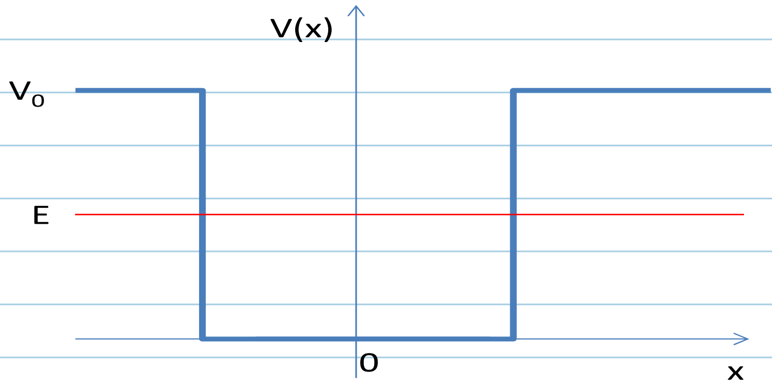
7.2 Finite depth potential well (bound states)



Region I Region II Region III

We are looking for now only for bound states, that is, $0 < E < V_0$

Preparation:

Solution to

$$\frac{\partial^2}{\partial x^2} f(x) = C f(x)$$

is given by $f(x) = A\, e^{\pm\sqrt{C}\, x}$

or more explicitly

exponential growth/damping

$$f(x) = \begin{cases} A_+ e^{\sqrt{C}\, x} + A_- e^{-\sqrt{C} x} & \text{for} \quad C \geq 0 \\ A_+ e^{i\sqrt{-C}\, x} + A_- e^{-i\sqrt{-C} x} & \text{for} \quad C < 0 \end{cases}$$

oscillation

7.2.1 Mathematical Ansatz

<u>**Regions I and III:**</u>

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_0\right)\psi_E(x) = E\,\psi_E(x)$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_E(x) = (E - V_0)\,\psi_E(x)$$

$$\boxed{\frac{d^2}{dx^2}\psi_E(x) = \underbrace{\frac{2m(V_0 - E)}{\hbar^2}}_{>0}\psi_E(x)}$$

Formal mathematical solutions in Regions I and III:

Region I:

$$\psi_E(x) = A_+ e^{\kappa x} + A_- e^{-\kappa x}$$

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

Region III:

$$\psi_E(x) = C_+ e^{\kappa x} + C_- e^{-\kappa x}$$

Region II:

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_E(x) = E\,\psi_E(x)$$

$$E > 0$$

$$\frac{d^2}{dx^2}\psi_E(x) = \underbrace{-\frac{2mE}{\hbar^2}}_{<0}\psi_E(x)$$

Formal solution in Region II

$$\psi_E(x) = B_+ e^{ikx} + B_- e^{-ikx}$$

alternative parametrization:

$$\psi_E(x) = B_c \cos kx + B_s \sin kx$$

$$k = \frac{\sqrt{2mE}}{\hbar}$$

overall:

$$\boxed{\psi_E(x) = \begin{cases} A_+ e^{\kappa x} + A_- e^{-\kappa x} & \text{I} \\ B_c \cos kx + B_s \sin kx & \text{II} \\ C_+ e^{\kappa x} + C_- e^{-\kappa x} & \text{III} \end{cases} \qquad \kappa = \frac{\sqrt{2m(V_0-E)}}{\hbar}\,;\quad k = \frac{\sqrt{2mE}}{\hbar}}$$

7.2.2 Condition that wave-function must be square-integrable

we cannot have exponential growth of wave function going to +/- infinity!

$$\Rightarrow \quad A_- = 0$$

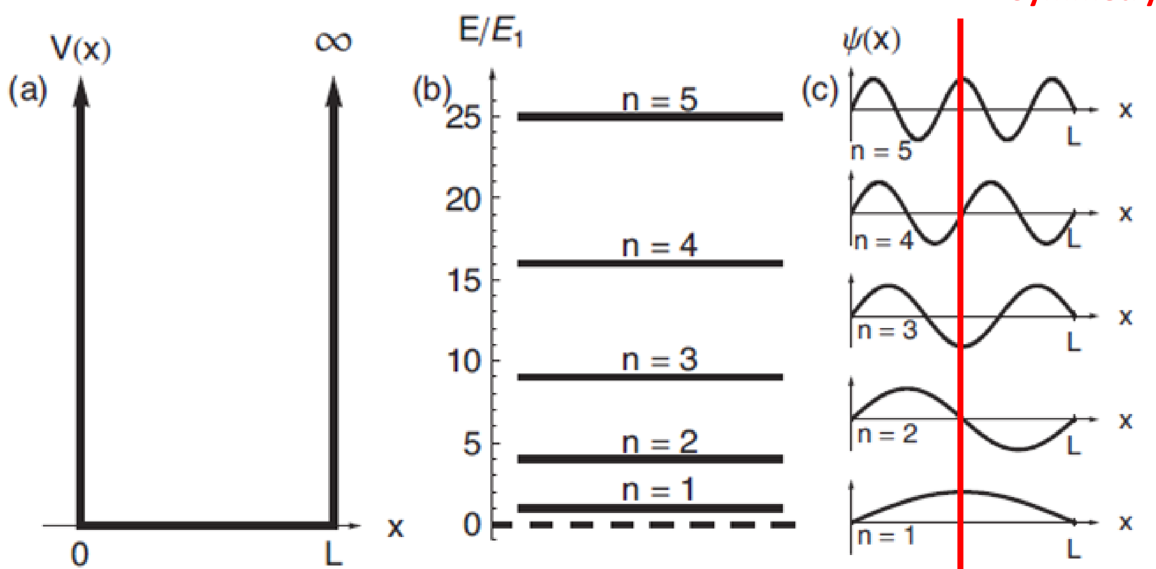
$$C_+ = 0$$

$$\boxed{\begin{aligned} \psi_E(x) &= \begin{cases} A_+ e^{\kappa x} & \text{I} \\ B_c \cos kx + B_s \sin kx & \text{II} \\ C_- e^{-\kappa x} & \text{III} \end{cases} \\ \kappa &= \frac{\sqrt{2m(V_0 - E)}}{\hbar} \; ; \quad k = \frac{\sqrt{2mE}}{\hbar} \end{aligned}}$$

7.2.3 General: Symmetry of Eigenfunctions (Parity operator)

Looking at the infinite potential well, we notice a symmetry of the eigenfunctions:

Symmetry



all functions are symmetric with respect to the middle of the well!

This could have been predicted:

Symmetry

Parity Operator:

$$\hat{\Pi}|x\rangle = |-x\rangle$$

If Parity Operator commutes with Hamilton operator:
➔ all eigenfunctions of H are either
➔ symmetric, or
➔ anti-symmetric

$$\hat{H}|\Psi\rangle \doteq \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\Psi_E(x)$$

$$\hat{\Pi}\;\hat{H}|\Psi\rangle \doteq \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(-x)\right)\Psi_E(-x)$$

$$\hat{H}\;\hat{\Pi}|\Psi\rangle \doteq \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\Psi_E(-x)$$

Parity Operator commutes with this Hamilton Operator whenever V(x) is symmetric!

(This statement depends on the choice of the coordinate system!)

Our finite potential well is symmetric with respect to the parity operator in the coordinate system that we used!
Therefore, all eigenfunctions are either symmetric or anti-symmetric, and we can seach for them separately.

7.2.4 Symmetry Simplifications

All energy eigenfunctions are either symmetric or anti-symmetric:

Symmetric solutions: $\psi(x) = \psi(-x)$

$B_s = 0$

$A_+ = C_-$

anti-symmetric solutions: $\psi(x) = -\psi(-x)$

$B_c = 0$

$A_+ = -C_-$

symmetric:

$$\psi_E(x) = \begin{cases} A_+ e^{\kappa x} & \text{I} \\ B_c \cos kx & \text{II} \\ A_+ e^{-\kappa x} & \text{III} \end{cases}$$

anti-symmetric

$$\psi_E(x) = \begin{cases} A_+ e^{\kappa x} & \text{I} \\ B_s \sin kx & \text{II} \\ (-A_+) e^{-\kappa x} & \text{III} \end{cases}$$

$$\kappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar} \quad ; \quad k = \frac{\sqrt{2m E}}{\hbar}$$

7.2.5 General: Matching conditions at interface

Math: Time independent Schrödinger Equation for particles in a potential are second-order differential equations

==> solutions of such Schrödinger Equation for particles in a potential
- are continuous functions, and also the
- first derivatives must be continuous

$\psi_E(x)$, $\frac{\partial}{\partial x}\psi_E(x)$ continuous

Exceptions:

at interfaces with infinite potential jumps, the first derivative can make (finite) jumps. (Check our solutions of the infinite well: they are continuous, but the first derivative makes jumps at the walls of the well!

7.2.6 Evaluation of Matching conditions

$\psi(x), \frac{\partial}{\partial x}\psi(x)$ continuous at $x = a$, $x = -a$

symmetry: it is sufficient to consider the condition either at $x=-a$ or at $x=a$!

symmetric solutions:

$$\psi\!: \quad A_+ e^{-\kappa a} = B_c \cos(ka) \qquad (\text{at } x = +a)$$

$$\tfrac{\partial}{\partial x}\psi\!: \quad -\kappa A_+ e^{-\kappa a} = -B_c k \sin(ka)$$

asymmetric solutions:

$$\psi\!: \quad -A_+ e^{-\kappa a} = B_s \sin(ka) \qquad (\text{at } x = +a)$$

$$\tfrac{\partial}{\partial x}\psi\!: \quad \kappa A_+ e^{-\kappa a} = k B_s \cos(ka)$$

In each situation (symmetric, anti-symmetric) both conditions need to be fulfilled simultaneously! That means, that the two equations need to become linear dependent in each case, as we would have otherwise only trivial solutions!!!
This will be possible only special values of the energy E (energy spectrum)

for these allowed energy values we will then be able to write down the solution of the wave function!

7.2.7 Eigenenergy spectrum

From the matching condition it follows:

$$\kappa = +k \frac{\sin ka}{\cos ka} \qquad (\text{symmetric})$$

$$\kappa = -k \frac{\cos ka}{\sin ka} \qquad (\text{anti-symmetric})$$

These are transcendental equations that cannot be solved analytically!
This situation is quite common in quantum mechanical problems. Only very special cases allow for a nice analytic formula. For this reason we started with the infinite potential!