Required properties of Hilbert space operators:

- Linearity
- Hermiticity
- Commutation relations
- General HUR

Unitary transformations and operators
Heisenberg vs. Schrödinger pictures
Heisenberg’s matrix formulation of QM
Matrix representation of wfs & operators
Invariants (Trace)
Unitary Operations

Unitary operations: transformations between different (orthogonal) bases. Different expansions of wave functions/vectors. Preserving norm (length) and relative projections, shapes (scalar products) Rotations, inversions, and translations in space.

Unitary op $\hat{U}$; wave functions or Dirac kets (Hilbert vectors) $|\varphi\rangle, |\psi\rangle$:

In particular, norm of a vector is preserved:

$$\|\hat{U}\varphi\|^2 = \langle \hat{U}\varphi | \hat{U}\varphi \rangle = \langle \varphi | \hat{U}^\dagger \hat{U} | \varphi \rangle = \langle \varphi | \varphi \rangle$$

Also scalar products (projections) are conserved.

$$\langle \hat{U}\varphi | \hat{U}\psi \rangle = \langle \varphi | \hat{U}^\dagger \hat{U} | \psi \rangle = \langle \varphi | \psi \rangle \rightarrow \hat{U}^\dagger \hat{U} = \mathbf{1} \text{ identity op}$$

Inverse operator $\hat{U}^\dagger = \hat{U}^{-1}$

Eigen kets $\{|\psi_u\rangle\}$ of $\hat{U}$ → calculate eigen values

$$\langle \psi_u | \psi_u \rangle = \langle \psi_u | \hat{U}^\dagger \hat{U} | \psi_u \rangle = \langle \hat{U}\psi_u | \hat{U}\psi_u \rangle = u^* \langle \psi_u | \hat{U}\psi_u \rangle = |u|^2 \langle \psi_u | \psi_u \rangle$$

Hence $|u|^2 = 1 \rightarrow u = e^{i\phi}$, $u$ is just a phase factor

$$\hat{U} |\psi\rangle \leftrightarrow |\psi\rangle$$
Unitary Coordinate Transformations

Unitary operators represent transformations between different bases.

Transformation between equivalent bases \( \{ \psi_j \} \leftrightarrow \{ \varphi_i \} \)

by rotations & translations: \( \{ \psi_j \} = \hat{U} \{ \varphi_i \} \)

\( \rightarrow \) Preserve volumes/norm

Define \((\hat{U})\):

Express basis \( \{ \psi_j \} \) components in terms of basis \( \{ \varphi_i \} \) →

\[
\psi_j = \sum_k U_{jk} \cdot \varphi_k
\]

Matrix element \( U_{jk} = \langle \varphi_k | \psi_j \rangle \)

\( U^\ast_{jk} = \langle \varphi_k | \psi_j \rangle^\ast = \langle \psi_j | \varphi_k \rangle = U_{kj} \)

\[
\langle \hat{U} \varphi | \hat{U} \psi \rangle = \langle \varphi | \hat{U}^\dagger \hat{U} | \psi \rangle = \langle \varphi | \psi \rangle
\]

\( \hat{U}^\dagger \hat{U} = \mathbf{1} \) identity op \( \rightarrow \hat{U}^\dagger = \hat{U}^{-1} \)

Eigen kets \( \{ | \psi_u \rangle \} \) of \( \hat{U} \) → EV: \( u = e^{i \cdot \phi_u} \) (= \( \cos \phi_u + i \cdot \sin \phi_u \))
Switch Bases (Coordinate Systems)

**Transformation between bases** \( \{ \varphi_i \} \overset{\hat{U}}{\longrightarrow} \{ \psi_j \} \), \quad \psi_j = \sum_k U_{jk} \cdot \varphi_k

**Matrix element** \( U_{jk} = \langle \varphi_k | \psi_j \rangle \iff U^*_{jk} = \langle \varphi_k | \psi_j \rangle^* = \langle \psi_j | \varphi_k \rangle = U^\dagger_{kj} \)

determine once, use for all wfs/kets

Arbitrary \( \Psi = \sum_i a_i \cdot \varphi_i \) with \( a_i = \langle \varphi_i | \Psi \rangle = \) projection of \( \Psi \) on \( \varphi_i \)

Also : \( \Psi = \sum_j c_j \cdot \psi_j \) with \( c_j = \langle \psi_j | \Psi \rangle = \) projection of \( \Psi \) on \( \psi_j \)

\[
\Psi = \sum_j c_j \cdot \psi_j = \sum_j c_j \cdot \left( U_{jk} \cdot \varphi_k \right) = \sum_k a_k \cdot \varphi_k
\]

\[
a_k = \sum_j U_{jk} \cdot c_j \rightarrow \text{invert} \quad c_j = \sum_k U^*_{jk} \cdot a_k = \sum_k U^*_{jk} \langle \varphi_k | \Psi \rangle
\]

→ Transformed vector components expressed in terms of originals

Because \( c_j = \langle \psi_j | \Psi \rangle = \sum_k \langle \psi_j | \varphi_k \rangle \langle \varphi_k | \Psi \rangle = \sum_k U^*_{jk} \cdot a_k \)

Also used closure relation \( \sum_k |\varphi_k\rangle \langle \varphi_k| = \hat{1} \)
Unitary Coordinate Transformations

Unitary operators represent transformations between different bases.

Transformation between equivalent bases \( \{ \psi_j \} \leftrightarrow \{ \varphi_i \} \)

by rotations & translations: \( \{ \psi_j \} = \hat{U} \{ \varphi_i \} \) \quad \rightarrow \text{Preserve volumes/norm}

Define \( (\hat{U}) \):

Express basis \( \{ \psi_j \} \) components in terms of basis \( \{ \varphi_i \} \) →

\[
\psi_j = \sum_k U_{jk} \cdot \varphi_k
\]

Matrix element \( U_{jk} = \langle \varphi_k | \psi_j \rangle \)

\[
U_{jk}^* = \langle \varphi_k | \psi_j \rangle^* = \langle \psi_j | \varphi_k \rangle = U_{kj}^\dagger
\]

\[
\langle \hat{U} \varphi | \hat{U} \psi \rangle = \langle \varphi | \hat{U}^\dagger \hat{U} | \psi \rangle = \langle \varphi | \psi \rangle \quad \hat{U}^\dagger \hat{U} = \mathbf{1} \text{ identity op} \rightarrow \hat{U}^\dagger = \hat{U}^{-1}
\]

Eigen kets \( \{ | \psi_u \rangle \} \) of \( \hat{U} \) \( \rightarrow \) EV: \( u = e^{i \cdot \phi_u} \) (= \cos \phi_u + i \cdot \sin \phi_u)
Unitary Coordinate Transformation

**Unitary op** $\hat{U}$; **wave functions / Dirac kets** (Hilbert vectors) $|\varphi\rangle, |\psi\rangle$:

**Derivations use implicit shorthand** $\varphi(x) = \langle x | \varphi \rangle$, $|x\varphi\rangle^2 = \|\varphi(x)\|^2 \triangleq \int_{-\infty}^{+\infty} dx \varphi^*(x) \varphi(x)$

\[
\langle \hat{U}\varphi | \hat{U}\psi \rangle = \langle \psi | \hat{U}^+\hat{U} | \psi \rangle = \langle \varphi | \psi \rangle \rightarrow \hat{U}^+\hat{U} = \hat{1} \text{ identity op}
\]

Specifically: norm of a vector: $\|\hat{U}\varphi\|^2 = \langle \hat{U}\varphi | \hat{U}\varphi \rangle = \langle \varphi | \hat{U}^+\hat{U} | \varphi \rangle = \langle \varphi | \varphi \rangle$

\[
i\hbar \frac{\partial}{\partial t} \psi = \hat{H}\psi
\]

If $\hat{H} \neq \hat{H}(t)$ (no explicit time dependence) \rightarrow

formal solution of TDSE $\psi(t) = \exp\left\{ \frac{1}{i\hbar} \cdot t \cdot \hat{H} \right\} \psi(0)$

Time evolution operator (propagator)

$\hat{U}(t,t_0) = e^{-\frac{i}{\hbar}\hat{H}(t-t_0)}$

$\hat{H}$ = conservative Hamilton op, $\psi(t) = \hat{U}(t,t_0)\psi(t_0) = e^{-\frac{i}{\hbar}\hat{H}(t-t_0)}\psi(t_0)$
Example: Time Evolution

Unitary op $\hat{U}$; wave functions / Dirac kets (Hilbert vectors) $|\varphi\rangle, |\psi\rangle$:

Derivations use implicit shorthand $\varphi(x) = \langle x | \varphi \rangle$, $|\langle x | \varphi \rangle|^2 = \|\varphi(x)\|^2 \equiv \int_{-\infty}^{+\infty} dx \varphi^*(x) \varphi(x)$

Time evolution of an arbitrary wf $\psi \leftrightarrow |\psi\rangle$ (use various reps)

Since $\hat{U}(t) \leftrightarrow \hat{H}$: choose $\hat{H}\varphi_n = E_n\varphi_n \rightarrow \text{basis } \{\varphi_n\}$

Expand $\psi(t_0)$ in basis of $H$-eigen states $\psi(t_0) = \sum_n c_{En} \cdot \varphi_{En}$ with $\|\psi(t_0)\|^2 = \sum_n |c_{En}|^2$

\[\hat{U}(t,t_0) = e^{-\frac{i}{\hbar}\hat{H}(t-t_0)}\]

\[
\|\psi(t)\|^2 = \left\| e^{-\frac{i}{\hbar}\hat{H}(t-t_0)} \psi(t_0) \right\|^2 = \left\| \sum_n c_{En} \cdot \varphi_{En} \right\|^2 = \left\| \sum_n c_{En} e^{-\frac{i}{\hbar}\hat{H}(t-t_0)} \cdot \varphi_{En} \right\|^2 = \sum_n \left| c_{En} \right|^2 = \int_{-\infty}^{+\infty} dx \varphi^*(x) \varphi(x) = \sum_n |c_{En}|^2 = \|\psi(t_0)\|^2
\]
What kind of unitary operations exist, what is effect on $|\psi\rangle$?

$$\hat{U}|\psi_u\rangle = e^{i\hat{\phi}_u}|\psi_u\rangle = e^{i\phi_u}|\psi_u\rangle \rightarrow \text{how does } \hat{\phi}_u \text{ transform } \psi \text{ or } |\psi\rangle \neq |\psi_u\rangle?$$

Determine from infinitesimlal transformations

$$\hat{U} = f(\hat{A}) = e^{i\hat{A}} = \sum_{n=0}^{\infty} \left(\frac{i}{n!}\right)^n \hat{A}^n = 1 + i \cdot \hat{A} + \frac{-1}{2!} \cdot \hat{A}^2 + \ldots$$

sum over odd and even powers of $\hat{A}$

Taylor expansion for translation by finite displacement $\vec{\varepsilon} : \psi(\vec{r} + \vec{\varepsilon}) = \psi(\vec{r}) + \vec{\varepsilon} \cdot \vec{\nabla} \psi(\vec{r}) + \ldots$

Differential displacement operator $\vec{\nabla} \rightarrow \hat{p} = (\hbar/i) \cdot \vec{\nabla}$

Finite translations

$$\psi(\vec{r}') = \psi(\vec{r}) + \sum_{n=1}^{\infty} \frac{(i/\hbar)^n}{n!} [(\vec{r}' - \vec{r}) \cdot \hat{p}]^n \psi(\vec{r}) = \exp \left\{ \frac{i}{\hbar} (\vec{r}' - \vec{r}) \cdot \hat{p} \right\}$$

$$\hat{U}_d = \exp \left\{ \frac{i}{\hbar} \vec{d} \cdot \hat{p} \right\} \text{ has required properties: } \hat{U}_d^{-1} = \hat{U}_{-d} = e^{\frac{-i}{\hbar} \vec{d} \cdot \hat{p}} = \hat{U}_d \rightarrow \hat{U}_d^+ \hat{U}_d^- = 1$$
Properties of Unitary Ops

Unitary operators represent transformations between different bases.

**Theorem:** If $\hat{A}^\dagger = \hat{A}$ Hermitian $\rightarrow \hat{U} = e^{i\cdot\hat{A}}$ is unitary

*What does $\hat{A}^\dagger = \hat{A}$ mean?* $\rightarrow$ Consider $\hat{p}^\dagger = \hat{p}$

**Proof of theorem:**

$\hat{U}^{-1} = e^{-i\cdot\hat{A}} = \sum_{n=0}^{\infty} \frac{1}{n!}(-\hat{A})^n = \hat{1} + (i\hat{A}) + \frac{1}{2!}(i\hat{A})^2 + \ldots = \left[\hat{1} + (i\hat{A})^\dagger + \frac{1}{2!}(i\hat{A}^\dagger)^2 + \ldots\right] = \left[\hat{1} + (i\hat{A}) + \frac{1}{2!}(i\hat{A})^2 + \ldots\right]^\dagger = e^{+i\cdot\hat{A}^\dagger} = \hat{U}^\dagger \rightarrow \hat{U}^\dagger = \hat{U}^{-1}$ and $\hat{U}^\dagger\hat{U} = \hat{1}$

\[
(i\hat{A})^n = i^n \cdot \hat{A}^n = \begin{cases} (-1)^{[n/2]} & \text{if } n = \text{even} \\ i \cdot (-1)^{[n/2]} & \text{if } n = \text{odd} \end{cases}
\]

Series over odd $n \rightarrow \text{Im}\hat{U}$

Series over even $n \rightarrow \text{Re}\hat{U}$
Instant Quiz

Show that unitary operators have eigen values of magnitude (norm) = 1

Unitary operator: \( \hat{U}^\dagger = \hat{U}^{-1} \) or \( \hat{U}^\dagger \hat{U} = \hat{1} \)

Assume, \( \psi_u \) is normalized eigen function (vector) of \( \hat{U} \) with \( \hat{U} \psi_u = u \cdot \psi_u \)

Prove that \( |u|^2 = 1 \)!

Eigen functions \( \{\varphi_u\} \) of linear, unitary \( \hat{U} \) form a basis

Arbitrary wave function \( \psi = \sum_u c_u \cdot \varphi_u \rightarrow \hat{U} \psi = \sum_u c_u \cdot (\hat{U} \varphi_u) = \sum_u (e^{i\phi_u} c_u) \cdot \varphi_u \)
Instant Quiz

Show that unitary operators have eigen values of magnitude (norm) = 1

Unitary operator: \( \hat{U}^\dagger = \hat{U}^{-1} \) or \( \hat{U}^\dagger \hat{U} = \hat{1} \)

Assume, \( \psi_u \) is normalized eigen function (vector) of \( \hat{U} \) with \( \hat{U} \psi_u = u \cdot \psi_u \)

Prove that \( |u|^2 = 1 \)!

Since \( \psi_u \) is normalized, \( \langle \psi_u | \psi_u \rangle = \| \psi_u \|^2 = 1 \) and \( \hat{U} \psi_u = u \cdot \psi_u \)

On the other hand, since \( \hat{U}^\dagger \hat{U} = \hat{1} \) \( \rightarrow \)

\[ \langle \psi_u | \psi_u \rangle = \langle \psi_u | \hat{U}^\dagger \hat{U} | \psi_u \rangle = \langle \hat{U} \psi_u | \hat{U} \psi_u \rangle = u^* \langle \psi_u | \hat{U} \psi_u \rangle = |u|^2 \langle \psi_u | \psi_u \rangle = |u|^2 \]

\( \rightarrow \) Hence \( |u|^2 = 1 \) qed

Further, \( u = e^{i \cdot \varphi_u} \), \( u \) is just a phase factor

Eigen functions \( \{ \varphi_u \} \) of linear, unitary \( \hat{U} \) form a basis

Arbitrary wave function \( \psi = \sum_u c_u \cdot \varphi_u \rightarrow \hat{U} \psi = \sum_u c_u \cdot (\hat{U} \varphi_u) = \sum_u \left( e^{i \cdot \varphi_u} c_u \right) \cdot \varphi_u \)
Instant Quiz

Inverse of products of unitary operators

Unitary operators: \( \hat{A} \) and \( \hat{B} \)

Is \( \hat{C} = \hat{A}\hat{B} \) also a unitary operator, or not?
Instant Quiz

Inverse of products of unitary operators

Unitary operators: $\hat{A}$ and $\hat{B}$

Is $\hat{C} = \hat{A}\hat{B}$ also a unitary operator, or not?

\[
\hat{A}\psi \leftrightarrow \langle \psi | \hat{A}^\dagger = \langle \hat{A}\psi |
\]

\[
\hat{A}\hat{B}\psi = \hat{A}\hat{B}_\psi : \text{rightmost operation } \hat{B} \text{ first, then } \hat{A}
\]

\[
\leftrightarrow \langle \psi | (\hat{A}\hat{B})^\dagger = \langle \hat{B}_\psi | \hat{A}^\dagger = \langle \hat{A}\hat{B}_\psi | = \langle \psi | \hat{B}^\dagger\hat{A}^\dagger
\]

\[
\hat{C}^\dagger = (\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger \rightarrow
\]

\[
\hat{C}^\dagger\hat{C} = (\hat{B}^\dagger\hat{A}^\dagger)\hat{A}\hat{B} = \hat{B}^\dagger(\hat{A}^\dagger\hat{A})\hat{B} = \hat{B}^\dagger\hat{B} = \hat{1}
\]

Yes!
Unitary Transformations of Ops and WFs

Many unitary ops $\hat{U}$ are not Hermitian $\rightarrow \hat{U}$ do not represent observables $A$, but are useful for effecting convenient transformations of Hermitian ops $A$:

Unitary $[\hat{U}^\dagger = U^{-1}]$, Hermitian $\hat{A} = \hat{A}^\dagger$, wf $\varphi, \psi$ & corresponding kets

$$ME \langle \varphi | \hat{A} | \psi \rangle = \langle \varphi | U^{-1} \hat{U} \hat{A} | \psi \rangle = \langle \hat{U} \varphi | \hat{U} \hat{A} | \psi \rangle = \langle \hat{U} \varphi | \hat{U} \hat{A} U^{-1} \hat{U} | \psi \rangle = \langle \hat{U} \varphi | \hat{U} \hat{A} U^{-1} | \hat{U} \psi \rangle$$

Transformed op $[\hat{A}' = \hat{U} \hat{A} U^{-1}]$ has same effect on transformed $\psi' = \hat{U} \psi$, etc. as $\hat{A}$ has on the originals $\psi$.

Example: time evolution op $\hat{U}(t, t') = \exp \{-i\hat{H}(t - t')/\hbar\}$

**Hermiticity is retained in unitary transforms**: If $\hat{A} = \hat{A}^\dagger \rightarrow$

$$\left( \hat{A}' \right)^\dagger = \left( \hat{U} \hat{A} U^{-1} \right)^\dagger = \left( \hat{U} \hat{A} U^\dagger \right)^\dagger = \left( \hat{U}^\dagger \right)^\dagger \hat{A}^\dagger \left( \hat{U}^\dagger \right) = \hat{U} \hat{A}^\dagger U^\dagger = \hat{U} \hat{A} U^{-1} = \hat{A}'$$

Eigen values of $\hat{A}' = \hat{U} \hat{A} U^{-1}$ in transformed basis are the same as EV of $\hat{A}$ in original basis $\rightarrow$

If basis is transformed with $\hat{U}$, use $\hat{A}' = \hat{U} \hat{A} U^{-1} = \hat{U} \hat{A} U^\dagger$
Example: Unitary Spin Rotation

Spin $S=1/2$ particles (mass $m$, magnetic moment $\mu$) at rest in homogeneous field

$\vec{\mu} = -\gamma \cdot \vec{S}$, gyromagnetic ratio: $\gamma = \left( g_s e / (2m) \right)$,

Magnetic field $\vec{B} = B_z \cdot \vec{z} / |\vec{z}|$

System Hamiltonian: $\hat{H} = -\vec{\mu} \cdot \vec{B} = \gamma \cdot \vec{S} \cdot \vec{B} = \gamma B_z S_z$ (conserv.)

Larmor frequency $\Omega := \gamma B_z \to \hat{H} = (\hbar/2) \gamma B_z \cdot \sigma_z = (\hbar/2) \Omega \cdot \sigma_z$

$\to$ Spin wave functions $X_+ = \langle \ up \ | z_+ \rangle$ and $X_- = \langle \ down \ | z_- \rangle$

Eigen vectors $\hat{\sigma}_z | z_+ \rangle = +1 \cdot | z_+ \rangle$ and $\hat{\sigma}_z | z_- \rangle = -1 \cdot | z_- \rangle$

Time evolution: $\hat{U}(t) = e^{-i \hat{H} \cdot t / \hbar} = e^{-i \Omega t \cdot \sigma_z / 2}$ ($\hbar$ cancels)

$X_\pm(t) = e^{-i \Omega t \cdot \sigma_z / 2} X_\pm(0) = \pm i \cdot \Omega t \cdot \sigma_z / 2$ $X_\pm(0) = \left( \cos \left( \frac{\Omega}{2} t \right) \mp i \cdot \sin \left( \frac{\Omega}{2} t \right) \right) X_\pm(0)
Example: Spin Rotation

Spin \( S = 1/2 \) particles (mass \( m \), magnetic moment \( \mu \)) at rest in homogeneous field

System Hamiltonian: \( \hat{H} = -\vec{\mu} \cdot \vec{B} = \gamma \cdot \vec{S} \cdot \vec{B} = \gamma B_z S_z \)

Larmor frequency \( \Omega := \gamma B_z \rightarrow \hat{H} = (\hbar/2) \cdot \Omega \cdot \hat{\sigma}_z \)

Arbitrary initial state

\( \mathbf{X}(\theta_o, \phi_o) = e^{-i\phi_o/2} \cos(\theta_o/2) \, \mathbf{X}_+ + e^{+i\phi_o/2} \sin(\theta_o/2) \, \mathbf{X}_- \)

\( \mathbf{X}(t) = \hat{U}(t) \mathbf{X}(0) = e^{-i/2 \cdot \Omega \cdot t \cdot \hat{\sigma}_z} \mathbf{X}(0) = e^{-i(\phi_o + \Omega t)/2} \cos(\theta_o/2) \, \mathbf{X}_+ + e^{+i(\phi_o + \Omega t)/2} \sin(\theta_o/2) \, \mathbf{X}_- \)

Expectation of direction of \( \vec{S} \) : \( \langle \mathbf{X} | \vec{S} | \mathbf{X} \rangle = \frac{\hbar}{2} \vec{n}_\mathbf{X}(t) \)

\( \vec{n}_\mathbf{X}(t) = \begin{pmatrix} \sin \theta_o \cos(\phi_o + \Omega t) \\ \sin \theta_o \sin(\phi_o + \Omega t) \\ \cos \theta_o \end{pmatrix} \)

Rotates in 3D space about \( z \) (\( B \)) axis at const. \( \theta_o \).
End (for now)