end{aligned}$$

$$\Psi_{E_n}(x) = A_+ \begin{cases} e^{\kappa_n x} & x \leq -a \\ e^{-\kappa_n a} \frac{\cos k_n x}{\cos(k_n a)} & |x| < a \\ e^{-\kappa_n x} & x \geq a \end{cases}$$

$$\text{Normalization: } \int dx |\Psi_E(x)|^2 = 1 \quad \rightarrow \quad A_+ = \dots$$

7.2.8 Graphical solution of eigenenergy spectrum

Graphical Solutions

Condition for energy eigenstates:

$$\kappa = k \frac{\sin(ka)}{\cos(ka)}$$

(symmetric)

$$\kappa = -k \frac{\cos(ka)}{\sin(ka)}$$

(anti-symmetric)

$$\kappa \equiv \kappa(E) = \frac{1}{\hbar} \sqrt{2m(V_0 - E)}$$

$$k \equiv k(E) = \frac{1}{\hbar} \sqrt{2mE}$$

Define:

$$ka \rightarrow z := \sqrt{2mE} \frac{a}{\hbar}$$

$$z_0 := \sqrt{2mV_0} \frac{a}{\hbar}$$

(constant)

Then we can set

$$\kappa a \rightarrow \sqrt{z_0^2 - z^2}$$

$$\sqrt{z_0^2 - z^2} = z \tan z$$

(symmetric)

$$\sqrt{z_0^2 - z^2} = -z \cot z$$

(anti-symmetric)

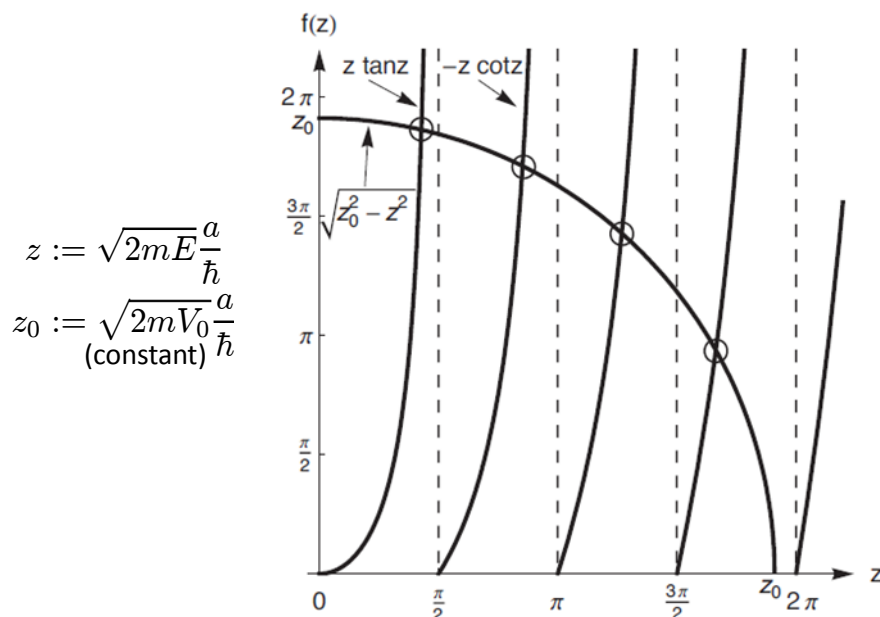


Figure 5.16 Graphical solution of the transcendental equations for the allowed energies of a finite square well ($z_0 = 6$).

Taken from McIntyre, Paradigm in Physics: Quantum Mechanics

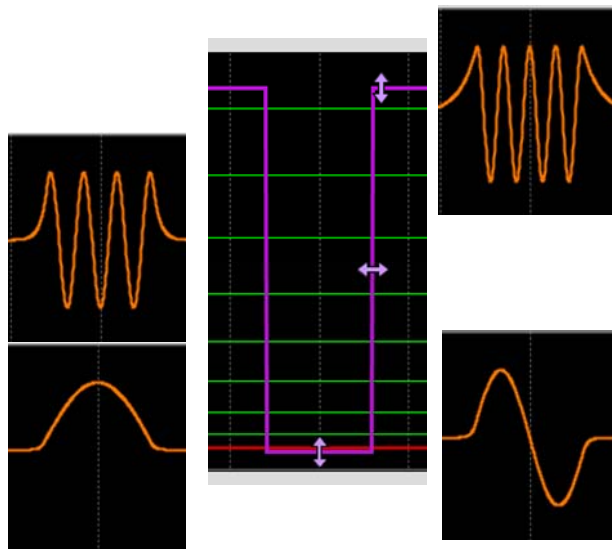
7.2.9 Discussion of eigenstates

There is at least one eigenstate, no matter which value z_0 takes, because the circle intersects at least with the first branch of $z \tan z$!!!

This includes the case of small potential depth ($V_0 \rightarrow 0$) or small width of the potential ($a \rightarrow 0$)

Note that the latter statement is not in contradiction with the uncertainty relation! One might wonder whether a narrow potential well would confine the particle in a small area, thus limiting the spread in position to a small value. Heisenberg's Uncertainty relations would then force the momentum spread to be large, leading to a large amount of kinetic energy related to the momentum spread. Wouldn't then the particle always have enough energy to escape the well? (meaning, there would be no bound states for narrow wells)

The math above tells us, that this is not happening, but why? The reason is that a narrow well does not confine the particle to be inside the well: the particle can leak into the wall, and the probability to find the particle in the wall becomes more substantial as one narrows the well! So the spread in position stays large enough, so that the momentum spread corresponds to kinetic energies well below the potential outside the well. Hence the particle is bound to the well.



- 1) There is always at least one bound eigenstate
- 2) The wave function 'leaks' into the wall!
- 3) The closer the eigenenergy to the height of potential wall, the more the wave function enters the wall

7.2.10. Additional material: Limit of infinite well

We expect to recover the analytical solution. And indeed, in that case we can recover from the graphics the solutions (intersection of circle and lines)

For $V \rightarrow 0$ we find $z_n = \frac{n\pi}{2}$ z_n : intersection

This corresponds again to the already derived energy levels

$$E_n = \frac{2\pi^2 \hbar^2}{a^2 m} n^2$$

moreover, we find that the wave function at $x = a/2$ satisfies

$n = 1, 3, 5$ symmetric

$$\cos ka = \cos \frac{n\pi}{2} = 0$$

similar

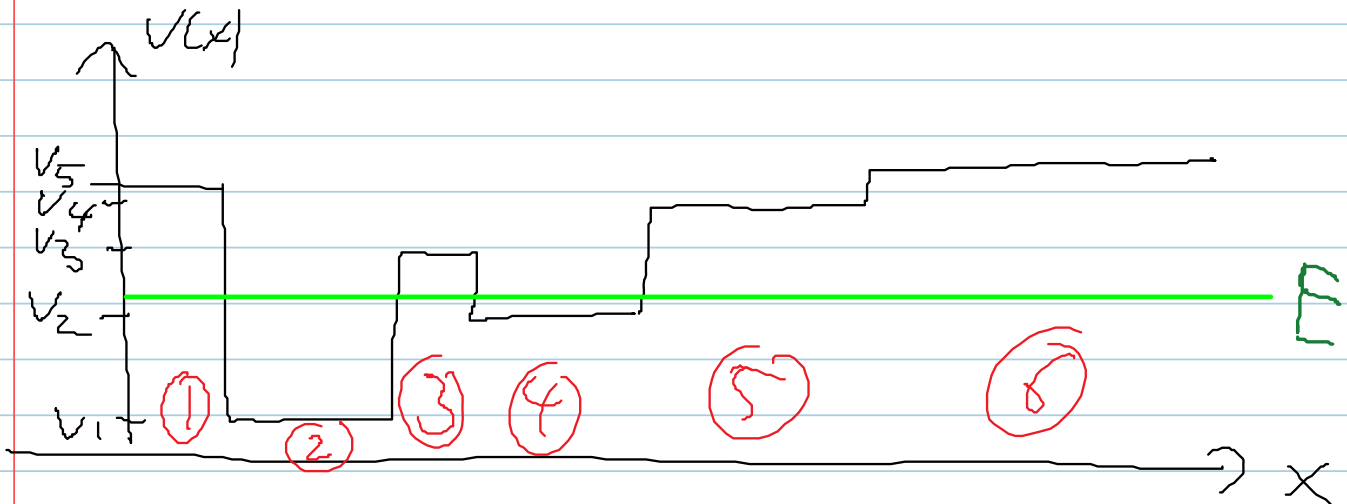
$n = 2, 4, 6 \dots$ anti-symmetric

$$\sin ka = \sin \frac{n\pi}{2} = 0$$

7.3 Bound states in Step potentials

7.3.1 Eyeball Solutions for step potential (See McIntyre 5.10.1)

You have now seen all tricks to solve step-wise potentials, at least as long as we look for eigenstates of energy E which satisfies



In principle, you have now all tools to find energy eigenstates of a Hamiltonian with a step-potential as drawn above.

1)

Whenever the energy of an eigenstate is above the potential, you get an oscillatory behaviour

$$A_+ e^{ikx} + A_- e^{-ikx}$$

with a wave number

$$k = \frac{1}{\hbar} \sqrt{2m(E - V_j)}$$

Whenever the energy is above the potential you get a superposition of exponential growth and decay

$$A_+ e^{\kappa x} + A_- e^{-\kappa x}$$

with length scale

$$\kappa = \frac{1}{\hbar} \sqrt{2m(V_j - E)}$$

2)

At $x \rightarrow \pm \infty$

the wave function has to decay exponentially

3) The wave function is continuous, as is its derivative (exception: infinite potential steps)

4) if the potential is symmetric around some coordinate, then all energy eigen functions are either symmetric or anti-symmetric with respect to that point.

7.3.2 Why do bound states show a discrete energy spectrum?

Consider a step-potential with N sections. We call an energy eigenstate a bound state if its energy is below the step potential for $x \rightarrow \pm \infty$

1) the mathematical ansatz introduces

$2N$ amplitudes

(2 for each section)

2) the requirement that there is no exponential growth as $x \rightarrow \pm \infty$ means that there will be

2 constraints (amplitudes set to zero)

3) at each interface, we have two linear constraints on the amplitudes coming from the continuity of the wave function and its derivative

$2(N-1)$ constraints

dependent

4) so we have $2N$ amplitudes and $2N$ constraints. This means in general, that the constraints have to be linear ~~independent~~ in order to get non-trivial solutions! (determinant condition)

As the constraints depend on the wave number and the decay/growth constant in each section, which are energy dependent, this determinant condition will impose constraints on the value of energy E where the determinant condition reveals linear dependency of constraints. \Rightarrow discrete energy spectrum!

5) once the constraints are linear ~~independent~~, we can eliminate amplitudes. for bound states, we are then left with one amplitude (one constraint was already contained in the other $2N-1$ ones), and then this amplitude is fixed by the normalization condition of the wave function.

dependent