PHOT 301: Quantum Photonics

LECTURE 05

Michaël Barbier, Fall semester (2024-2025)

SUMMARY

So far we looked at bound states

- Infinite well
- Linear potential well (Electrical field, not seen yet)
- Harmonic oscillator

Different well potentials lead to different allowed energy levels

Narrower wells $\longrightarrow$ less energy levels (more spread)

FREE PARTICLES

FREE PARTICLE: PROPAGATING WAVES

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x), \qquad \text{as } V(x) = 0$$

$$\Rightarrow \qquad \frac{d^2\psi(x)}{dx^2} = -k^2\psi(x), \qquad \text{with } k = \frac{\sqrt{2mE}}{\hbar}$$

- Solutions are unconstrained: all energy values
- Similar to a very wide well (with infinite walls)

$$\psi(x) = Ae^{ikx} + Be^{-ikx}$$

FREE PARTICLE SOLUTIONS

$$\psi(x) = Ae^{ikx} + Be^{-ikx}$$

- Problem 1: Not normalizable
- Problem 2: Velocity is half of classical velocity

PROBLEM 1: NOT NORMALIZABLE

$$\psi(x) = Ae^{ikx} + Be^{-ikx}$$

$$\begin{aligned}
|\psi(x)|^2 &= \psi(x)^* \, \psi(x) \\
&= (A^* e^{-ikx} + B^* e^{ikx})(Ae^{ikx} + Be^{-ikx}) \\
&= |A|^2 + |B|^2 + (AB^* e^{i2kx} + A^* Be^{-i2kx}) \\
&= |A|^2 + |B|^2 + \Re\left(AB^* e^{i2kx}\right)
\end{aligned}$$

$$\Rightarrow \int_{-\infty}^{+\infty} |\psi(x)|^2 dx = (|A|^2 + |B|^2)\,\infty + \int_{-\infty}^{+\infty} \Re\left(AB^* e^{i2kx}\right) dx$$

The last integral is bounded (oscillating between finite values)

The total integral $\int |\psi|^2 dx \longrightarrow +\infty$, and therefore doesn't exist.

PROBLEM 2: VELOCITY TOO SLOW

We can rewrite $\Psi(x,t) = \psi(x)e^{-iEt/\hbar}$ with $E = \frac{\hbar^2 k^2}{2m}$:

$$\begin{aligned}\Psi(x,t) &= Ae^{ikx - iEt/\hbar} + Be^{-ikx - iEt/\hbar} \\ &= Ae^{ikx - iEt/\hbar} + Be^{-ikx - iEt/\hbar} \\ &= Ae^{ik(x - \frac{\hbar k}{2m}t)} + Be^{-ik(x - \frac{\hbar k}{2m}t)}\end{aligned}$$

- This is a function of $x \pm vt$, a "wave" moving with velocity v
- The velocity is $v_{\text{quantum}} = \frac{\hbar k}{2m} = \sqrt{\frac{E}{2m}}$
- Classically the velocity $v_{\text{classical}} = \sqrt{\frac{2E}{m}}$ because $E = \frac{1}{2}mv^2$
- The classical velocity is twice the one according to quantum mechanics!

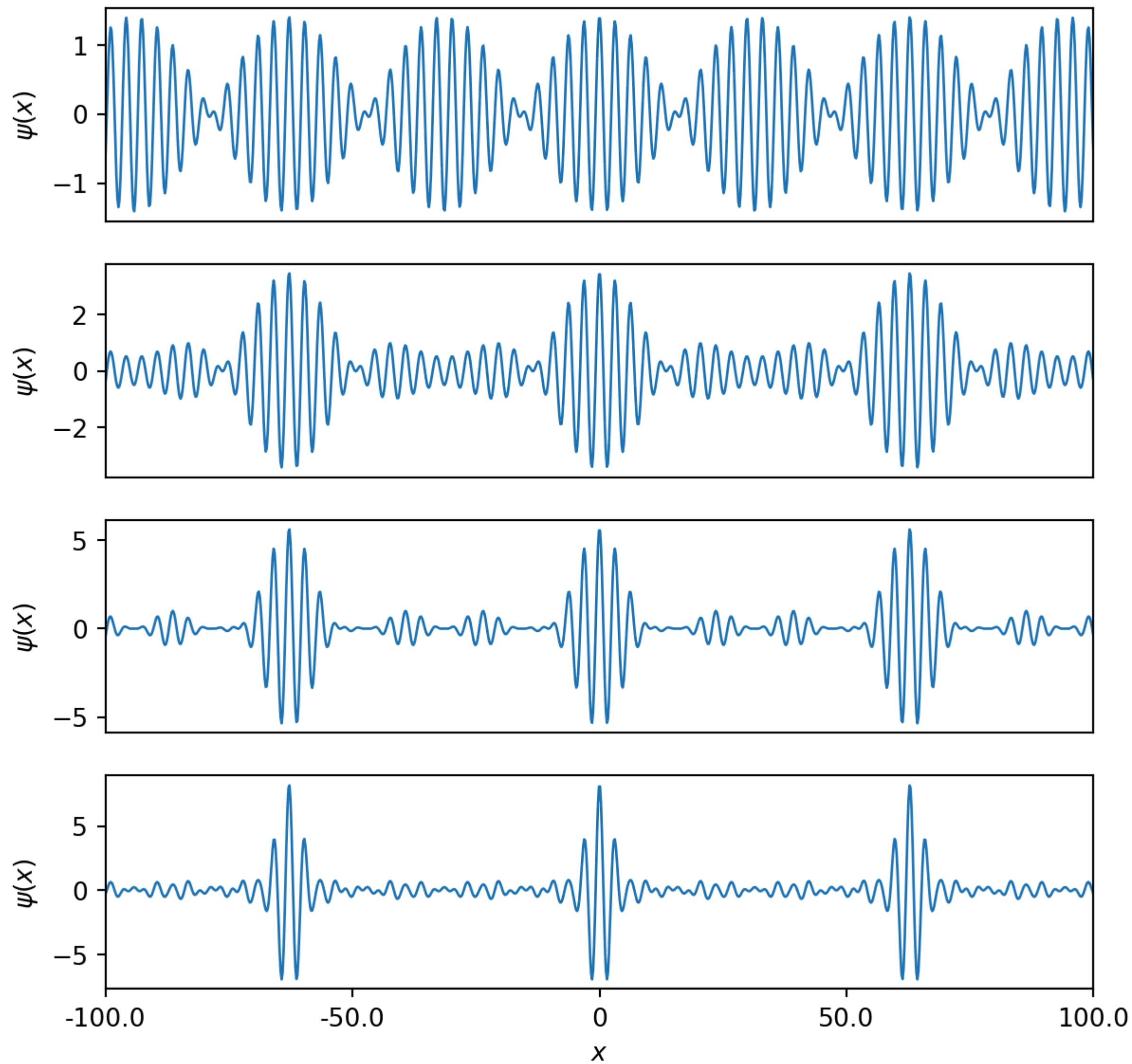
WAVE PACKET

- Superposition of propagating waves is normalizable
- Solves the velocity problem as well!
- Is consistent with uncertainty principle
- Fourier's trick to find coefficients

WAVE PACKET

- Superposition of waves
- Momentum around main $\sum_{n=-N}^{N} k_0 \pm n\delta k$
- Plots from top to bottom $N = 1, 2, 4, 8$

$$\psi(x) = \sum_{n=-N}^{N} e^{i(k_0+n\delta k)x}$$



WAVE PACKET

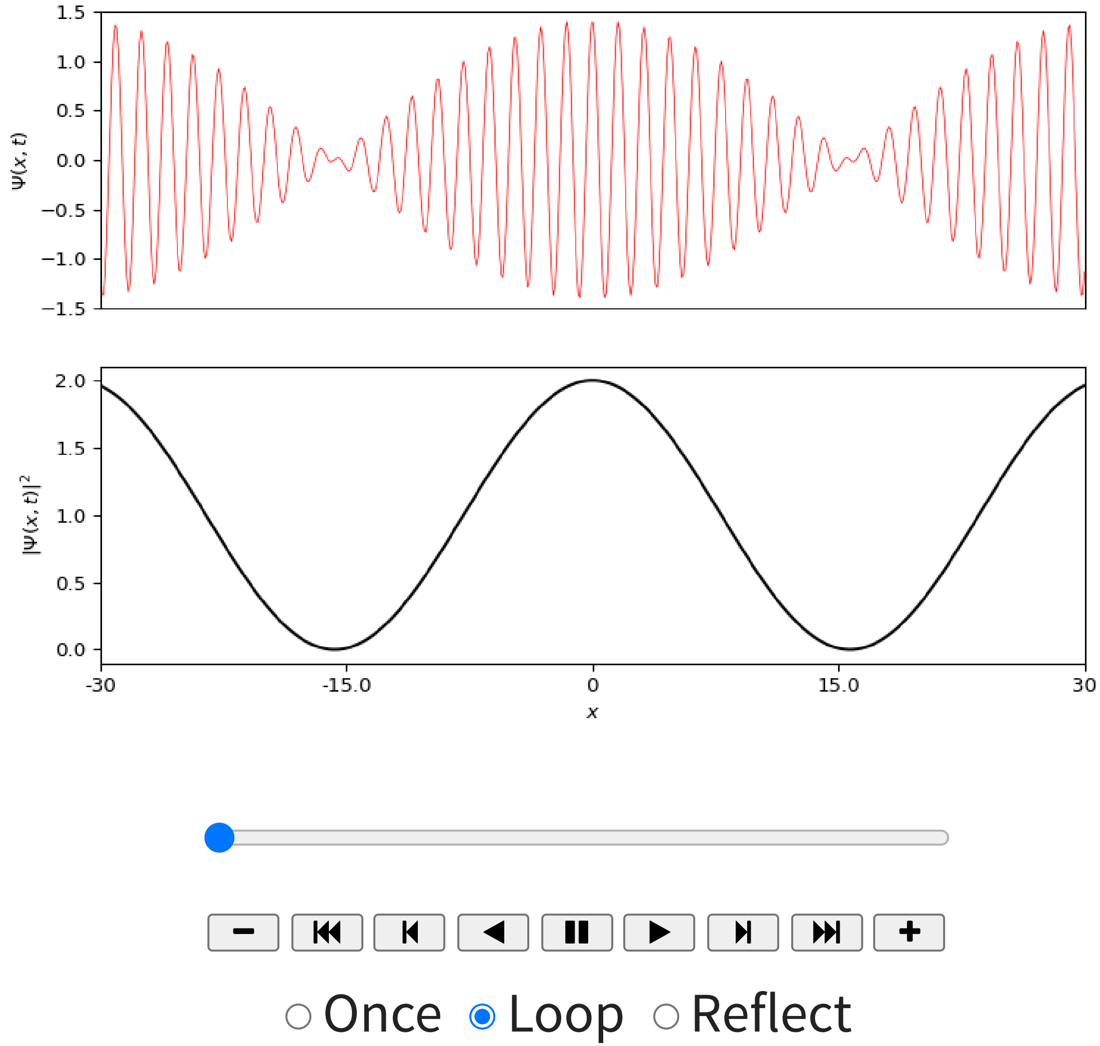
Phase velocity v

$$v = \frac{\omega}{k}$$

Group velocity:

$$v_g = \frac{d\omega}{dk}$$

$$\Psi(x,t) = \sum_{n=-N}^{N} e^{i(k_0 + n\delta k)x}$$



PHASE AND GROUP VELOCITY

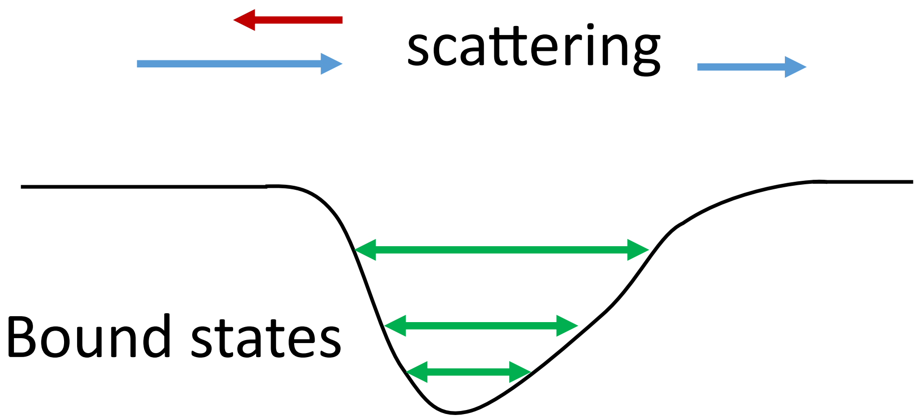
$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int \phi(k) e^{i(kx-\omega t)}$$

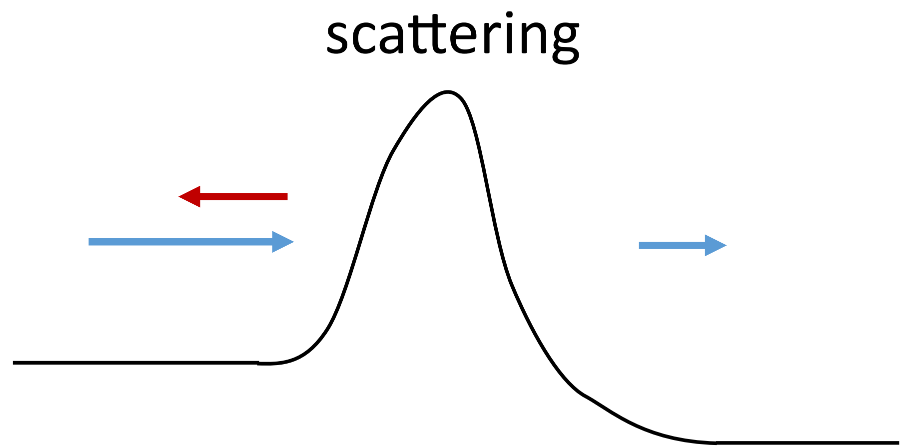
Assume $\phi(k)$ around k_0

$$\begin{aligned}\Psi(x,t) &\approx \frac{1}{\sqrt{2\pi}} \int \phi(k_0+s) e^{i((k_0+s)x-(\omega_0+s\omega_0')t)} \\ &\approx \frac{1}{\sqrt{2\pi}} e^{i(k_0 x-\omega_0 t)} \int \phi(k_0+s) e^{is(x-\omega_0' t)}\end{aligned}$$

BOUND STATES AND SCATTERING

BOUND STATES AND FREE PARTICLES

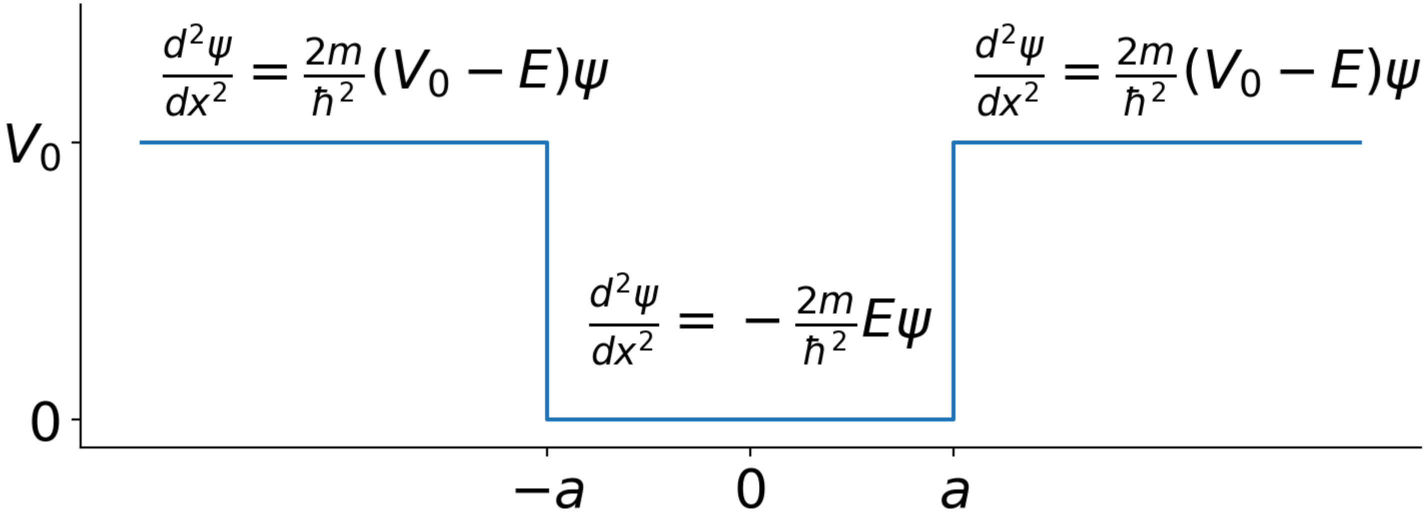




- Bound states have a bounded domain
- Particle is stuck in a potential valley
- Free particles can go everywhere
- **Scattering** of particles with $E > V_{\text{max}}$
- **Tunneling** of particles with $E < V_{\text{max}}$

FINITE POTENTIAL BARRIERS/STEPS/WELLS

FINITE SQUARE WELL

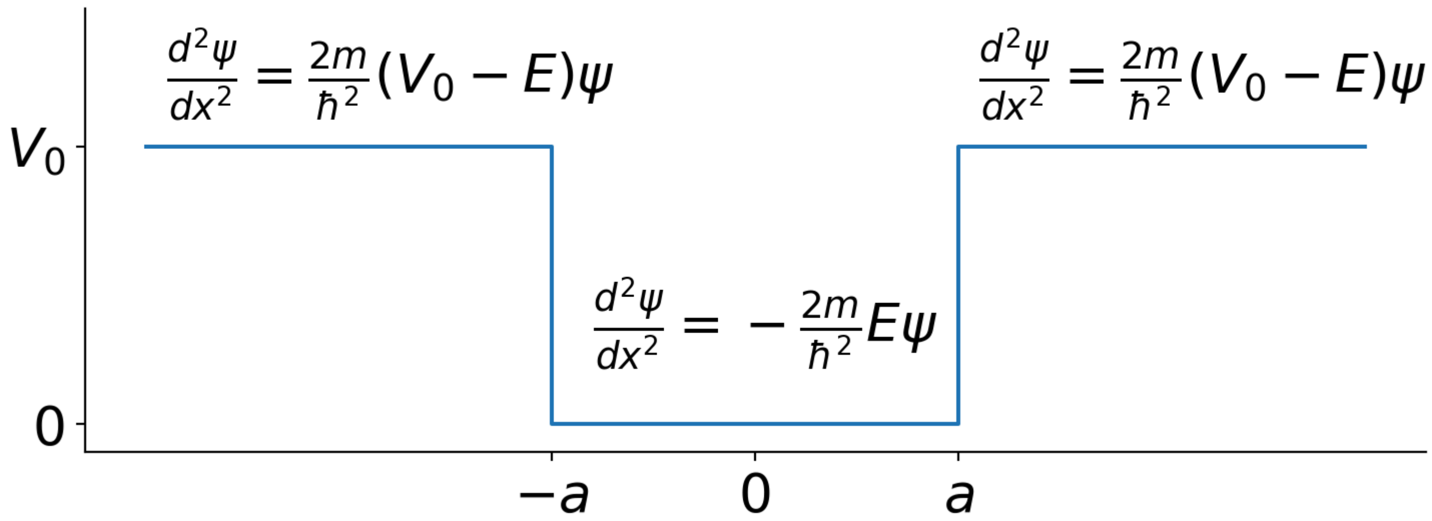


- Finite square potential well
- Bound states $0 < E < V_0$
- Scattering states $E > V_0$

Schrodinger equation:

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

FINITE WELL: BOUND STATES

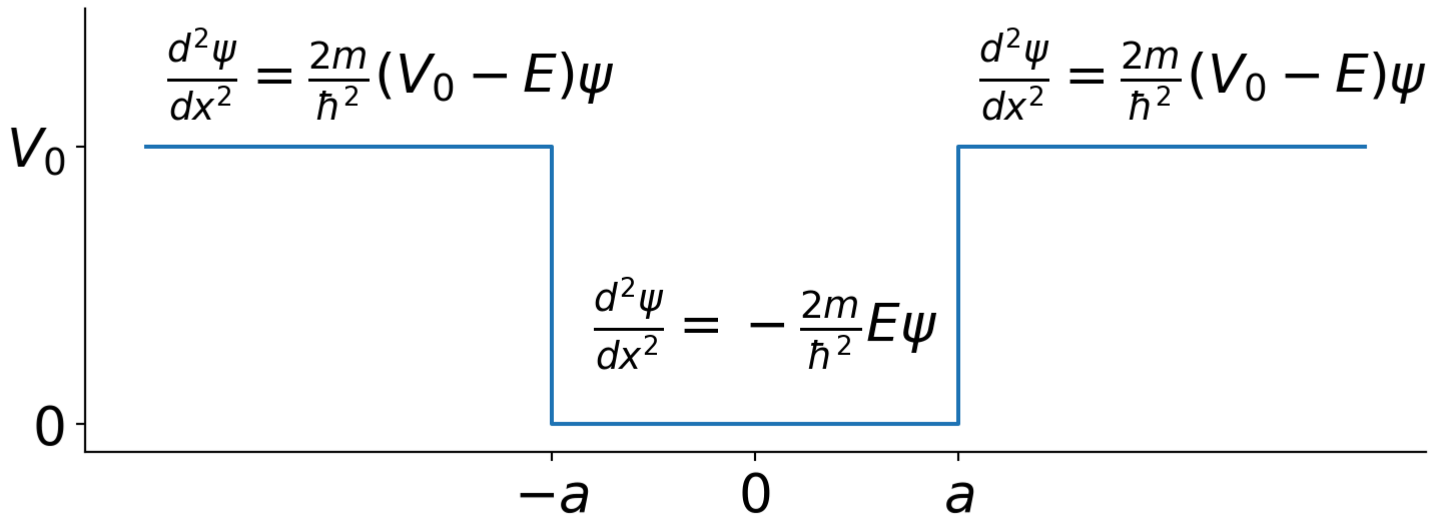


For **bound states** $0 < E < V_0$

$$\text{inside:} \quad \psi(-a < x < a) = C\sin(\lambda x) + D\cos(\lambda x) \qquad \lambda = \frac{\sqrt{2mE}}{\hbar}$$

$$\text{outside:} \quad \begin{aligned} \psi(x < -a) &= Ae^{-\kappa x} + Be^{\kappa x} = Be^{\kappa x} \\ \psi(x > a) &= Fe^{-\kappa x} + Ge^{\kappa x} = Fe^{-\kappa x} \end{aligned} \qquad \kappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

FINITE WELL: BOUND STATES



Since $\psi(x)$ is continuous in $x = -a$ and $x = a$:

$$\begin{aligned} Be^{-\kappa a} &= -C\sin(\lambda a) + D\cos(\lambda a) \\ Fe^{-\kappa a} &= C\sin(\lambda a) + D\cos(\lambda a) \end{aligned}$$

$\psi(x)$ continuous in $x = -a, a$

$$\begin{aligned} B\kappa e^{-\kappa a} &= \lambda C\cos(\lambda a) + D\sin(\lambda a) \\ -F\kappa e^{-\kappa a} &= \lambda C\cos(\lambda a) - \lambda D\sin(\lambda a) \end{aligned}$$

$\frac{d\psi(x)}{dx}$ continuous in $x = -a, a$

FINITE WELL: BOUND STATES

$$\begin{aligned} Be^{-\kappa a} &= -C\sin(\lambda a) + D\cos(\lambda a) \\ Fe^{-\kappa a} &= C\sin(\lambda a) + D\cos(\lambda a) \end{aligned}$$

$\psi(x)$ continuous in $x = -a, a$

$$\begin{aligned} B\kappa e^{-\kappa a} &= \lambda C\cos(\lambda a) + \lambda D\sin(\lambda a) \\ -F\kappa e^{-\kappa a} &= \lambda C\cos(\lambda a) - \lambda D\sin(\lambda a) \end{aligned}$$

$\dfrac{d\psi(x)}{dx}$ continuous in $x = -a, a$

Add the first two equations and subtract the others:

$$\begin{aligned} (B+F)e^{-\kappa a} &= 2D\cos\lambda a \\ (B+F)\frac{\kappa}{\lambda}e^{-\kappa a} &= 2D\sin\lambda a \end{aligned}$$

And divide them $\Leftrightarrow B \neq -F$

$$\frac{\kappa}{\lambda} = \tan\lambda a$$

FINITE WELL: BOUND STATES

$$\begin{aligned} Be^{-\kappa a} &= -C\sin(\lambda a) + D\cos(\lambda a) \\ Fe^{-\kappa a} &= C\sin(\lambda a) + D\cos(\lambda a) \end{aligned}$$

$\psi(x)$ continuous in $x = -a, a$

$$\begin{aligned} B\kappa e^{-\kappa a} &= \lambda C\cos(\lambda a) + \lambda D\sin(\lambda a) \\ -F\kappa e^{-\kappa a} &= \lambda C\cos(\lambda a) - \lambda D\sin(\lambda a) \end{aligned}$$

$\frac{d\psi(x)}{dx}$ continuous in $x = -a, a$

Now subtract the first two equations and add the others:

$$\begin{aligned} (B-F)e^{-\kappa a} &= -2C\sin\lambda a \\ (B-F)\frac{\kappa}{\lambda}e^{-\kappa a} &= 2C\cos\lambda a \end{aligned}$$

And divide them $\Leftrightarrow B \neq F$

$$\begin{aligned} \frac{\kappa}{\lambda} &= -\cot\lambda a \qquad \text{if } B \neq F \\ \frac{\kappa}{\lambda} &= \tan\lambda a \qquad \text{if } B \neq -F \text{ from before} \end{aligned}$$

FINITE WELL: BOUND STATES

$$\frac{\kappa}{\lambda} = -\cot \lambda a \qquad \text{if } B \neq F$$
$$\frac{\kappa}{\lambda} = \tan \lambda a \qquad \text{if } B \neq -F \text{ from before}$$

- The relations are inconsistent!
- Only possible if one of them is invalid: $B = F$ or $B = -F$

$$B = F \quad \Rightarrow \quad \begin{aligned} (B-F)e^{-\kappa a} &= -2C \sin \lambda a \\ (B-F)\frac{\kappa}{\lambda}e^{-\kappa a} &= 2C \cos \lambda a \end{aligned} \quad \Rightarrow C = 0, \psi(x) = D\cos(\lambda x)$$

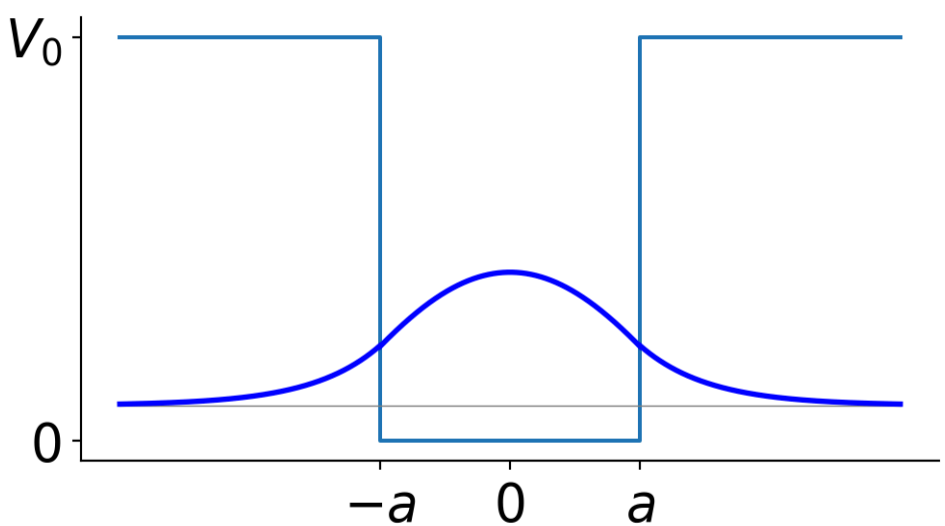
$$B = -F \quad \Rightarrow \quad \begin{aligned} (B+F)e^{-\kappa a} &= 2D \cos \lambda a \\ (B+F)\frac{\kappa}{\lambda}e^{-\kappa a} &= 2D \sin \lambda a \end{aligned} \quad \Rightarrow D = 0, \psi(x) = C\sin(\lambda x)$$

FINITE WELL: BOUND STATES (WAVE FUNCTION)

Symmetric solutions

$$\begin{cases} \psi(x < -a) = Be^{\kappa x} \\ \psi(-a < x < a) = D\cos(\lambda x) \\ \psi(x > a) = Be^{-\kappa x} \end{cases}$$

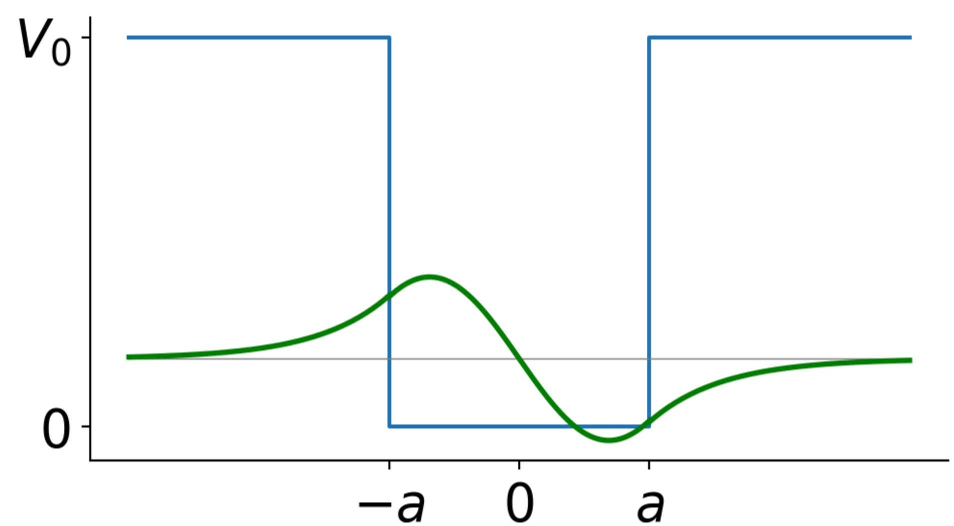
with $F = B \quad \& \quad \kappa = \lambda \tan \lambda a$



Asymmetric solutions

$$\begin{cases} \psi(x < -a) = Be^{\kappa x} \\ \psi(-a < x < a) = C\sin(\lambda x) \\ \psi(x > a) = -Be^{-\kappa x} \end{cases}$$

with $F = -B \quad \& \quad \kappa = -\lambda \cot \lambda a$



FINITE WELL: BOUND STATES

Symmetric solutions

$$\begin{cases} \psi(x < -a) = Be^{\kappa x} \\ \psi(-a < x < a) = D\cos(\lambda x) \\ \psi(x > a) = Be^{-\kappa x} \end{cases}$$

with $F = B \quad \& \quad \kappa = \lambda \tan \lambda a$

Asymmetric solutions

$$\begin{cases} \psi(x < -a) = Be^{\kappa x} \\ \psi(-a < x < a) = C\sin(\lambda x) \\ \psi(x > a) = -Be^{-\kappa x} \end{cases}$$

with $F = -B \quad \& \quad \kappa = -\lambda \cot \lambda a$

Let's first obtain the energy from κ and λ:

$$\kappa^2 = \frac{2m}{\hbar^2}(V_0 - E), \qquad \lambda^2 = \frac{2m}{\hbar^2}(E)$$

Define $z = \lambda\, a$ and $z_0 = a\, \frac{\sqrt{2mV_0}}{\hbar}$

$$\implies \quad \kappa^2 + \lambda^2 = \frac{2m}{\hbar^2}(V_0) = z_0^2/a^2 \quad \implies \quad \kappa^2 a^2 = z_0^2 - z^2$$

FINITE WELL: BOUND STATES

Symmetric solutions

$$\begin{cases} \psi(x < -a) = Be^{\kappa x} \\ \psi(-a < x < a) = D\cos(\lambda x) \\ \psi(x > a) = Be^{-\kappa x} \end{cases}$$

with $F = B \quad \& \quad \kappa = \lambda \tan \lambda a$

$$\implies \tan z = \sqrt{\frac{z_0^2}{z^2} - 1}$$

Asymmetric solutions

$$\begin{cases} \psi(x < -a) = Be^{\kappa x} \\ \psi(-a < x < a) = C\sin(\lambda x) \\ \psi(x > a) = -Be^{-\kappa x} \end{cases}$$

with $F = -B \quad \& \quad \kappa = -\lambda \cot \lambda a$

$$\implies -\cot z = \sqrt{\frac{z_0^2}{z^2} - 1}$$

where we made use of:

$$\kappa^2 a^2 = z_0^2 - z^2 \implies \kappa/\lambda = \sqrt{z_0^2/z^2 - 1}$$

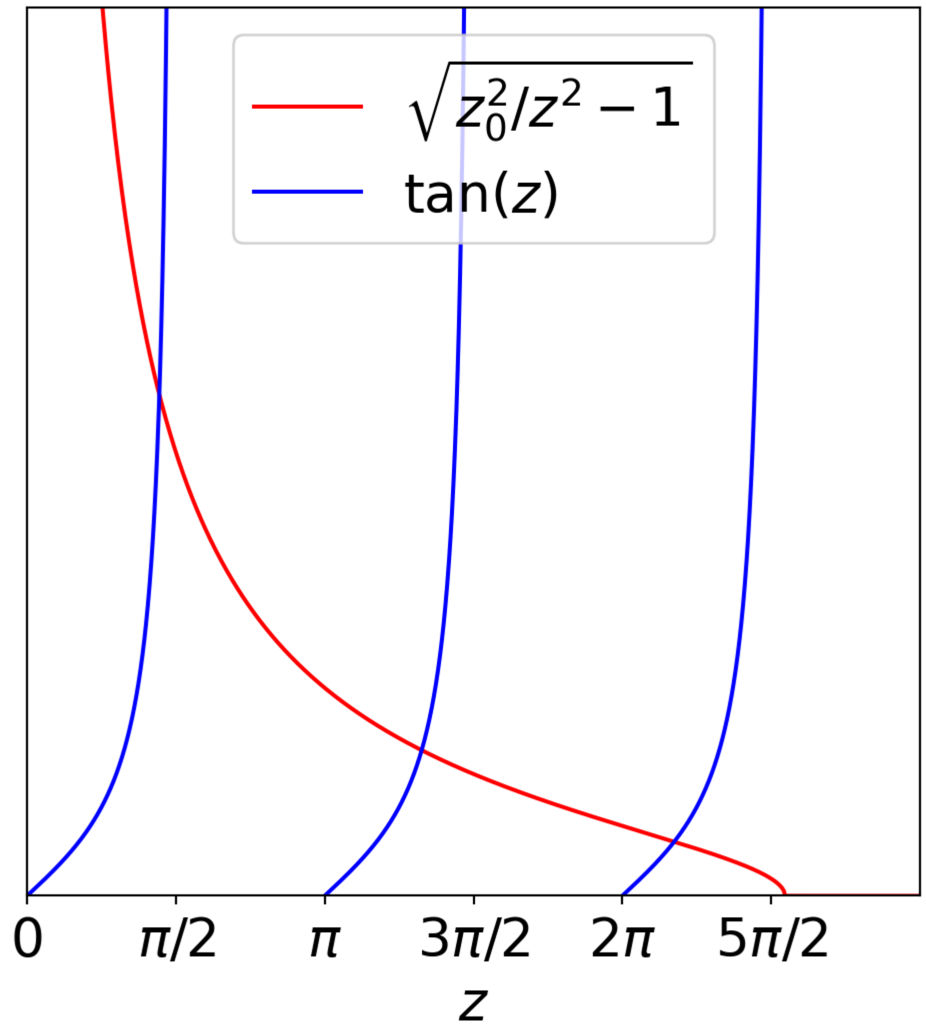
FINITE WELL: E FOR SYMMETRIC BOUND STATES

Symmetric solutions

$$\begin{cases} \psi(x < -a) = Be^{\kappa x} \\ \psi(-a < x < a) = D\cos(\lambda x) \\ \psi(x > a) = Be^{-\kappa x} \end{cases}$$

with $F = B \quad \& \quad \kappa = \lambda \tan \lambda a$

$$\implies \tan z = \sqrt{\frac{z_0^2}{z^2} - 1}$$



FINITE WELL: E FOR ASYMMETRIC BOUND STATES

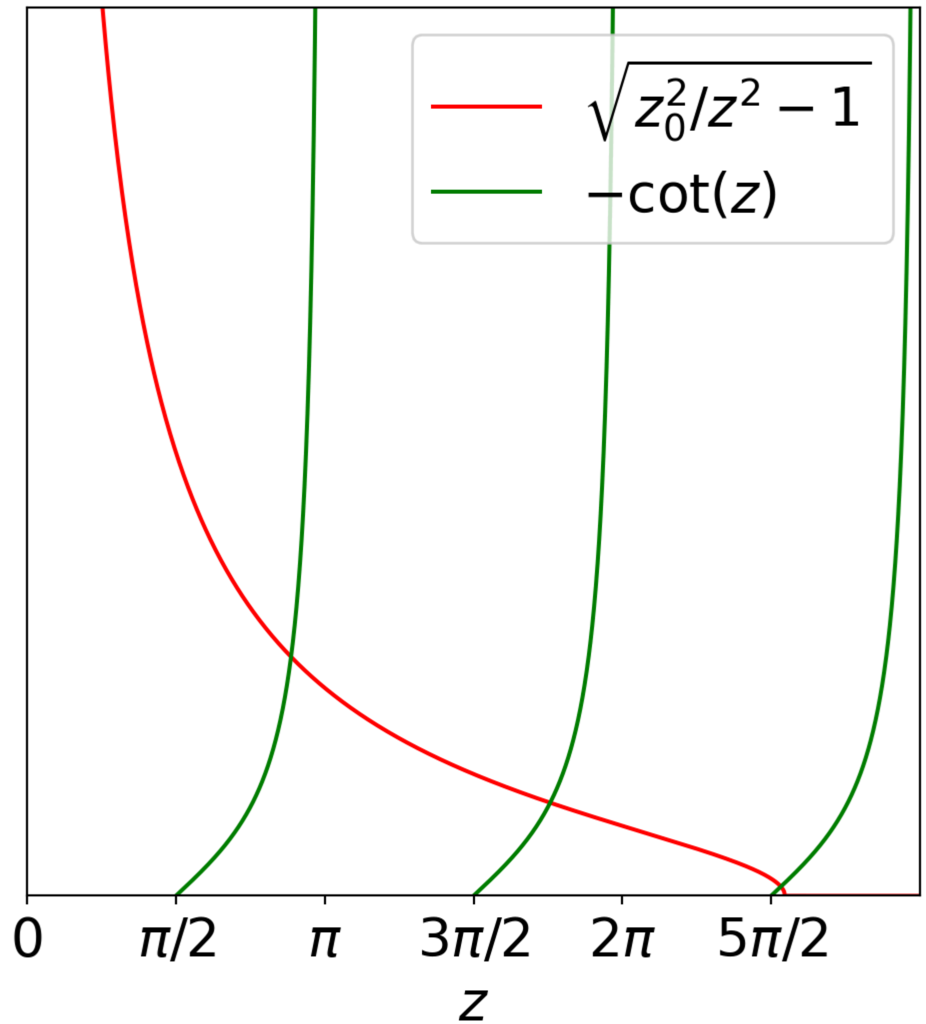
Asymmetric solutions

$$\begin{cases} \psi(x < -a) = Be^{\kappa x} \\ \psi(-a < x < a) = C\sin(\lambda x) \\ \psi(x > a) = -Be^{-\kappa x} \end{cases}$$

with $F = -B \quad \& \quad \kappa = -\lambda \cot \lambda a$

$$\implies -\cot z = \sqrt{\frac{z_0^2}{z^2} - 1}$$

Asymmetric energies approximately "shifted" to the right

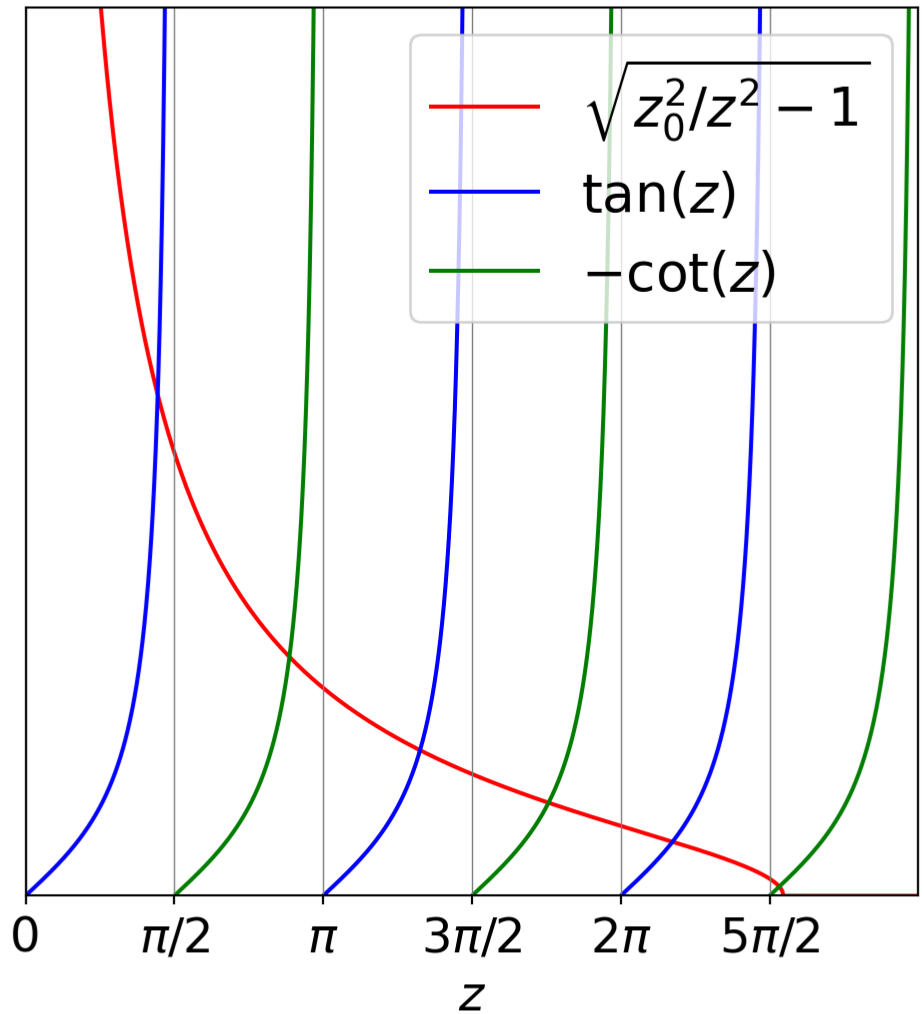


FINITE WELL: GRAPHICAL ENERGY-LEVELS

- Symmetric and asymmetric solutions
- Energy levels at intersections of red curve with blue/green curves.
- Energies close to infinite well energies (vertical asymptotes):

$$E_n = \frac{\hbar^2 z^2}{2ma^2} \lessapprox E_n^\infty = \frac{\hbar^2}{2m}\frac{n^2\pi^2}{(2a)^2}$$

- z_0 is intersection of red curve with x-axis
- Increasing $z_0 \implies$ more energy-levels
- Decreasing $z_0 \implies$ less energy-levels
- $z_0 = \frac{\sqrt{2mV_0}}{\hbar} a \propto \sqrt{V_0}\, a$



FINITE WELL: NUMERICAL SOLUTIONS

Numerically solving for z:

$$\tan z = \sqrt{z_0^2/z^2 - 1},$$
$$-\cot z = \sqrt{z_0^2/z^2 - 1}$$

Gives us:

- Energy levels $E_n = \frac{\hbar^2\lambda^2}{2m} = \frac{\hbar^2 z^2}{2ma^2}$
- Values for C or D as function of B:

$$B = D\cos(\lambda a)e^{\kappa a}$$
$$B = -C\sin(\lambda a)e^{\kappa a}$$

- Normalization $\longrightarrow$ final unknown B