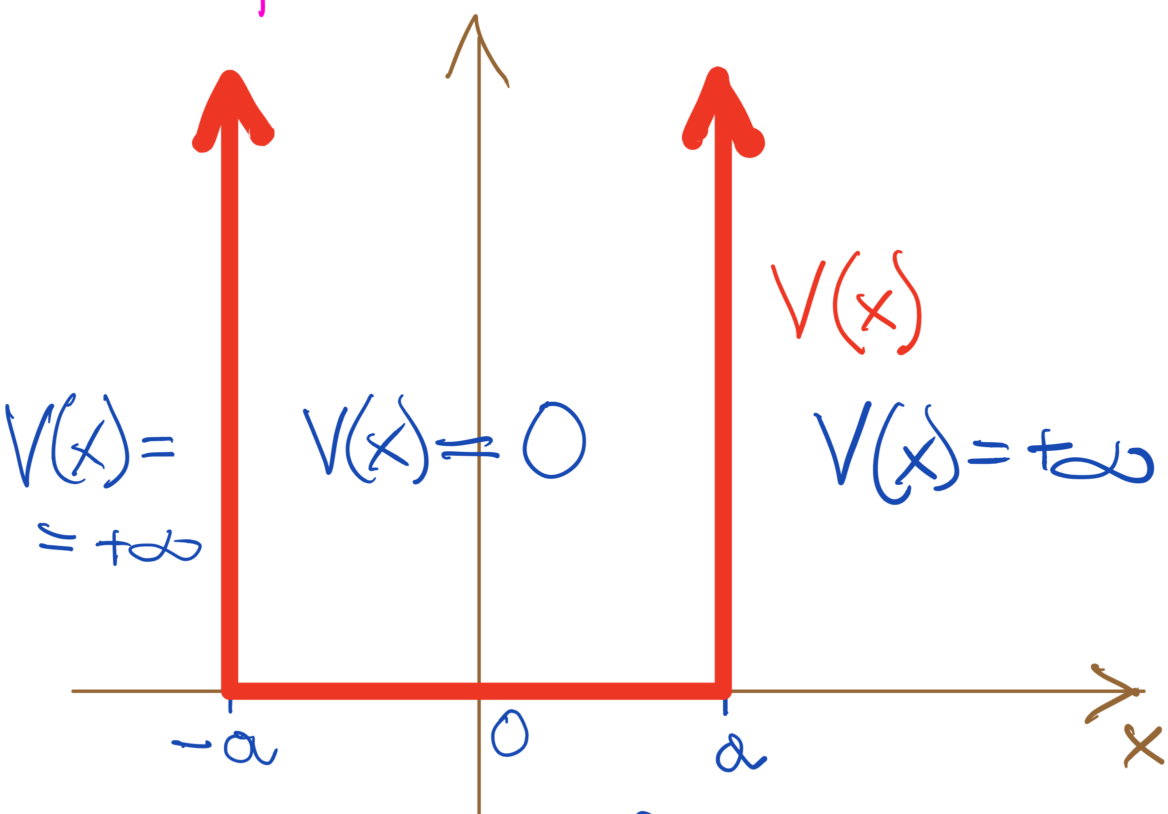
One-dimensional square-well potential



$$V(x) = \begin{cases} 0 & |x| < a \\ +\infty & |x| \geq a \end{cases}$$

1. $u(x) = 0$ for $|x| \geq a$.
2. No scattering states.
3. Infinite number of discrete energy levels, $E_n > V_{min} = 0$

$$Hu = Eu, \quad |x| < a$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}u = Eu$$

$$u(x) = A\sin\alpha x + B\cos\alpha x$$

$$\alpha = \sqrt{\frac{2mE}{\hbar^2}}$$ ✓

Boundary conditions at $x = \pm a$:

$$0 = u(a) = A\sin\alpha a + B\cos\alpha a \quad (1)$$

$$0 = u(-a) = -A\sin\alpha a + B\cos\alpha a \quad (2)$$

$(1)-(2)$: $\quad A\sin\alpha a = 0$

$(1)+(2)$: $\quad B\cos\alpha a = 0$

- $A = B = 0$

  $u(x) = 0 \quad \forall x \rightarrow$ not a solution

- $A, B \neq 0$

$$\left.\begin{aligned} \sin\alpha a &= 0 \\ \cos\alpha a &= 0 \end{aligned}\right\} \text{not possible}$$

We are left with

- $A = 0,\ B \neq 0$ or $A \neq 0,\ B = 0$

- $A = 0,\ B \neq 0$

$$\cos \alpha a = 0$$

✓ $$\alpha a = n\frac{\pi}{2}, \quad n = \overset{+}{\cancel{\pm}}1, \overset{+}{\cancel{\pm}}3, \overset{+}{\cancel{\pm}}5, \dots$$

$$u_n(x) = B \cos \frac{n\pi}{2a} x, \quad |x| \leq a$$

- $A \neq 0,\ B = 0$

$$\sin \alpha a = 0$$

✓ $$\alpha a = n\frac{\pi}{2}, \quad n = \cancel{0}, \overset{+}{\cancel{\pm}}2, \overset{+}{\cancel{\pm}}4, \dots$$

$$u_n(x) = A \sin \frac{n\pi}{2a} x, \quad |x| \leq a$$

$$\alpha a = n\frac{\pi}{2}$$

$$\alpha = \frac{n\pi}{2a}, \quad \sqrt{\frac{2mE}{\hbar^2}} = \frac{n\pi}{2a}$$

$$E = E_n = \frac{n^2\pi^2\hbar^2}{8ma^2},$$

$$n = 1, 2, 3, \ldots$$

$$E_1 = \frac{\pi^2\hbar^2}{8ma^2}$$

$$E_n = n^2 E_1$$

$\boxed{\text{n=1 is a ground state}}$

Normalization of $u_n(x)$:

$$\int_{-\infty}^{\infty} |u_n(x)|^2 dx = 1$$

$$\int_{-a}^{a} |u_n(x)|^2 dx = 1$$

Determine B:

$$1 = B^2 \int_{-a}^{a} \cos^2\left(\frac{n\pi}{2a}x\right) dx$$

$$\cos^2 y = \frac{1+\cos 2y}{2}$$

$$= B^2 \int_{-a}^{a} \frac{\left(1+\cos\frac{n\pi}{a}x\right)}{2} dx$$

$$= B^2 \left\{ \frac{1}{\cancel{2}} \cancel{2}a + \frac{1}{2}\int_{-a}^{a} \cos\frac{n\pi}{a}x\,dx \right\}$$

$$= B^2 \left\{ a + \cancel{\frac{1}{2}\frac{a}{n\pi}\sin\frac{n\pi}{a}x \Big|_{x=-a}^{x=a}} \right\} \quad 0$$

$$= aB^2$$

$$B = \frac{1}{\sqrt{a}}$$

Similarly, $A = \frac{1}{\sqrt{a}}$.

$$u_n(x) = \frac{1}{\sqrt{a}} \cos \frac{n\pi}{2a} x$$

$n = 1, 3, \ldots$

$$u_n(x) = \frac{1}{\sqrt{a}} \sin \frac{n\pi}{2a} x$$

$n = 2, 4, \ldots$

$$E_n = \frac{n^2 \pi^2 \hbar^2}{8 m a^2}$$

$l = 2a$ (width of the well)

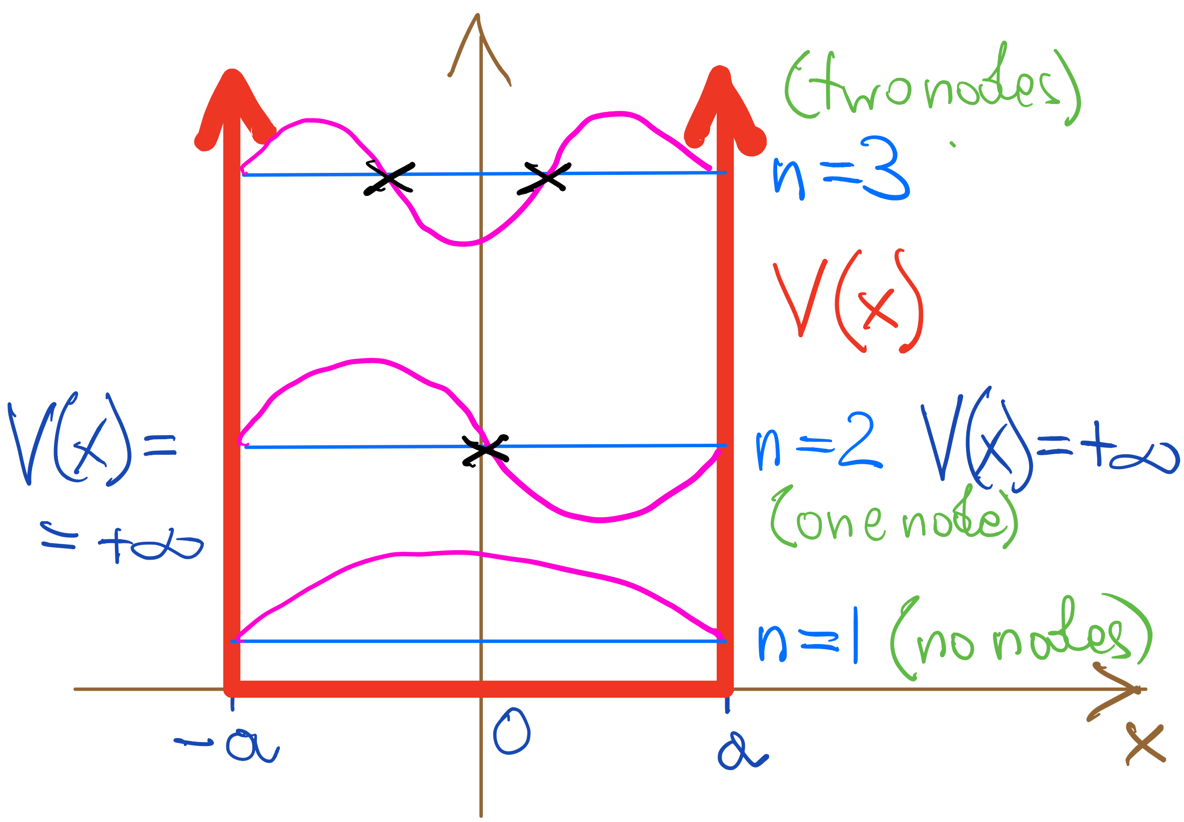
$$u_n(x) = \sqrt{\frac{2}{\ell}} \cos \frac{n\pi}{\ell} x$$

$n = 1, 3, \ldots$

$$u_n(x) = \sqrt{\frac{2}{\ell}} \sin \frac{n\pi}{\ell} x$$

$n = 2, 4, \ldots$

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2m\ell^2} = n^2 E_1$$



Each energy level is NONDEGENERATE

$$E_1 \to u_1, \; E_2 \to u_2, \; E_n \to u_n$$

We say that E_n is degenerate if

$$H u_{nj} = E_n u_{nj}$$

$$j = 1, \ldots, k_n \quad (k_n > 1)$$

Degeneracies occur when there are symmetries in H

$G \to$ symmetry group

$R \in G$,

$[H, R] = 0$, $\forall R \in G$

If irreps are multidimensional, we can anticipate degeneracies.

For particle in a box, we found even solutions,

$$u_n(x) = u_n(-x), \quad n = 1, 3, 5, \ldots$$

and odd solutions

$$u_n(x) = -u_n(-x) \quad n = 2, 4, \ldots$$

This is because $V(x) = V(-x)$

[V is an EVEN function of x]

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

At x:

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

At $(-x)$:

$$-\frac{\hbar^2}{2m}\frac{d^2 u(-x)}{dx^2} + \underset{\substack{\| \\ V(x)}}{V(-x)}\,u(-x) = E u(-x)$$

If $V(x) = V(-x)$,

$u(x)$ and $u(-x)$ are solutions of the same energy.

Assume that E is nondegenerate,

$$u(-x) = \varepsilon\, u(x) \quad \forall x$$

$$u(x) = \varepsilon\, u(-x) = \varepsilon^2 u(x)$$

$$\varepsilon^2 = 1 \Rightarrow \varepsilon = \pm 1$$

Either

$$u(x) \overset{\text{even}}{=} u(-x) \quad [\varepsilon = +1]$$

or

$$u(x) \overset{\text{odd}}{=} -u(-x) \quad [\varepsilon = -1]$$

What if E is degenerate?
In this case $u(x)$ does not have to be even or odd.

However, we can always make $u(x)$ even or odd:

$$u_{even}(x) = \frac{1}{2}\left[u(x) + u(-x)\right]$$

$$u_{odd}(x) = \frac{1}{2}\left[u(x) - u(-x)\right]$$

$$u(x), u(-x) \longrightarrow u_{even}(x), u_{odd}(x)$$

Conclusion:

If V is even, solutions are either even or odd.

or can be made

(they have well-defined parity).

Going back to particle in a box,

$$u(x) = A\sin\alpha x + B\cos\alpha x$$

Since V is even,

$$u(x) = B\cos\alpha x \quad \text{(even)}$$
$$(B \neq 0)$$

or

$$u(x) = A\sin\alpha x \quad \text{(odd)}$$
$$(A \neq 0)$$

For example, consider

$$u(x) = A\sin\alpha x, \; A \neq 0$$

$$u(a) = A\sin\alpha a = 0$$

$$\alpha a = n\frac{\pi}{2}, \; n = \cancel{0}, \cancel{\pm}2, \ldots$$

$$u_n(x) = A\sin\frac{n\pi}{2a}x, \; n = 2, 4, \ldots$$

$$V = V(r),$$
$$V(-x,-y,-z) = V(x,y,z)$$

MATHEMATICAL FOUDATIONS OF QM

- $\Psi(q_1,\dots,q_f,t)$ represents the state of a quantum-mechanical system
- $c_1\Psi_1 + c_2\Psi_2$ may represent a state if Ψ_1 and Ψ_2 are quantum states

- bound states satisfy

$$\int_{\Gamma} \psi^* \psi \, d\tau < \infty \qquad (A)$$

- expectation values

$$\langle \hat{F} \rangle = \int_{\Gamma} \psi^* \hat{F} \psi \, d\tau \qquad (B)$$

(assuming that ψ is normalized)

- operators representing observables are linear

$$\hat{F}(c_1\psi_1 + c_2\psi_2) = c_1 \hat{F}\psi_1 + c_2 \hat{F}\psi_2$$

— it is anticipated that

$$\int_\Gamma \varphi^*(\hat{F}\psi)\,d\tau \quad (C)$$

$$= \int_\Gamma (\hat{F}\varphi)^*\psi\,d\tau$$

(we proved this for $\hat{\nabla}^2, \hat{T}$)
easy to see for V

(A), (B), (C) belong to

$$\int_\Gamma \varphi^*(\hat{F}\psi)\,d\tau \quad \checkmark$$

[In (A), $\varphi=\psi$, $\hat{F}=\mathbb{1}$ the unit operator; in (B), $\varphi=\psi$]

$$\int \varphi^* (\hat{F}\psi)\, d\tau$$

$$= (\varphi, \hat{F}\psi)$$

inner **product** (scalar product)

IN THE **HILBERT SPACE**

$$\langle \varphi | \underbrace{\hat{F}\psi}_{\text{ket}} \rangle \equiv (\varphi, \hat{F}\psi)$$

bra ket bracket

$\hat{F}$ satisfying (C) is hermitian or **SELF-ADJOINT.**

HILBERT SPACE is an infinite or finite-dimensional LINEAR INNER PRODUCT (UNITARY) SPACE WHICH IS ALSO A COMPLETE METRIC SPACE with respect to the metric generated by the INNER (SCALAR) PRODUCT.

$$
\begin{tikzcd}
& \underset{(\alpha f+\beta g \in \mathcal{H})}{\text{LINEAR}} \arrow[dr] & & \underset{D[f,g]}{\text{METRIC}} \arrow[dl] & \\
\text{(SPACES)} & & \underset{\|f\|}{\text{NORM}} \arrow[r, "\text{complete}"] \arrow[d] & \text{BANACH} \arrow[d] & \\
& & \overset{(f,g)}{\text{UNITARY}} \arrow[r, "\text{complete}"'] & \text{HILBERT} &
\end{tikzcd}
$$

LINEAR SPACES ($\mathcal{H}$)

Set $\mathcal{H}$, $f, g, h, \ldots \in \mathcal{H}$

vectors in $\mathcal{H}$

"$+$", "$\cdot$"

add

multiply by a scalar

1. (i) $f+g \in \mathcal{H}$

(ii) $f+(g+h)$

$= (f+g)+h$

(iii) $\exists\ \Theta\ \forall f$ $f+\Theta = \Theta + f$

$= f$

zero vector

(iv) $\forall f\ \exists -f$ $f+(-f)$

$= (-f)+f = \Theta$

(v) $f+g = g+f$

$\mathcal{H}$ is an Abelian group with respect to "+".

$K \to$ number field (scalars) [complex numbers]

(i) $\alpha f \in \mathcal{H}$ $\forall \alpha \in K$ $\forall f \in \mathcal{H}$

(ii) $\alpha(f+g) = \alpha f + \alpha g$

(iii) $(\alpha+\beta) f = \alpha f + \beta f$

(iv) $\alpha(\beta f) = (\alpha\beta) f$

(v) $1 \cdot f = f$, $0 \cdot f = \Theta$

$\alpha_1 f_1 + \alpha_2 f_2 \in \mathcal{H}$

Elements (vectors) $f_1, \ldots, f_n$ in $\mathcal{H}$ are linearly independent if

$$\alpha_1 f_1 + \ldots + \alpha_n f_n = \Theta$$

implies that

$$\alpha_1 = \ldots = \alpha_n = 0.$$

Otherwise, $f_1, \ldots, f_n$ are linearly dependent.

A set $\{f_1, \ldots, f_n\}$ such that $f_1, \ldots, f_n$ are linearly independent, but

$f_1, \dots, f_n, g$ are linearly dependent for every g is called a BASIS.

n is called a dimension of $\mathcal{H}$,

$$n = \dim \mathcal{H}.$$

If one can find arbitrarily many linearly independent vectors in $\mathcal{H}$, $\dim \mathcal{H} = \infty$.

Example of a linear space: $\mathbb{R}^n$

$x \equiv (x_1, \dots, x_n) \in \mathbb{R}^n$. Basis: $e_1 = (1, 0, \dots, 0)$, $e_2 = (0, 1, \dots, 0), \dots, e_n = (0, 0, \dots, 1)$

$$x = x_1 e_1 + \dots + x_n e_n = \sum_{i=1}^{n} x_i e_i$$

METRIC SPACES $(\mathcal{H})$

We can define a DISTANCE between element $f, g, \ldots \in \mathcal{H}$

$D[f,g] \leftarrow$ distance between f and g

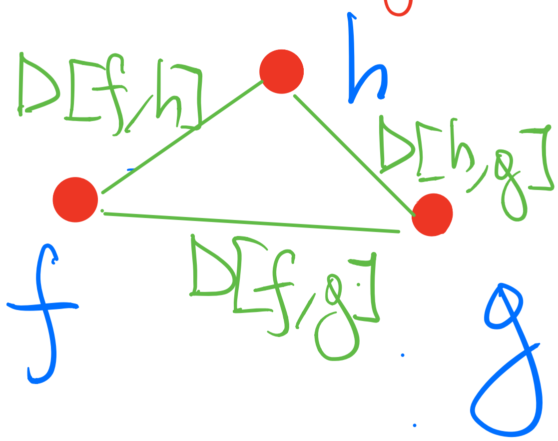
(a) $D[f,g] = D[g,f] > 0$ for $f \neq g$

(b) $D[f,f] = 0$

(c) $D[f,g] \leqslant$

$\leqslant D[f,h] + D[h,g]$

(triangle inequality)



Example, Euclidean space $\mathbb{R}^n$

$\mathbb{R}^n \ni (x_1, \dots, x_n)$

$$D[x,y] = \sqrt{\sum_{i=1}^{n} |x_i - y_i|^2}$$