

A CM system is described by

- $2n$ real coordinates z_i of the phase space
- the Hamiltonian $H(z, t)$,
- the Poisson bracket of z_i

$$\{z_i, z_j\} - \omega_{ij}(z) = 0 \quad (0.1)$$

- z_i satisfy Hamilton's eom

$$\frac{dz_i}{dt} = \{H, z_i\} = \frac{\partial H}{\partial z_j} \omega_{ji}(z) \quad (0.2)$$

- Observables are real-valued functions $f(z, t)$,
e.g. z_i , H , angular momentum and so on.

To quantise such a system one performs the following two steps

1. z^i become elements \mathcal{Z}^i of a unital associative algebra \mathcal{A} over \mathbb{C} .

\mathcal{A} is generated by the identity element \mathcal{I} and the elements \mathcal{Z}^i that satisfy ($i^2 = -1$)

$$\mathcal{F}^{ij} \equiv \frac{i}{\hbar} [\mathcal{Z}^i, \mathcal{Z}^j] - \Omega^{ij}(\mathcal{Z}) = 0, \quad \lim_{\hbar \rightarrow 0} \Omega^{ij}(z) = \omega^{ij}(z) \quad (0.3)$$

2. One finds an irreducible representation of \mathcal{A} in a Hilbert space \mathcal{H} such that \mathcal{Z}^i are represented by Hermitian operators \hat{Z}^i acting in the space.

The quantum physics is encoded in this representation. In particular

- Vectors $|\psi\rangle$ of \mathcal{H} are quantum mechanical states of the system.
- Observables are Hermitian operators acting in \mathcal{H} , and they include a Hamiltonian $\hat{H} = H(\hat{Z}, t) + \mathcal{O}(\hbar)$ which governs the quantum dynamics of the system.
- The spectrum of a Hermitian operator is measurable.
Measurements are represented by projection operators.
- The symmetries of the system are represented by unitary operators.

An elementary (point) particle may have spin \vec{S} that is intrinsic angular momentum.

The projection of the spin on any axes can take only discrete values

$$\frac{S^z}{\hbar} = s, s - 1, s - 2, \dots, -s, \quad s = 0, \frac{1}{2}, 1, \frac{3}{2}, \dots \quad (0.4)$$

- The number s is also called the spin of a particle
- Particles of half-integer spin s are called fermions, e.g. electron and proton have spin $1/2$
- Particles of integer spin are called bosons, e.g. Higgs boson has spin 0, photon has spin 1, graviton has spin 2

To describe spin one enlarges the phase space of a point particle by adding to $\vec{x} = (x, y, z)$ and $\vec{p} = (p^x, p^y, p^z)$ a spin vector $\vec{s} = (s^x, s^y, s^z)$ of constant length.

- \vec{s} obeys the Poisson algebra of $\vec{\ell} = \vec{x} \times \vec{p}$ and Poisson-commutes with \vec{x} and \vec{p} .
- Since $\vec{s}^2 = \text{const}$ the spin phase space is S^2 .
- The phase space of a particle with a spin is $\mathbb{R}^6 \times S^2$

$$\begin{aligned} \{p^\alpha, x^\beta\} &= \delta^{\alpha\beta}, \quad \{x^\alpha, x^\beta\} = 0, \quad \{p^\alpha, p^\beta\} = 0, \quad \alpha, \beta = 1, 2, 3, \\ \{s^\alpha, s^\beta\} &= -\epsilon^{\alpha\beta\gamma} s^\gamma, \quad \sum_\alpha (s^\alpha)^2 = \text{const}, \quad \{s^\alpha, x^\beta\} = 0, \quad \{s^\alpha, p^\beta\} = 0 \end{aligned} \quad (0.5)$$

- One can require $\vec{s}^2 = \text{const}$ because \vec{s}^2 Poisson-commutes with all s^α and therefore with $H(\vec{x}, \vec{p}, \vec{s}, t)$.
- The total angular momentum \vec{j} is given by

$$\vec{j} = \vec{\ell} + \vec{s} \quad (0.6)$$

and it is the one which is conserved if the system is invariant under rotations.

In quantum theory x^α , p^α and ℓ_α become generators of an algebra

$$\begin{aligned} \frac{i}{\hbar}[\mathcal{P}^\alpha, \mathcal{X}^\beta] &= \delta^{\alpha\beta} \mathcal{I}, \quad [\mathcal{X}^\alpha, \mathcal{X}^\beta] = 0, \quad [\mathcal{P}^\alpha, \mathcal{P}^\beta] = 0, \quad \alpha, \beta = 1, 2, 3, \\ \frac{i}{\hbar}[\mathcal{S}^\alpha, \mathcal{S}^\beta] &= -\epsilon^{\alpha\beta\gamma} \mathcal{S}^\gamma, \quad \sum_\alpha (\mathcal{S}^\alpha)^2 = \text{const } \mathcal{I}, \quad [\mathcal{S}^\alpha, \mathcal{X}^\beta] = 0, \quad [\mathcal{S}^\alpha, \mathcal{P}^\beta] = 0 \end{aligned} \quad (0.7)$$

We will see in due course that $\sum_\alpha (\mathcal{S}^\alpha)^2 = s(s+1)\hbar^2 \hat{I}$ for a particle of spin s .

Comparing (0.7) with (0.5), we see that the quantisation is just the replacement

$$\{\bullet, \bullet\} \mapsto \frac{i}{\hbar}[\bullet, \bullet] \quad (0.8)$$

The relations between \mathcal{X} 's and \mathcal{P} 's are called **canonical commutation relations**.

The algebra generated by \mathcal{X} and \mathcal{P} for each value of α

$$[\mathcal{X}, \mathcal{P}] = i \hbar \mathcal{I} \quad (0.9)$$

is called the Heisenberg algebra

$\mathcal{T}^\alpha \equiv \frac{\mathcal{S}^\alpha}{i\hbar}$ satisfy the $\mathfrak{su}(2) \cong \mathfrak{so}(3)$ Lie algebra commutation relations

$$[\mathcal{S}^\alpha, \mathcal{S}^\beta] = i \hbar \epsilon^{\alpha\beta\gamma} \mathcal{S}^\gamma \quad \Leftrightarrow \quad [\mathcal{T}^\alpha, \mathcal{T}^\beta] = \epsilon^{\alpha\beta\gamma} \mathcal{T}^\gamma, \quad \mathcal{T}^\alpha \equiv \frac{\mathcal{S}^\alpha}{i\hbar} \quad (0.10)$$

1 MATHEMATICS OF QUANTUM MECHANICS

1.1 Matrix operations

An $m \times n$ matrix $A = (A_{ia})$, $i = 1, 2, \dots, m$, $a = 1, 2, \dots, n$ is the following table with m rows and n columns

$$A = \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1n} \\ A_{21} & A_{22} & \dots & A_{2n} \\ \vdots & \vdots & & \vdots \\ A_{m1} & A_{m2} & \dots & A_{mn} \end{pmatrix} \quad (1.11)$$

- A_{ia} are called matrix elements, components or entries.
- We only consider matrix elements which are either real or complex numbers, and often refer to numbers as scalars.
- The set of all $m \times n$ real matrices will be denoted by $\text{Mat}(m, n, \mathbb{R})$
- The set of all $m \times n$ complex matrices will be denoted by $\text{Mat}(m, n, \mathbb{C})$ or simply by $\text{Mat}(m, n)$.
- Sets of square matrices will be denoted by $\text{Mat}(n, \mathbb{R})$ and $\text{Mat}(n, \mathbb{C})$ or $\text{Mat}(n)$.
- Unless otherwise specified matrices are assumed to be complex.

Any matrix can be written as a linear combination of the matrices E_{ia} which have one on the intersection of the i -th row and a -th column and zeroes everywhere else

$$(E_{ia})_{jb} = \delta_{ij}\delta_{ab} \quad \Rightarrow \quad A = \sum_{i=1}^m \sum_{a=1}^n A_{ia} E_{ia} \quad (1.12)$$

The matrices E_{ia} form the standard basis of the space of $m \times n$ matrices.

The following three operations can be performed with matrices

(I) The **sum** of two $m \times n$ matrices $A = (A_{ia})$ and $B = (B_{ia})$ is the matrix $A + B$

$$A + B = (A_{ia} + B_{ia}) \quad \Leftrightarrow \quad (A + B)_{ia} = A_{ia} + B_{ia} \quad (1.13)$$

Obviously, the matrix addition is commutative: $A + B = B + A$.

(II) The product of a scalar c and a matrix A is the matrix cA

$$cA = (cA_{ia}) \quad \Leftrightarrow \quad (cA)_{ia} = cA_{ia} \quad (1.14)$$

Since matrix elements are scalars too they commute with c and therefore $cA = Ac$.

The matrix addition and multiplication by scalars make $\text{Mat}(m, n, \mathbb{C})$ a vector space.

(III) The **product** of an $m \times n$ matrix $A = (A_{ia})$ and an $n \times p$ matrix $B = (B_{a\beta})$ is the $m \times p$ matrix AB

$$AB = (\sum_a A_{ia} B_{a\beta}) \quad \Leftrightarrow \quad (AB)_{i\beta} = \sum_{a=1}^n A_{ia} B_{a\beta}, \quad \beta = 1, 2, \dots, p \quad (1.15)$$

Clearly, if $p \neq m$ then the product of B and A does not exist.

Obviously, the matrix product is associative

$$A(BC) = (AB)C \quad (1.16)$$

The matrix product and the existence of the identity matrix makes the space of square matrices $\text{Mat}(n, \mathbb{C})$ a unital associative algebra over \mathbb{C} .

Def. Let \mathcal{A} be a **vector space** over \mathbb{F} where \mathbb{F} is either \mathbb{C} or \mathbb{R} , and let \mathcal{A} be equipped with a **multiplication** (or binary) operation, $\mathcal{A} \times \mathcal{A} \mapsto \mathcal{A}$ denoted by $*$ so that $\forall \mathcal{S}, \mathcal{T} \in \mathcal{A}, \mathcal{S} * \mathcal{T} \in \mathcal{A}$. Then, \mathcal{A} is an **algebra** over \mathbb{F} if $\forall \mathcal{S}, \mathcal{T}, \mathcal{U} \in \mathcal{A}$ and $\forall a, b \in \mathbb{F}$ (“scalars”)

1. $(\mathcal{S} + \mathcal{T}) * \mathcal{U} = \mathcal{S} * \mathcal{U} + \mathcal{T} * \mathcal{U} \quad \leftarrow \quad \text{right distributivity}$
2. $\mathcal{U} * (\mathcal{S} + \mathcal{T}) = \mathcal{U} * \mathcal{S} + \mathcal{U} * \mathcal{T} \quad \leftarrow \quad \text{left distributivity}$
3. $(a \mathcal{S}) * (b \mathcal{T}) = (ab)(\mathcal{S} * \mathcal{T}) \quad \leftarrow \quad \text{compatibility with “scalars”}$

These three properties mean that the operation is **bilinear**.

Thus, given a basis $\mathcal{E}_i, i = 1, \dots, \dim \mathcal{A}$ of \mathcal{A} the product $*$ is completely determined by the structure constants $f_{ij}^k \in \mathbb{F}$ defined by

$$\mathcal{E}_i * \mathcal{E}_j = \sum_{k=1}^{\dim \mathcal{A}} f_{ij}^k \mathcal{E}_k \quad (1.17)$$

The dimension of an algebra is its dimension as a vector space.

Def. An algebra \mathcal{A} is called

- **commutative** if $S * T = T * S \quad \forall S, T \in \mathcal{A}$.
- **unital** if $\exists \mathcal{I} \in \mathcal{A} : \mathcal{I} * S = S * \mathcal{I} = S \quad \forall S \in \mathcal{A}$.
 \mathcal{I} is called a unit or identity element of \mathcal{A}
- **associative** if $(S * T) * \mathcal{U} = S * (T * \mathcal{U}) \quad \forall S, T, \mathcal{U} \in \mathcal{A}$

1.2 Dirac's bra and ket notation

$$|\alpha\rangle \leftrightarrow \alpha = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix}, \quad \langle\alpha| \equiv |\alpha\rangle^\dagger \leftrightarrow \alpha^\dagger = (a_1^*, a_2^*, \dots, a_n^*) \quad (1.18)$$

The dot product of $|\alpha\rangle$ and $|\beta\rangle$

$$\langle\alpha|\beta\rangle \equiv \langle\alpha| \cdot |\beta\rangle = \alpha^\dagger \cdot \beta = (a_1^*, a_2^*, \dots, a_n^*) \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix} = \sum_{i=1}^m a_i^* b_i, \quad \langle\beta|\alpha\rangle = \langle\alpha|\beta\rangle^* \quad (1.19)$$

$|\alpha| \equiv \sqrt{\langle\alpha|\alpha\rangle}$ is the length of the vector.

Let us denote $c|\alpha\rangle \equiv |c\alpha\rangle$. Then, $\langle c\alpha| = |c\alpha\rangle^\dagger = c^* \langle\alpha|$, and

$$\langle\alpha|c\beta\rangle = c\langle\alpha|\beta\rangle = \langle c^* \alpha|\beta\rangle, \quad \langle c\alpha|\beta\rangle = c^* \langle\alpha|\beta\rangle = \langle\alpha|c^* \beta\rangle \quad (1.20)$$

The dot product is linear wrt the second factor, and antilinear wrt the first factor.

Similarly, given a matrix A and a ket $|\alpha\rangle$ we denote their product as

$$A|\alpha\rangle \equiv |A\alpha\rangle \quad (1.21)$$

and find

$$\langle A\alpha| = (|A\alpha\rangle)^\dagger = (A|\alpha\rangle)^\dagger = |\alpha\rangle^\dagger A^\dagger = \langle\alpha|A^\dagger \quad (1.22)$$

Thus,

$$\langle\alpha|A|\beta\rangle = \langle\alpha|A\beta\rangle = \langle A^\dagger\alpha|\beta\rangle, \quad \langle\alpha|A|\beta\rangle^* = \langle\beta|A^\dagger|\alpha\rangle \quad (1.23)$$

If A is Hermitian $A^\dagger = A$ then $\langle\alpha|A|\alpha\rangle^* = \langle\alpha|A|\alpha\rangle \in \mathbb{R}$.

If $A = U$ is unitary then $\langle\alpha|\beta\rangle$ is invariant under transformation of ket vectors by U

$$\langle U\alpha|U\beta\rangle = \langle\alpha|U^\dagger U|\beta\rangle = \langle\alpha|\beta\rangle \quad (1.24)$$

Consider now an equation consisting of kets, scalars, and operators, such as

$$A_1|\alpha_1\rangle = c_2|\alpha_2\rangle + c_3|\alpha_3\rangle\langle\alpha_4|A_2|\alpha_5\rangle + c_6A_3^\dagger A_4|\alpha_6\rangle \quad (1.25)$$

To find its bra form we hermitian conjugate, and get

$$\langle\alpha_1|A_1^\dagger = \langle\alpha_2|c_2^* + \langle\alpha_5|A_2^\dagger|\alpha_4\rangle\langle\alpha_3|c_3^* + \langle\alpha_6|A_4^\dagger A_3 c_6^* \quad (1.26)$$

The rule for taking the hermitian conjugate or adjoint of the most general eq is:

When a product of matrices, bras, kets, and explicit numerical coefficients is encountered, reverse the order of all factors and make the substitutions $A \leftrightarrow A^\dagger$, $|\alpha\rangle \leftrightarrow \langle\alpha|$, $c \leftrightarrow c^*$.

The standard basis vectors E_i and E_i^t will be denoted by $|i\rangle$ and $\langle i|$, $i = 1, 2, \dots, n$

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad |2\rangle = \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix}, \quad \dots \quad |n\rangle = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix} \quad (1.27)$$

The kets $|i\rangle$ are mutually orthogonal and normalised

$$\langle i|j\rangle = \delta_{ij} \quad (1.28)$$

and form the **canonical** orthonormal basis over which $|\alpha\rangle$ and $\langle\alpha|$ can be decomposed as

$$|\alpha\rangle = \sum_{i=1}^n a_i |i\rangle, \quad \langle\alpha| = \sum_{i=1}^n a_i^* \langle i| \quad (1.29)$$

Their components are

$$a_i = \langle i|\alpha\rangle \Rightarrow |\alpha\rangle = \sum_{i=1}^n |i\rangle \langle i|\alpha\rangle, \quad a_i^* = \langle\alpha|i\rangle \Rightarrow \langle\alpha| = \sum_{i=1}^n \langle\alpha|i\rangle \langle i| \quad (1.30)$$

- Vectors

$$|Ui\rangle = U|i\rangle = \sum_{j=1}^n U_{ji}|j\rangle, \quad \langle Ui|Uj\rangle = \delta_{ij}, \quad U^\dagger U = I \quad (1.31)$$

also form an orthonormal basis of the ket vector space.

- Kets are columns, i.e. $n \times 1$ matrices, and bras are rows, i.e. $1 \times n$ matrices.

The matrix product of a ket and a bra is an $n \times n$ matrix

$$(|\mu\rangle\langle\nu|)|\alpha\rangle = |\mu\rangle\langle\nu|\alpha\rangle = |\mu\rangle\langle\nu|\alpha\rangle, \quad \langle\alpha|(|\mu\rangle\langle\nu|) = \langle\alpha|\mu\rangle\langle\nu| \quad (1.32)$$

- If c is a scalar

$$c|\mu\rangle\langle\nu| = |\mu\rangle c\langle\nu| = |\mu\rangle\langle\nu|c \quad (1.33)$$

Let $c = \langle\alpha|\beta\rangle$

$$\langle\alpha|\beta\rangle|\mu\rangle\langle\nu| = |\mu\rangle\langle\alpha|\beta\rangle\langle\nu| = (|\mu\rangle\langle\alpha|)(|\beta\rangle\langle\nu|) \quad (1.34)$$

The r.h.s. of this equation is the product of two matrices.

- Consider the matrices $|i\rangle\langle j|$

$$(|i\rangle\langle j|)|\alpha\rangle = |i\rangle\langle j|\alpha\rangle = a_j|i\rangle, \quad \langle\alpha|(|i\rangle\langle j|) = \langle\alpha|i\rangle\langle j| = a_i^*\langle j| \quad (1.35)$$

This action coincides with the product of $E_{ij} = (\delta_{ik}\delta_{jl})$ with α , and therefore

$$|i\rangle\langle j| = E_{ij}, \quad (E_{ij})_{kl} = \delta_{ik}\delta_{jl} \quad (1.36)$$

- Thus, any $n \times n$ matrix can be decomposed as

$$A = (A_{ij}) = \sum_{i,j=1}^n A_{ij}|i\rangle\langle j| = \sum_{i,j=1}^n \langle i|A|j\rangle |i\rangle\langle j| = \sum_{i,j=1}^n |i\rangle\langle i|A|j\rangle\langle j|, \quad A_{ij} = \langle i|A|j\rangle \quad (1.37)$$

- Its action on basis kets is

$$A|i\rangle = \sum_{j,k=1}^n |j\rangle\langle j|A|k\rangle\langle k|i\rangle = \sum_{j=1}^n |j\rangle A_{ji} = \sum_{j=1}^n A_{ji}|j\rangle \quad (1.38)$$

- The product of two matrices

$$\begin{aligned} AB &= \sum_{i,j=1}^n A_{ij}|i\rangle\langle j| \sum_{k,l=1}^n B_{kl}|k\rangle\langle l| = \sum_{i,j,k,l=1}^n A_{ij}B_{kl}|i\rangle\langle j||k\rangle\langle l| \\ &= \sum_{i,j,k,l=1}^n A_{ij}B_{kl}|i\rangle\langle j|k\rangle\langle l| = \sum_{i,j,k,l=1}^n A_{ij}B_{kl}|i\rangle\delta_{jk}\langle l| = \sum_{i,j,l=1}^n A_{ij}B_{jl}|i\rangle\langle l| \\ &= \sum_{i,l=1}^n (AB)_{il}|i\rangle\langle l| \end{aligned} \quad (1.39)$$

- The identity matrix I is given by

$$I = \sum_{i=1}^n |i\rangle\langle i| = \sum_{i=1}^n P_i, \quad P_i \equiv |i\rangle\langle i| \quad (1.40)$$

- (i) The matrix P_i is called the projection operator for the ket $|i\rangle$ because its action on any ket $|\alpha\rangle$ produces $a_i|i\rangle$ that is the projection of $|\alpha\rangle$ along the direction $|i\rangle$.
- (ii) They satisfy

$$P_i P_j = |i\rangle\langle i||j\rangle\langle j| = |i\rangle\langle i|j\rangle\langle j| = \delta_{ij}|i\rangle\langle j| = \delta_{ij}P_j \quad (1.41)$$

- (iii) Equation (1.40) is called the **completeness relation**

- (iv) The matrix multiplication rule can be obtained by using (1.40)

$$(AB)_{ij} = \langle i|AB|j\rangle = \langle i|AIB|j\rangle = \langle i|A \sum_{k=1}^n |k\rangle\langle k|B|j\rangle = \sum_{k=1}^n A_{ik}B_{kj} \quad (1.42)$$

- The projection operator along the direction of any normalised vector $|\nu\rangle$ is

$$P_{|\nu\rangle} = |\nu\rangle\langle\nu| = \sum_{i,j=1}^n \nu_i^* \nu_j |i\rangle\langle j|, \quad P_{|\nu\rangle}^\dagger = P_{|\nu\rangle}, \quad P_{|\nu\rangle} P_{|\nu\rangle} = P_{|\nu\rangle} \quad (1.43)$$

In QM measurements are represented by projection operators applied to a state vector.

The Pauli matrices σ^α (sometimes also denoted by τ_α) are

$$\sigma^1 \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2 \equiv \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^3 \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (1.44)$$

- In bra-ket notation

$$\sigma^1 = |1\rangle\langle 2| + |2\rangle\langle 1|, \quad \sigma^2 = -i|1\rangle\langle 2| + i|2\rangle\langle 1|, \quad \sigma^3 = |1\rangle\langle 1| - |2\rangle\langle 2| \quad (1.45)$$

- They form a basis of traceless 2×2 matrices, are hermitian and unitary
- They act on the basis vectors as

$$\sigma^1|1\rangle = |2\rangle, \quad \sigma^1|2\rangle = |1\rangle, \quad \sigma^2|1\rangle = i|2\rangle, \quad \sigma^2|2\rangle = -i|1\rangle, \quad \sigma^3|1\rangle = |1\rangle, \quad \sigma^3|2\rangle = -|2\rangle$$

Thus, $|1\rangle$ and $|2\rangle$ are eigenvectors of σ^3 with eigenvalues 1 and -1 .

- Products $\sigma^\alpha \sigma^\beta$

$$\begin{aligned} \sigma^1 \sigma^2 &= (|1\rangle\langle 2| + |2\rangle\langle 1|)(-i|1\rangle\langle 2| + i|2\rangle\langle 1|) = i|1\rangle\langle 1| - i|2\rangle\langle 2| = i\sigma^3 \\ \sigma^2 \sigma^1 &= -i\sigma^3, \quad \sigma^1 \sigma^3 = -i\sigma^2, \quad \sigma^3 \sigma^1 = i\sigma^2, \quad \sigma^2 \sigma^3 = i\sigma^1, \quad \sigma^3 \sigma^2 = -i\sigma^1 \end{aligned}$$

- They satisfy the relations

$$\sigma^\alpha \sigma^\beta + \sigma^\beta \sigma^\alpha = 2\delta^{\alpha\beta} I \quad (1.46)$$

$$[\sigma^\alpha, \sigma^\beta] = 2i \sum_{\gamma=1}^3 \epsilon^{\alpha\beta\gamma} \sigma^\gamma \quad \Leftrightarrow \quad \left[\frac{\sigma^\alpha}{2i}, \frac{\sigma^\beta}{2i} \right] = \sum_{\gamma=1}^3 \epsilon^{\alpha\beta\gamma} \frac{\sigma^\gamma}{2i} \quad (1.47)$$

Def. A unital associative algebra \mathcal{A} over \mathbb{C} is said to be generated by elements $\mathcal{I}, \mathcal{Z}_1, \mathcal{Z}_2, \dots, \mathcal{Z}_N$ that satisfy the defining relations

$$\mathcal{F}_\alpha(\mathcal{Z}_1, \dots, \mathcal{Z}_N) = \mathcal{O}, \quad \alpha = 1, \dots, M \quad (1.48)$$

where \mathcal{O} is the zero vector of \mathcal{A} , if

- (i) The vectors of \mathcal{A} are linear combinations of the identity element \mathcal{I} and all words made of \mathcal{Z}_i 's

$$\mathcal{I}, \mathcal{Z}_i, \mathcal{Z}_i\mathcal{Z}_j, \mathcal{Z}_i\mathcal{Z}_j\mathcal{Z}_k, \dots, \mathcal{Z}_{i_1}\cdots\mathcal{Z}_{i_n}, \dots \quad (1.49)$$

- (ii) The multiplication is defined in a natural way by “gluing” words

$$(\mathcal{Z}_{i_1}\cdots\mathcal{Z}_{i_k}) * (\mathcal{Z}_{j_1}\cdots\mathcal{Z}_{j_n}) = \mathcal{Z}_{i_1}\cdots\mathcal{Z}_{i_k}\mathcal{Z}_{j_1}\cdots\mathcal{Z}_{j_n} \quad (1.50)$$

- (iii) The relations (1.48) are taken into account by identifying vectors \mathcal{T}_1 and \mathcal{T}_2 if

$$\mathcal{T}_2 - \mathcal{T}_1 = \sum_{a,\beta} \mathcal{V}_a^\beta * \mathcal{F}_\beta * \mathcal{W}_a^\beta \quad (1.51)$$

for some elements $\mathcal{V}_a^\beta, \mathcal{W}_a^\beta$ of \mathcal{A} .

If we now forget that σ^α are 2×2 matrices, and think about them as generators of an algebra then the relations (1.46) are the defining relations of the Clifford algebra $\mathbb{C}l_3$ where 3 refers to the number of generators in the algebra.

Def. A representation of a unital associative algebra \mathcal{A} (also called a left \mathcal{A} -module) denoted by (ρ, \mathcal{V}) is a vector space \mathcal{V} together with a homomorphism of algebras $\rho : \mathcal{A} \mapsto \text{End}(\mathcal{V})$, i.e., a linear map preserving the multiplication and unit

$$\rho : \mathcal{A} \mapsto \text{End}(\mathcal{V}), \quad \mathcal{A} \ni \mathcal{T} \mapsto \rho(\mathcal{T}) \in \text{End}(\mathcal{V}), \quad \rho(\mathcal{S} * \mathcal{T}) = \rho(\mathcal{S})\rho(\mathcal{T}) \quad (1.52)$$

Clearly, $\rho(\mathcal{A})$ is a subalgebra of the algebra of operators acting in \mathcal{V} . The dimension of the representation is equal to the dimension of \mathcal{V} . If $\mathcal{V} = \mathbb{C}^n$ then

$$\text{End}(\mathcal{V}) = \text{Mat}(n) \quad \Rightarrow \quad \rho(\mathcal{A}) \subset \text{Mat}(n) \quad (1.53)$$

and the algebra \mathcal{A} is represented by $n \times n$ matrices acting in \mathbb{C}^n . Thus, the Pauli matrices provide a two-dimensional representation of the generators of the Clifford algebra $\mathbb{C}l_3$.

Def. A **Lie algebra** is a vector space \mathcal{G} over a field \mathbb{F} with a bilinear operation $[\cdot, \cdot]: \mathcal{G} \times \mathcal{G} \mapsto \mathcal{G}$ which is called a commutator or a Lie bracket, such that the following axioms are satisfied:

- It is skew symmetric: $[\mathcal{J}, \mathcal{J}] = \mathcal{O}$ which implies $[\mathcal{J}, \mathcal{K}] = -[\mathcal{K}, \mathcal{J}]$ for all $\mathcal{J}, \mathcal{K} \in \mathcal{G}$
- It satisfies the Jacobi Identity: $[\mathcal{J}, [\mathcal{K}, \mathcal{L}]] + [\mathcal{K}, [\mathcal{L}, \mathcal{J}]] + [\mathcal{L}, [\mathcal{J}, \mathcal{K}]] = \mathcal{O}$
where \mathcal{O} is the zero vector of \mathcal{G} .

Clearly, a Lie algebra is in general a non-associative algebra with the multiplication $*$ given by the bracket $[\cdot, \cdot]$. Given a basis \mathcal{E}_i , $i = 1, \dots, \dim \mathcal{G}$ of \mathcal{G} its Lie algebra structure is determined by commutators of the basis vectors

$$[\mathcal{E}_i, \mathcal{E}_j] = \sum_{k=1}^{\dim \mathcal{G}} c_{ij}^k \mathcal{E}_k \quad (1.54)$$

Here $c_{ij}^k \in \mathbb{F}$ are called the structure constants of the Lie algebra \mathcal{G} .

A representation of a Lie algebra is defined similar to the one for associative algebras.

Def. A representation of a Lie algebra \mathcal{G} (also called a left \mathcal{G} -module) denoted by (ρ, \mathcal{V}) is a vector space \mathcal{V} together with a homomorphism of Lie algebras $\rho : \mathcal{G} \mapsto \text{End}(\mathcal{V})$, i.e., a linear map preserving the commutator

$$\rho : \mathcal{G} \mapsto \text{End}(\mathcal{V}), \quad \mathcal{G} \ni \mathcal{J} \mapsto \rho(\mathcal{J}) \in \text{End}(\mathcal{V}), \quad \rho([\mathcal{J}, \mathcal{K}]) = [\rho(\mathcal{J}), \rho(\mathcal{K})] \quad (1.55)$$

In particular, the Lie algebra commutation relations (1.54) are preserved by ρ

$$T_i = \rho(\mathcal{E}_i) \quad \Rightarrow \quad [T_i, T_j] = \sum_{k=1}^{\dim \mathcal{G}} c_{ij}^k T_k \quad (1.56)$$

Clearly, if a Lie algebra is a subspace of the space of $n \times n$ matrices then, the Lie bracket is the usual commutator of matrices.

Def. The Lie algebra $\mathfrak{sl}(n, \mathbb{F})$ over \mathbb{F} , where \mathbb{F} is either \mathbb{C} or \mathbb{R} is isomorphic to the Lie algebra of $n \times n$ **traceless matrices**, $\text{tr} A = 0 \quad \forall A \in \mathfrak{sl}(n, \mathbb{F})$.

Since σ^α form a basis of 2×2 complex traceless matrices, the relations

$$[\sigma^\alpha, \sigma^\beta] = 2i\epsilon^{\alpha\beta\gamma}\sigma^\gamma$$

are the commutation relations of $\mathfrak{sl}(2, \mathbb{C})$.

The Pauli matrices provide a **defining representation** of the $\mathfrak{sl}(2, \mathbb{C})$ algebra.

Another widely used basis of 2×2 traceless matrices is

$$\sigma^+ \equiv \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = |1\rangle\langle 2|, \quad \sigma^- \equiv \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = |2\rangle\langle 1|, \quad \sigma^3 \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = |1\rangle\langle 1| - |2\rangle\langle 2| \quad (1.57)$$

They satisfy the commutation relations

$$[\sigma^+, \sigma^-] = \sigma_3, \quad [\sigma^3, \sigma^\pm] = \pm 2\sigma^\pm \quad (1.58)$$

Since these matrices are real, this basis is suitable for both $\mathfrak{sl}(2, \mathbb{C})$ and $\mathfrak{sl}(2, \mathbb{R})$.

It is said that $\mathfrak{sl}(n, \mathbb{R})$ is a **real form** of $\mathfrak{sl}(n, \mathbb{C})$.

The representation of $\mathfrak{sl}(2, \mathbb{C})$ is not unique. We can also realise $\mathfrak{sl}(2, \mathbb{C})$ by the matrices

$$\sigma_{\Phi}^{\alpha} = \Phi \sigma^{\alpha} \Phi^{-1}, \quad \Phi \in GL(2, \mathbb{C}) \quad (1.59)$$

which obviously satisfy the $\mathfrak{sl}(2, \mathbb{C})$ commutation relations.

The same is true for any Lie algebra \mathcal{G} .

Given a representation (1.56), and an invertible linear operator Φ , the operators

$$T_i^{\Phi} = \Phi T_i \Phi^{-1} = \Phi \rho(\mathcal{E}_i) \Phi^{-1} \quad (1.60)$$

form a basis of another representation of \mathcal{G} .

This leads to the following natural definition

Def. Two representations (ρ_1, \mathcal{V}_1) and (ρ_2, \mathcal{V}_2) of \mathcal{G} (or \mathcal{A}) are called equivalent, or isomorphic, if there is an invertible linear operator $\Phi : \mathcal{V}_1 \mapsto \mathcal{V}_2$ which commutes with the action of \mathcal{G} , i.e.,

$$\Phi \rho_1(\mathcal{J}) = \rho_2(\mathcal{J})\Phi \quad \Leftrightarrow \quad \rho_2(\mathcal{J}) = \Phi \rho_1(\mathcal{J})\Phi^{-1} \quad (1.61)$$

For example, the representation of $\mathfrak{sl}(2, \mathbb{C})$ by the Pauli matrices is equivalent to the following one

$$\rho_2(\mathcal{J}^1) = \sigma^2, \quad \rho_2(\mathcal{J}^2) = \sigma^3, \quad \rho_2(\mathcal{J}^3) = \sigma^1 \quad (1.62)$$

with the matrix Φ equal to

$$\Phi = \begin{pmatrix} \frac{1}{2} + \frac{i}{2} & \frac{1}{2} + \frac{i}{2} \\ -\frac{1}{2} + \frac{i}{2} & \frac{1}{2} - \frac{i}{2} \end{pmatrix} \quad (1.63)$$

Def. The Lie algebra $\mathfrak{su}(n)$ over \mathbb{R} is the vector space of $n \times n$ **traceless anti-hermitian matrices**, $A^\dagger = -A$, $\text{tr} A = 0 \ \forall A \in \mathfrak{su}(n)$.

- $\sigma^\alpha/2i$ is a basis of 2×2 traceless anti-hermitian matrices, the relations (1.47)

$$[\sigma^\alpha, \sigma^\beta] = 2i \epsilon^{\alpha\beta\gamma} \sigma^\gamma \quad \Leftrightarrow \quad \left[\frac{\sigma^\alpha}{2i}, \frac{\sigma^\beta}{2i} \right] = \epsilon^{\alpha\beta\gamma} \frac{\sigma^\gamma}{2i}$$

are the commutation relations of $\mathfrak{su}(2)$

- The matrices $T^\alpha = \sigma^\alpha/2i$ provide a defining representation of the $\mathfrak{su}(2)$ algebra.
- T^α being traceless also provide a basis of $\mathfrak{sl}(2, \mathbb{C})$
- Thus, $\mathfrak{su}(2)$ is a real form of $\mathfrak{sl}(2, \mathbb{C})$ while $\mathfrak{sl}(2, \mathbb{C})$ is said to be the complexification of $\mathfrak{su}(2)$.
- The two real forms $\mathfrak{sl}(2, \mathbb{R})$ and $\mathfrak{su}(2)$ of $\mathfrak{sl}(2, \mathbb{C})$ are not isomorphic as real Lie algebras.

In the case of the $\mathfrak{su}(n)$ algebra we are interested in representations by traceless anti-hermitian matrices (or in general by operators).

- Such a representation is called unitary
- Equivalent representations are called unitarily equivalent because for them Φ must be unitary
- For example, Φ given by (1.63)

$$\Phi = \begin{pmatrix} \frac{1}{2} + \frac{i}{2} & \frac{1}{2} + \frac{i}{2} \\ -\frac{1}{2} + \frac{i}{2} & \frac{1}{2} - \frac{i}{2} \end{pmatrix}$$

is unitary, and therefore the representations by $T^\alpha = \sigma^\alpha/2i$ and $T_\Phi^\alpha = \Phi T^\alpha \Phi^\dagger$ are unitarily equivalent.

The spin operators \hat{S}^α are related to \hat{T}^α as $\hat{S}^\alpha = i\hbar \hat{T}^\alpha$

- The hermitian matrices $S^\alpha = \frac{\hbar}{2}\sigma^\alpha$ represent the spin operators.
- As $(\sigma^\alpha)^2 = I$, we get

$$\sum_{\alpha} (S^\alpha)^2 = s(s+1)\hbar^2 I = \frac{3}{4}\hbar^2 I$$

and therefore, it is a spin 1/2 representation.

- The canonical basis vectors $|1\rangle$ and $|2\rangle$ are eigenvectors of σ^3 with eigenvalues $\hbar/2$ and $-\hbar/2$.
- In QM they are interpreted as spin up and spin down state vectors
- They are usually denoted by

$$|\uparrow\rangle \equiv |1\rangle, \quad |\downarrow\rangle \equiv |2\rangle \quad \text{or} \quad |+\rangle \equiv |1\rangle, \quad |-\rangle \equiv |2\rangle \quad (1.64)$$

- In this notation

$$S^x = \frac{\hbar}{2}(|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|), \quad S^y = \frac{\hbar}{2}(-i|\uparrow\rangle\langle\downarrow| + i|\downarrow\rangle\langle\uparrow|), \quad S^z = \frac{\hbar}{2}(|\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|)$$

- If a particle is in an eigenstate of S^z then S^x and S^y acting on the state flip the spin.

One might think that the representation theories of unital associative algebras and Lie algebras are different. There is however no difference.

Def. A universal enveloping algebra of a Lie algebra \mathcal{G} over \mathbb{F} with basis elements \mathcal{E}_i satisfying the commutation relations

$$[\mathcal{E}_i, \mathcal{E}_j] = \sum_{k=1}^{\dim \mathcal{G}} c_{ij}^k \mathcal{E}_k \quad (1.65)$$

is a unital associative algebra $\mathcal{U}(\mathcal{G})$ over \mathbb{F} generated by elements $\mathcal{I}, \mathcal{E}_i, i = 1, \dots, \dim \mathcal{G}$ that satisfy the relations (1.65).

Obviously, any representation of $\mathcal{U}(\mathcal{G})$ is a representation of \mathcal{G} , and the other way around.

In what follows when we say a representation of \mathcal{G} we also mean $\mathcal{U}(\mathcal{G})$ that is we allow ourself to consider not only commutators but also products of the operators representing \mathcal{G} .

Generalisation to arbitrary orthonormal basis $|e_i\rangle$ of kets

$$\langle e_i | e_j \rangle = \delta_{ij}, \quad |e_i\rangle = U|i\rangle, \quad U = \sum_i |e_i\rangle \langle i|, \quad U^\dagger U = U U^\dagger = I \quad (1.66)$$

- The completeness relation has the same form as with canonical basis vectors

$$\sum_{i=1}^n |e_i\rangle \langle e_i| = \sum_{i=1}^n U|i\rangle \langle i|U^\dagger = U \sum_{i=1}^n |i\rangle \langle i|U^\dagger = U I U^\dagger = I \quad (1.67)$$

- Any α is expanded as

$$|\alpha\rangle = I|\alpha\rangle = \sum_{i=1}^n |e_i\rangle \langle e_i|\alpha\rangle \quad (1.68)$$

where $\langle e_i|\alpha\rangle$ are the components of the ket $|\alpha\rangle$ with respect to the basis $|e_i\rangle$.

- Any matrix A is expanded as

$$A = I A I = \sum_{i=1}^n |e_i\rangle \langle e_i| A \sum_{j=1}^n |e_j\rangle \langle e_j| = \sum_{i,j=1}^n |e_i\rangle \langle e_i| A |e_j\rangle \langle e_j| = \sum_{i,j=1}^n \langle e_i| A |e_j\rangle |e_i\rangle \langle e_j| \quad (1.69)$$

where $\langle e_i| A |e_j\rangle$ are the elements of the matrix A with respect to the basis $|e_i\rangle$.

- (1.68) and (1.69) allow us to define an abstract vector space with an inner product and consider linear operators or transformations acting in the space. Components and matrix elements appear after one has chosen a particular basis in the space.

- A change of a basis is called a **passive transformation** because it does not change vectors and matrices.
- An **active transformation** changes vectors and matrices but keeps the basis untouched.
- We require that the transformed vector and matrix would have the components $\langle e_i|\alpha\rangle$ and the matrix elements $\langle e_i|A|e_j\rangle$

$$|\alpha\rangle \mapsto |\tilde{\alpha}\rangle = \sum_{i=1}^n |i\rangle \langle e_i|\alpha\rangle = U^\dagger |\alpha\rangle \quad (1.70)$$

$$A \mapsto \tilde{A} = \sum_{i,j=1}^n |i\rangle \langle e_i|A|e_j\rangle \langle j| = U^\dagger A U \quad (1.71)$$

- A basis is transformed by U while vectors are by U^\dagger , and

$$\langle \alpha|A|\beta\rangle = \langle \tilde{\alpha}|\tilde{A}|\tilde{\beta}\rangle \quad (1.72)$$

- In QM $\langle \alpha|A|\beta\rangle$ encode physical properties of a mechanical system. Physical transformations are represented by unitary operators, and if the properties of the system do not change under one, then the matrix elements do not change either. Active and passive transformations provide us with two equivalent ways of describing the same symmetries.

Hilbert space

Let us set the dimension of the ket and bra vector spaces to infinity.

- Kets and bras become semi-infinite columns and rows while matrices become unbounded from below and from the right.
- Refer to these “matrices” as operators acting in the infinite dimensional space. To stress that they act in an infinite dimensional space we place a hat above them – \hat{T} .
- There is no problem in describing vectors and operators by using the bra-ket formalism. We can still define the addition of vectors and their multiplication by scalars in the same way as for finite-dimensional spaces.
- The dot product cannot be defined for any vector, e.g. $\sum_{i=1}^{\infty} |i\rangle$
- We consider vectors of finite length which we call normalisable.
- These vectors form a vector space because the addition of normalisable vectors and their multiplication by scalars also produce normalisable vectors.

This obviously holds for the multiplication by a scalar. As to the addition, it follows from the triangle inequality

$$|\alpha + \beta| \leq |\alpha| + |\beta| < \infty \quad (1.73)$$

- Thus, the set of vectors of finite length is closed under the vector addition and the scalar multiplication, and is a vector space with a dot product.

This space is an example of a **Hilbert space**.

- An operator may transform a finite-length vector to a non-normalisable one.

(i) As an example, consider an operator \hat{N} acting on the basis kets as

$$\hat{N}|i\rangle = i|i\rangle \quad (1.74)$$

(ii) Then, acting with \hat{N} on the ket

$$|\alpha\rangle = \sum_{i=1}^{\infty} \frac{1}{i} |i\rangle, \quad \langle\alpha|\alpha\rangle = \sum_{i=1}^{\infty} \frac{1}{i^2} = \frac{\pi^2}{6} \quad (1.75)$$

one gets the non-normalisable vector $\hat{N}|\alpha\rangle = \sum_{i=1}^{\infty} |i\rangle$

- Thus, in general an operator is not well-defined on the whole Hilbert space.
- The domain of an operator is the subspace on which the operator is well-defined, i.e. the operator maps a vector from its domain to a normalisable vector.
- The trace and the determinant may not be defined for some operators.

For example, the trace does not exist for the identity operator \hat{I} , and both the trace and the determinant do not exist for the operator \hat{N} .

Creation and annihilation operators

It is common in QM to start numbering basis vectors not from 1 but from 0

$$|\psi\rangle = \sum_{n=0}^{\infty} \psi_n |n\rangle, \quad \sum_{n=0}^{\infty} |\psi_n|^2 < \infty \quad (1.76)$$

Consider two operators \hat{a} and \hat{a}^\dagger which satisfy

$$[\hat{a}, \hat{a}^\dagger] = \hat{I} \quad (1.77)$$

and act on the basis ket and bra vectors as

$$\begin{aligned} \hat{a}|0\rangle &= 0, & \hat{a}|n\rangle &= c_{n-1}|n-1\rangle, & \hat{a}^\dagger|n\rangle &= d_n|n+1\rangle \\ \langle 0|\hat{a}^\dagger &= 0, & \langle n|\hat{a}^\dagger &= \langle n-1|c_{n-1}^*, & \langle n|\hat{a} &= \langle n+1|d_n^* \end{aligned} \quad (1.78)$$

- \hat{a} and \hat{a}^\dagger are called the annihilation and creation operators, respectively.
- $|0\rangle$ is called the vacuum state or the vacuum because it is destroyed by \hat{a}

- Let us find the conditions c_n and d_n satisfy.

(i) $\hat{a} = (\hat{a}^\dagger)^\dagger \Rightarrow$

$$\langle n+1|\hat{a}^\dagger|n\rangle = \langle n+1|d_n|n+1\rangle = d_n \quad (1.79)$$

and

$$\langle n+1|\hat{a}^\dagger|n\rangle = \langle n|c_n^*|n\rangle = c_n^* \quad (1.80)$$

Thus,

$$d_n = c_n^* \quad (1.81)$$

(ii) Then,

$$\hat{a}\hat{a}^\dagger|0\rangle = d_0\hat{a}|1\rangle = d_0c_0|0\rangle \quad (1.82)$$

and

$$\hat{a}\hat{a}^\dagger|0\rangle = (\hat{I} + \hat{a}^\dagger\hat{a})|0\rangle = |0\rangle \Rightarrow |c_0| = 1 \quad (1.83)$$

(iii) Similarly,

$$\hat{a}\hat{a}^\dagger|n\rangle = d_n\hat{a}|n+1\rangle = d_nc_n|n\rangle \quad (1.84)$$

and

$$\hat{a}\hat{a}^\dagger|n\rangle = (\hat{I} + \hat{a}^\dagger\hat{a})|n\rangle = |n\rangle + \hat{a}^\dagger c_{n-1}|n-1\rangle = |n\rangle + c_{n-1}d_{n-1}|n\rangle \quad (1.85)$$

Thus,

$$|c_n|^2 = 1 + |c_{n-1}|^2, \quad |c_0| = 1 \quad (1.86)$$

(iv) These recursion relations can be easily solved

$$|c_0| = 1, \quad |c_1|^2 = 2, \quad |c_2|^2 = 3, \quad \dots \quad |c_n|^2 = n + 1 \quad (1.87)$$

(v) Thus, the most general solution is

$$c_n = \sqrt{n+1} e^{i\phi_n}, \quad d_n = \sqrt{n+1} e^{-i\phi_n}, \quad \phi_n \in \mathbb{R} \quad (1.88)$$

and

$$\hat{a}|n\rangle = \sqrt{n} e^{i\phi_{n-1}}|n-1\rangle, \quad \hat{a}^\dagger|n\rangle = \sqrt{n+1} e^{-i\phi_n}|n+1\rangle \quad (1.89)$$

- The simplest solution is obtained by setting $\phi_n = 0$ for all n (and dropping the hat)

$$a|n\rangle = \sqrt{n}|n-1\rangle, \quad a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle \quad (1.90)$$

- All basis vectors can be created by the repeated action of a^\dagger on the vacuum

$$\begin{aligned} |n+1\rangle &= \frac{1}{\sqrt{n+1}} a^\dagger|n\rangle = \frac{1}{\sqrt{n+1}} \frac{1}{\sqrt{n}} a^\dagger a^\dagger|n-1\rangle = \frac{1}{\sqrt{(n+1)n}} \frac{1}{\sqrt{n-1}} (a^\dagger)^3|n-2\rangle \\ &= \frac{1}{\sqrt{(n+1)n \cdots (n+2-k)}} \frac{1}{\sqrt{n+1-k}} (a^\dagger)^{k+1}|n-k\rangle = \frac{1}{\sqrt{(n+1)n \cdots 2}} (a^\dagger)^{n+1}|0\rangle \end{aligned}$$

- Thus,

$$|n\rangle = \frac{1}{\sqrt{n!}} (a^\dagger)^n |0\rangle \quad (1.91)$$

- (i) The number n labelling the basis vector is equal to the number of creation operators applied to the vacuum.
- (ii) Hilbert space created this way is often called the Fock space.
- (iii) In QM it is often said that it is a state with n quanta.
- (iv) (1.91) implies that any operator acting in the Hilbert space is a linear combination of the identity operator and products of creation and annihilation operators.
- From formulae (1.90) we get the bra-ket form of a and a^\dagger

$$a = \sum_{n=0}^{\infty} \sqrt{n} |n-1\rangle \langle n| = \sum_{n=0}^{\infty} \sqrt{n+1} |n\rangle \langle n+1|, \quad a^\dagger = \sum_{n=0}^{\infty} \sqrt{n+1} |n+1\rangle \langle n| \quad (1.92)$$

where we have written the formula for a so that it would be manifest that a and a^\dagger are Hermitian conjugate to each other.

- Let us use formulae (1.92) to check that the commutation relation (1.77) is satisfied

$$\begin{aligned}
[a, a^\dagger] &= aa^\dagger - a^\dagger a = \sum_{k=0}^{\infty} \sqrt{k+1} |k\rangle \langle k+1| \sum_{n=0}^{\infty} \sqrt{n+1} |n+1\rangle \langle n| \\
&\quad - \sum_{n=0}^{\infty} \sqrt{n+1} |n+1\rangle \langle n| \sum_{k=0}^{\infty} \sqrt{k+1} |k\rangle \langle k+1| \\
&= \sum_{n=0}^{\infty} (n+1) |n\rangle \langle n| - \sum_{n=0}^{\infty} (n+1) |n+1\rangle \langle n+1| \\
&= \sum_{n=0}^{\infty} (n+1) |n\rangle \langle n| - \sum_{n=0}^{\infty} n |n\rangle \langle n| = \sum_{n=0}^{\infty} |n\rangle \langle n| = \hat{I}
\end{aligned} \tag{1.93}$$

- The basis vectors are eigenvectors of the Hermitian operator $N = a^\dagger a$ (and aa^\dagger) with the eigenvalues

$$N|n\rangle = a^\dagger a|n\rangle = a^\dagger \sqrt{n} |n-1\rangle = n|n\rangle \tag{1.94}$$

- $N = a^\dagger a$ is called the number operator because its eigenvalue is equal to the number of quanta in an eigenstate.

\hat{a} and \hat{a}^\dagger can be used to construct a representation of the Heisenberg algebra

Def. The Heisenberg algebra \mathfrak{H} (also called the Weyl algebra) is a unital associative algebra over \mathbb{C} generated by elements \mathcal{I} , \mathcal{X} , \mathcal{P} that satisfy the relation

$$[\mathcal{X}, \mathcal{P}] \equiv \mathcal{X} * \mathcal{P} - \mathcal{P} * \mathcal{X} = i \hbar \mathcal{I} \quad (1.95)$$

- Ansatz for \hat{X} and \hat{P} which represent \mathcal{X} and \mathcal{P} as operators

$$\hat{X} = \eta_x \hat{a} + \eta_x^* \hat{a}^\dagger, \quad \hat{P} = \eta_p \hat{a} + \eta_p^* \hat{a}^\dagger \quad (1.96)$$

- Their commutator

$$[\hat{X}, \hat{P}] = [\eta_x \hat{a} + \eta_x^* \hat{a}^\dagger, \eta_p \hat{a} + \eta_p^* \hat{a}^\dagger] = (\eta_x \eta_p^* - \eta_x^* \eta_p) \hat{I} \quad (1.97)$$

- Thus, if

$$\eta_x \eta_p^* - \eta_x^* \eta_p = i \hbar \quad (1.98)$$

then \hat{X} and \hat{P} given by (1.96) satisfy the Heisenberg algebra commutation relation, and provide a representation of \mathfrak{H} in the Hilbert space.

- The standard choice is

$$\eta_x^* = \eta_x \equiv \eta, \quad \eta_p^* = -\eta_p = \frac{i \hbar}{2 \eta} \quad (1.99)$$

- \hat{X} and \hat{P} are expressed through \hat{a} and \hat{a}^\dagger as

$$\hat{X} = \eta(\hat{a}^\dagger + \hat{a}), \quad \hat{P} = \frac{i\hbar}{2\eta}(\hat{a}^\dagger - \hat{a}) \quad (1.100)$$

- The inverse transformation is

$$\hat{a} = \frac{1}{2\eta}\hat{X} + i\frac{\eta}{\hbar}\hat{P}, \quad \hat{a}^\dagger = \frac{1}{2\eta}\hat{X} - i\frac{\eta}{\hbar}\hat{P} \quad (1.101)$$

- In QM dynamics of a system is governed by a Hamiltonian and one is interested in its eigenvectors and eigenvalues.
- As an application of (1.100), let us rewrite the harmonic oscillator Hamiltonian

$$\hat{H} = \omega\left(\frac{m\omega\hat{X}^2}{2} + \frac{\hat{P}^2}{2m\omega}\right) \quad (1.102)$$

in terms of a and a^\dagger

$$\begin{aligned} \hat{H} &= \omega\left(\frac{m\omega\eta^2}{2}((a^\dagger)^2 + a^2 + a^\dagger a + aa^\dagger) - \frac{\hbar^2}{8\eta^2 m\omega}((a^\dagger)^2 + a^2 - a^\dagger a - aa^\dagger)\right) \\ &= \omega\left(\frac{m\omega\eta^2}{2} - \frac{\hbar^2}{8\eta^2 m\omega}\right)((a^\dagger)^2 + a^2) + \omega\left(\frac{m\omega\eta^2}{2} + \frac{\hbar^2}{8\eta^2 m\omega}\right)(2a^\dagger a + \hat{I}) \end{aligned} \quad (1.103)$$

- If we choose

$$\eta^2 = \frac{\hbar}{2m\omega} \quad (1.104)$$

then \hat{H} is

$$\hat{H} = \hbar\omega \left(\hat{a}^\dagger \hat{a} + \frac{\hat{I}}{2} \right) = \hbar\omega \left(\hat{N} + \frac{\hat{I}}{2} \right) \quad (1.105)$$

- The basis vector $|n\rangle$ is an eigenvector of \hat{H} with the eigenvalue $\hbar\omega(n + 1/2)$.

The representation $\rho(\mathcal{X}) = \hat{X}$, $\rho(\mathcal{P}) = \hat{P}$ of the Heisenberg algebra

$$\hat{X} = \eta(\hat{a}^\dagger + \hat{a}), \quad \hat{P} = \frac{i\hbar}{2\eta}(\hat{a}^\dagger - \hat{a}), \quad [\hat{a}, \hat{a}^\dagger] = \hat{I} \quad (1.106)$$

is infinite dimensional.

- What happens if we pick any nonzero vector and start acting on it by all operators from the Heisenberg algebra?
- The set of vectors obtained this way is a subspace of our representation space \mathcal{H} .
- If this subspace \mathcal{W} does not coincide with \mathcal{H} then we can restrict ρ to \mathcal{W} and get a **subrepresentation** of ρ .

This discussion applies to any representation of any algebra

Def. A subrepresentation of a representation \mathcal{V} of an algebra \mathcal{A} is a subspace $\mathcal{W} \subset \mathcal{V}$ which is invariant under all the operators $\rho(\mathcal{T}) : \mathcal{V} \mapsto \mathcal{V}$, $\mathcal{T} \in \mathcal{A}$, that is

$$\rho(\mathcal{T})\mathcal{W} \subset \mathcal{W} \quad \forall \mathcal{T}$$

Trivially, \mathcal{O} and \mathcal{V} are always subrepresentations.

Def. A representation $\mathcal{V} \neq \mathcal{O}$ of \mathcal{A} is irreducible if the only subrepresentations of \mathcal{V} are \mathcal{O} and \mathcal{V} .

- The spin 1/2 representation of $\mathcal{U}(\mathfrak{su}(2))$ is irreducible.
- The representation of the Heisenberg algebra is irreducible because
 - (i) any normalised vector in \mathcal{H} can be mapped to $|0\rangle$ by a unitary operator
 - (ii) the whole space is obtained by acting on the vacuum by linear combinations of products of the creation operator.

Irreducible representations are important due to

Schur's Lemma. Any two irreducible representations of \mathcal{A} of the same dimension are equivalent.

- Easy to prove for finite-dimensional representations.
- For representations in infinite dimensional Hilbert space there are subtleties related to domains of operators under consideration.

Resolving these subtleties leads to the following important theorem

The Stone-von Neumann theorem. Any two irreducible unitary representations of the Heisenberg algebra are unitarily equivalent.

- A precise formulation and the proof of the Stone-von Neumann theorem is complicated and far beyond the scope of the course.
- Any representation of the Heisenberg algebra we will encounter is unitarily equivalent to the representation by the creation and annihilation operators.

Example of a reducible representation

Def. The direct sum of two nonzero representations (ρ, \mathcal{V}) and (σ, \mathcal{W}) of an algebra \mathcal{A} is the representation $(\rho \oplus \sigma, \mathcal{V} \oplus \mathcal{W})$ defined by

$$(\rho \oplus \sigma)(\mathcal{T}) = \rho(\mathcal{T}) \oplus \sigma(\mathcal{T}) \quad (1.107)$$

If we choose a basis of $\mathcal{V} \oplus \mathcal{W}$ properly, then $\rho \oplus \sigma$ can be represented in the following block-diagonal form

$$(\rho \oplus \sigma)(\mathcal{T}) = \rho(\mathcal{T}) \oplus \sigma(\mathcal{T}) = \begin{pmatrix} \rho(\mathcal{T}) & 0 \\ 0 & \sigma(\mathcal{T}) \end{pmatrix} \quad (1.108)$$

and each block acts in its own space.

The eigenvectors and eigenvalues of a hermitian matrix have four crucial properties

1. The eigenvalues of a hermitian matrix are real.

Indeed, let $A|\alpha\rangle = \lambda|\alpha\rangle$, $\langle\alpha|\alpha\rangle = 1$. Then, $\langle\alpha|A|\alpha\rangle = \lambda$. On the other hand,

$$\lambda^* = \langle\alpha|A|\alpha\rangle^* = \langle\alpha|A^\dagger|\alpha\rangle = \langle\alpha|A|\alpha\rangle = \lambda$$

2. The eigenvectors of a hermitian matrix belonging to distinct eigenvalues are orthogonal.

Suppose $A|\alpha\rangle = \lambda|\alpha\rangle$, $A|\beta\rangle = \mu|\beta\rangle$, $\lambda \neq \mu$. Then

$$0 = \langle\alpha|A|\beta\rangle - \langle\alpha|A^\dagger|\beta\rangle = \mu\langle\alpha|\beta\rangle - \langle A\alpha|\beta\rangle = (\mu - \lambda)\langle\alpha|\beta\rangle \quad \Rightarrow \quad \langle\alpha|\beta\rangle = 0$$

3. The eigenvectors of a hermitian matrix span the space, and therefore there is an orthonormal basis $|e_i\rangle$ of eigenvectors of A .

4. Any hermitian matrix admits the spectral decomposition

$$A = \sum_{i=1}^n \lambda_i |e_i\rangle\langle e_i| = \sum_{i=1}^n \lambda_i P_{e_i}, \quad A|e_i\rangle = \lambda_i |e_i\rangle, \quad \langle e_i|e_j\rangle = \delta_{ij}, \quad \lambda_i \in \mathbb{R}$$

where $P_{e_i} = |e_i\rangle\langle e_i|$ is the projection operator along the direction of $|e_i\rangle$

$$P_{e_i}P_{e_j} = \delta_{ij}P_{e_j} \quad \forall i, j, = 1, \dots, n$$

This follows from the existence of an orthonormal basis $|e_i\rangle$ of eigenvectors of A .

- Any matrix which is a function of a hermitian matrix can be decomposed as

$$f(A) = \sum_{i=1}^n f(\lambda_i) |e_i\rangle \langle e_i| \quad (1.109)$$

- Since any unitary matrix U is an exponential of a hermitian matrix, $U = \exp(iA)$, it has the decomposition

$$U = e^{iA} = \sum_{i=1}^n e^{i\lambda_i} |e_i\rangle \langle e_i| \quad (1.110)$$

- There are infinitely many hermitian matrices A with the same U due to the periodicity of the exponential function, $\exp(i(\lambda_i + 2\pi)) = \exp(i\lambda_i)$.

Example. Consider a 2×2 hermitian matrix A

- It may have two distinct eigenvalues.
- If they coincide then A is proportional to I .
- Thus, any 2×2 traceless hermitian matrix A has two distinct eigenvalues
- Since $\text{tr} A = 0$ its eigenvalues differ by sign. Thus,

$$A = U \Lambda U^\dagger, \quad \Lambda = \begin{pmatrix} \lambda & 0 \\ 0 & -\lambda \end{pmatrix} = \lambda \sigma^3, \quad \lambda > 0, \quad U \in SU(2) \quad (1.111)$$

- Combine σ^α into a vector of matrices $\vec{\sigma} = (\sigma^1, \sigma^2, \sigma^3)$
- Write any 2×2 traceless hermitian matrix A in the form

$$A = \vec{a} \cdot \vec{\sigma} \equiv \sum_{\alpha=1}^3 a_\alpha \sigma^\alpha, \quad \vec{a} = (a_1, a_2, a_3), \quad a_i \in \mathbb{R} \quad \forall i \quad (1.112)$$

- 2×2 traceless hermitian matrices are identified with real 3-d vectors in \mathbb{R}^3 .

- Since

$$\text{tr} A^2 = \sum_{\alpha, \beta=1}^3 a_\alpha a_\beta \text{tr}(\sigma^\alpha \sigma^\beta) = \sum_{\alpha, \beta=1}^3 a_\alpha a_\beta 2\delta^{\alpha\beta} = 2 \sum_{\alpha=1}^3 a_\alpha^2 = 2\vec{a}^2 = 2\lambda^2 \quad (1.113)$$

the length of \vec{a} is equal to the positive eigenvalue of A .

- The set of 2×2 traceless hermitian matrices with the same eigenvalues $\pm\lambda$ can be identified with a sphere of radius λ .
- Introducing spherical coordinates

$$a_1 = \lambda \cos \phi \sin \theta, \quad a_2 = \lambda \sin \phi \sin \theta, \quad a_3 = \lambda \cos \theta, \quad \vec{a} = \lambda \vec{u}, \quad \vec{u}^2 = 1 \quad (1.114)$$

we can write

$$A = \lambda \vec{u} \cdot \vec{\sigma} \quad (1.115)$$

where \vec{u} is the unit vector in the direction of \vec{a} .

- Any 2×2 unitary matrix U with unit determinant can be written as an exponential of a 2×2 traceless hermitian matrix

$$U = e^{\frac{1}{2i}\vartheta \vec{n} \cdot \vec{\sigma}}, \quad \vec{n} \cdot \vec{\sigma} \equiv \sum_{\alpha=1}^3 n_\alpha \sigma^\alpha, \quad \vec{n}^2 = 1, \quad \vartheta \in \mathbb{R} \quad (1.116)$$

- Taking into account that $(\vec{n} \cdot \vec{\sigma})^2 = I$, it is easy to show that

$$U = e^{\frac{1}{2i}\vartheta \vec{n} \cdot \vec{\sigma}} = I \cos \frac{\vartheta}{2} + \frac{1}{i} \vec{n} \cdot \vec{\sigma} \sin \frac{\vartheta}{2} \quad (1.117)$$

- Choose

$$\vartheta = \theta, \quad \vec{n} = (-\sin \phi, \cos \phi, 0) \quad (1.118)$$

- Then

$$\begin{aligned} U &= \begin{pmatrix} \cos \frac{\theta}{2} & -e^{-i\phi} \sin \frac{\theta}{2} \\ e^{i\phi} \sin \frac{\theta}{2} & \cos \frac{\theta}{2} \end{pmatrix} \\ &= \cos \frac{\theta}{2} (|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|) - e^{-i\phi} \sin \frac{\theta}{2} |\uparrow\rangle\langle\downarrow| + e^{i\phi} \sin \frac{\theta}{2} |\downarrow\rangle\langle\uparrow| \end{aligned} \quad (1.119)$$

- Using (1.117), one shows

$$A = \lambda \vec{u} \cdot \vec{\sigma} = U \Lambda U^\dagger \quad (1.120)$$

- Thus, U diagonalises A , and therefore the eigenvectors of A are

$$\begin{aligned} |e_\uparrow\rangle &= U|\uparrow\rangle = \cos \frac{\theta}{2} |\uparrow\rangle + e^{i\phi} \sin \frac{\theta}{2} |\downarrow\rangle \\ |e_\downarrow\rangle &= U|\downarrow\rangle = \cos \frac{\theta}{2} |\downarrow\rangle - e^{-i\phi} \sin \frac{\theta}{2} |\uparrow\rangle \end{aligned} \quad (1.121)$$

- In QM the spin 1/2 operators S^α are related to the Pauli matrices as $S^\alpha = \hbar \sigma^\alpha / 2$.
- Thus, $\vec{u} \cdot \vec{S}$ is the projection of the spin vector \vec{S} along the unit vector \vec{u} , and the vectors (1.121) are its eigenvectors with eigenvalues $\pm \hbar/2$.

Geometric interpretation of

$$U = e^{\frac{1}{2i}\vartheta \vec{n} \cdot \vec{\sigma}}, \quad \vec{n} \cdot \vec{\sigma} \equiv \sum_{\alpha=1}^3 n_\alpha \sigma^\alpha, \quad \vec{n}^2 = 1, \quad \vartheta \in \mathbb{R} \quad (1.122)$$

- Consider the following transformation of traceless hermitian matrices

$$A \mapsto A' = e^{\frac{1}{2i}\vartheta \vec{n} \cdot \vec{\sigma}} A e^{-\frac{1}{2i}\vartheta \vec{n} \cdot \vec{\sigma}}, \quad A = \vec{a} \cdot \vec{\sigma}, \quad A' = \vec{a}' \cdot \vec{\sigma} \quad (1.123)$$

- Since it preserves traces of matrices, the lengths of \vec{a} and \vec{a}' are equal.
- Thus, this transformation can be interpreted as a rotation of \vec{a} .
- It is the rotation through the angle ϑ about the vector \vec{n} .
- Since for fixed \vec{n} the matrices $\exp(\frac{1}{2i}\vartheta \vec{n} \cdot \vec{\sigma})$ form a one-parameter subgroup of $SU(2)$ it is sufficient to consider transformations with infinitesimal ϑ

$$\begin{aligned} A \mapsto A' &= A + \frac{1}{2i}\vartheta \vec{n} \cdot \vec{\sigma} A - A \frac{1}{2i}\vartheta \vec{n} \cdot \vec{\sigma} = \vec{a} \cdot \vec{\sigma} + \frac{\vartheta}{2i} [\vec{n} \cdot \vec{\sigma}, \vec{a} \cdot \vec{\sigma}] \\ &= \vec{a} \cdot \vec{\sigma} + \frac{\vartheta}{2i} \sum_{\alpha, \beta, \gamma=1}^3 2i \epsilon^{\alpha\beta\gamma} n_\alpha a_\beta \sigma^\gamma = \vec{a} \cdot \vec{\sigma} + \vartheta (\vec{n} \times \vec{a}) \cdot \vec{\sigma} \end{aligned} \quad (1.124)$$

- Thus, as required

$$\delta \vec{a} = \vartheta \vec{n} \times \vec{a} \quad (1.125)$$

- In particular, since σ^3 is identified with $\vec{k} = (0, 0, 1)$ (and therefore Λ with $\lambda \vec{k}$), we find that \vec{n} in (1.118)

$$\vartheta = \theta, \quad \vec{n} = (-\sin \phi, \cos \phi, 0) \quad (1.126)$$

is orthogonal to both \vec{u} in (1.114)

$$\vec{u} = (\cos \phi \sin \theta, \sin \phi \sin \theta, \cos \theta) \quad (1.127)$$

and \vec{k} , and therefore to the plane spanned by these vectors.

- The vector \vec{u} is obtained by the rotation through the angle θ about the vector \vec{n} .

Tensor product

Def. . Given two matrices $A \in \text{Mat}(k, l)$ and $B \in \text{Mat}(m, n)$

$$A = \begin{pmatrix} a_{11} & \cdots & a_{1l} \\ \vdots & \vdots & \vdots \\ a_{k1} & \cdots & a_{kl} \end{pmatrix}, \quad B = \begin{pmatrix} b_{11} & \cdots & b_{1n} \\ \vdots & \vdots & \vdots \\ b_{m1} & \cdots & b_{mn} \end{pmatrix} \quad (1.128)$$

their tensor (or Kronecker) product $A \otimes B \in \text{Mat}(km, ln)$ is the following $km \times ln$ matrix

$$A \otimes B = \begin{pmatrix} a_{11}B & \cdots & a_{1l}B \\ \vdots & \vdots & \vdots \\ a_{k1}B & \cdots & a_{kl}B \end{pmatrix} \quad (1.129)$$

- The matrix elements of $A \otimes B$ have four indices: $(A \otimes B)_{a\alpha, pr} = a_{a\rho} b_{\alpha r}$.
- All $km \times ln$ matrices of the form $A \otimes B$ span $\text{Mat}(km, ln)$, and we can write $\text{Mat}(km, ln) = \text{Mat}(k, l) \otimes \text{Mat}(m, n)$.
- The tensor product of two columns is a column, of two rows is a row,

- The tensor product of a column α and a row β^\dagger is a matrix equal to the usual matrix product of the column and the row, and it is also equal to the tensor product of the row and the column $\alpha \otimes \beta = \alpha\beta^\dagger = \beta^\dagger \otimes \alpha$

$$\begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_m \end{pmatrix} \otimes (b_1^*, b_2^*, \dots, b_n^*) = \alpha\beta^\dagger = \begin{pmatrix} a_1 b_1^* & a_1 b_2^* & \dots & a_1 b_n^* \\ a_2 b_1^* & a_2 b_2^* & \dots & a_2 b_n^* \\ \vdots & \vdots & \ddots & \vdots \\ a_m b_1^* & a_m b_2^* & \dots & a_m b_n^* \end{pmatrix} = (b_1^*, b_2^*, \dots, b_n^*) \otimes \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_m \end{pmatrix}$$

In bra-ket notation we write

$$|\alpha\rangle\langle\beta| = |\alpha\rangle \otimes \langle\beta| = \langle\beta| \otimes |\alpha\rangle \neq \langle\beta|\alpha\rangle$$

- If we have the tensor product of several columns then it is natural to denote the tensor product of several kets as either

$$|\alpha_1\rangle|\alpha_2\rangle \cdots |\alpha_L\rangle \equiv |\alpha_1\rangle \otimes |\alpha_2\rangle \otimes \cdots \otimes |\alpha_L\rangle \quad (1.130)$$

or, if there is no ambiguity, as

$$|\alpha_1\alpha_2 \cdots \alpha_L\rangle \equiv |\alpha_1\rangle \otimes |\alpha_2\rangle \otimes \cdots \otimes |\alpha_L\rangle \quad (1.131)$$

- The tensor product in general is not commutative but $A \otimes B$ and $B \otimes A$ are of the same size and made of the same set of matrix elements $a_{\alpha\rho}b_{\alpha r}$.
- There is a $km \times km$ permutation matrix P and a $ln \times ln$ permutation matrix Q such that

$$B \otimes A = P(A \otimes B)Q$$

- If A and B are square matrices then $Q = P^t = P^\dagger = P^{-1}$, and $A \otimes B$ and $B \otimes A$ are similar.
- The tensor product is associative, and its other useful properties are

$$(i) \quad (A_1 \otimes A_2 \otimes \cdots \otimes A_L)^t = A_1^t \otimes A_2^t \otimes \cdots \otimes A_L^t$$

$$(ii) \quad (A_1 \otimes A_2 \otimes \cdots \otimes A_L)^\dagger = A_1^\dagger \otimes A_2^\dagger \otimes \cdots \otimes A_L^\dagger$$

(iii) If A_i and B_i are matrices such that the matrix product $A_i B_i$ exists for all i then

$$(A_1 \otimes A_2 \otimes \cdots \otimes A_L) \cdot (B_1 \otimes B_2 \otimes \cdots \otimes B_L) = A_1 B_1 \otimes A_2 B_2 \otimes \cdots \otimes A_L B_L$$

(iv) If A is $m \times m$ and B is $n \times n$ then

$$\text{tr}(A \otimes B) = \text{tr}(A) \text{tr}(B), \quad \det(A \otimes B) = (\det A)^n (\det B)^m$$

- For example

$$\begin{aligned}
|\uparrow\uparrow\rangle &\equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, & |\uparrow\downarrow\rangle &\equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \\
|\downarrow\uparrow\rangle &\equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, & |\downarrow\downarrow\rangle &\equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}
\end{aligned}$$

gives the canonical basis of \mathbb{C}^4 .

- Then,

$$\begin{aligned}
\sigma^1 \otimes \sigma^2 |\uparrow\downarrow\rangle &= \left[\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \right] \cdot \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ -i \\ 0 \end{pmatrix} \\
&= -i |\downarrow\uparrow\rangle \\
\sigma^1 \otimes \sigma^2 |\uparrow\downarrow\rangle &= \sigma^1 |\uparrow\rangle \otimes \sigma^2 |\downarrow\rangle = |\downarrow\rangle \otimes (-i |\uparrow\rangle) = -i |\downarrow\uparrow\rangle
\end{aligned}$$

The vector space of 2^L -dim columns can be represented as the tensor product of L 2-dim columns.

In QM and condensed matter physics it is identified with the space of states of a spin chain with L sites, in other words a length L spin chain

$$|\uparrow\uparrow\cdots\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \cdots \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \longleftrightarrow \begin{array}{c} \text{all spins up} \\ \uparrow \quad \uparrow \quad \cdots \quad \uparrow \\ \bullet \text{---} \bullet \text{---} \cdots \text{---} \bullet \end{array}$$

$$|\downarrow\uparrow\uparrow\cdots\uparrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \cdots \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \longleftrightarrow \begin{array}{c} \text{1st spin down} \\ \downarrow \quad \uparrow \quad \cdots \quad \uparrow \\ \bullet \text{---} \bullet \text{---} \cdots \text{---} \bullet \end{array}$$

$$|\uparrow\downarrow\uparrow\cdots\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \cdots \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \longleftrightarrow \begin{array}{c} \text{2nd spin down} \\ \uparrow \quad \downarrow \quad \cdots \quad \uparrow \\ \bullet \text{---} \bullet \text{---} \cdots \text{---} \bullet \end{array}$$

$$|\cdots\uparrow \underbrace{\downarrow}_{i\text{-th term}} \uparrow\cdots\rangle = \cdots \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \underbrace{\begin{pmatrix} 0 \\ 1 \end{pmatrix}}_{i\text{-th term}} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \cdots \longleftrightarrow \begin{array}{c} \text{\textit{i}-th spin down} \\ \cdots \text{---} \uparrow \text{---} \downarrow \text{---} \uparrow \text{---} \cdots \\ \bullet \text{---} \bullet \text{---} \bullet \text{---} \cdots \end{array}$$

$$\begin{aligned}
|\cdots \uparrow \underbrace{\downarrow}_{i\text{-th term}} \uparrow \cdots \underbrace{\downarrow}_{j\text{-th term}} \uparrow \cdots\rangle &= \cdots \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \underbrace{\begin{pmatrix} 0 \\ 1 \end{pmatrix}}_{i\text{-th term}} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \cdots \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \underbrace{\begin{pmatrix} 0 \\ 1 \end{pmatrix}}_{j\text{-th term}} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \cdots \\
&\longleftrightarrow \cdots \text{---} \overset{\uparrow}{\bullet} \text{---} \underset{\downarrow}{\bullet} \text{---} \overset{\uparrow}{\bullet} \text{---} \cdots \text{---} \overset{\uparrow}{\bullet} \text{---} \underset{\downarrow}{\bullet} \text{---} \overset{\uparrow}{\bullet} \text{---} \cdots
\end{aligned}$$

- Dynamics of such a spin chain is governed by a Hamiltonian which is a hermitian matrix acting in the space.
- The most famous model of this type is called the Heisenberg spin chain

$$H = \sum_{i=1}^L (J_x S_i^x S_{i+1}^x + J_y S_i^y S_{i+1}^y + J_z S_i^z S_{i+1}^z + \vec{h} \cdot \vec{S}_i) \quad (1.132)$$

- (i) \vec{S}_i is the spin 1/2 operator on site i
- (ii) J_α are exchange couplings
- (iii) \vec{h} is a magnetic field

(iv) \vec{S}_i acts only on the particle at the i -th site, and can be written as

$$\vec{S}_i = I \otimes I \otimes \cdots \otimes I \otimes \underbrace{\vec{S}}_{i\text{-th term}} \otimes I \otimes \cdots \otimes I \quad (1.133)$$

where I is the 2×2 identity matrix.

- (v) The same notation is used in general: given the tensor product of several vectors (of any dimensions) a matrix A_i only transforms the i -th vector.
- (vi) Note that A_i and B_j commute if $i \neq j$.
- (vii) If all J_α are distinct then the model is called a XYZ spin 1/2 chain
- (viii) If $J_x = J_y \neq J_z$ it is a XXZ spin 1/2 chain
- (ix) If $J_x = J_y = J_z$ it is a XXX spin 1/2 chain.
- In QM the Hilbert space of several particles is isomorphic to the tensor product of Hilbert spaces of each of the particles.

Def. A **vector space** \mathcal{V} over \mathbb{C} is a set of **vectors** ($|\alpha\rangle, |\beta\rangle, |\gamma\rangle, \dots$) equipped with two operations: **vector addition** and **scalar multiplication** which satisfy

I. Vector addition

(a) The set is **closed** under vector addition,

that is the “sum” of any two vectors is another vector: $|\alpha\rangle + |\beta\rangle = |\gamma\rangle$

(b) Vector addition is **commutative**: $|\alpha\rangle + |\beta\rangle = |\beta\rangle + |\alpha\rangle$

(c) Vector addition is **associative**: $|\alpha\rangle + (|\beta\rangle + |\gamma\rangle) = (|\alpha\rangle + |\beta\rangle) + |\gamma\rangle$

(d) There exists a **zero** or **null** vector, $|0\rangle$, such that for every vector $|\alpha\rangle$: $|\alpha\rangle + |0\rangle = |\alpha\rangle$

(e) For every $|\alpha\rangle$ there is an associated **inverse** vector, $|- \alpha\rangle$, such that: $|\alpha\rangle + |- \alpha\rangle = |0\rangle$

II. Scalar multiplication

(a) The set is **closed** under scalar multiplication,

that is the “product” of any scalar with any vector is another vector: $c|\alpha\rangle = |\gamma\rangle$

(b) Scalar multiplication is **distributive** with respect to

(i) vector addition: $c(|\alpha\rangle + |\beta\rangle) = c|\alpha\rangle + c|\beta\rangle$

(ii) scalar addition: $(c + d)|\alpha\rangle = c|\alpha\rangle + d|\alpha\rangle$

(c) Scalar multiplication is **associative**

with respect to the ordinary multiplication of scalars: $c(d|\alpha\rangle) = (cd)|\alpha\rangle$

(d) Multiplication by 0 and 1 gives: $0|\alpha\rangle = |0\rangle$, $1|\alpha\rangle = |\alpha\rangle$

(e) Obviously, $|- \alpha\rangle = (-1)|\alpha\rangle \equiv -|\alpha\rangle$

Examples of vector spaces are

1. The set of all complex $n \times m$ matrices is nm -dimensional
 2. The set of all polynomials of degree less than N in x is N -dimensional
 3. The set of all functions defined in an interval $[0, L]$ is infinite-dimensional
- Let the space dimension n be finite, and let $|e_1\rangle, |e_2\rangle, \dots, |e_n\rangle$ be a basis.

(i) Any vector $|\alpha\rangle$ can be written as a linear combination of $|e_i\rangle$

$$|\alpha\rangle = a_1|e_1\rangle + a_2|e_2\rangle + \dots + a_n|e_n\rangle = \sum_{i=1}^n a_i|e_i\rangle \quad (1.134)$$

(ii) The complex numbers a_i are called the **components** of $|\alpha\rangle$ with the given basis

(iii) The vector can be uniquely represented by the ordered n -tuple of its components

$$|\alpha\rangle \leftrightarrow (a_1, a_2, \dots, a_n) \quad (1.135)$$

- If the space dimension is infinite but there is a countable basis, then we just write

$$|\alpha\rangle = \sum_{i=1}^{\infty} a_i |e_i\rangle, \quad |\alpha\rangle \leftrightarrow (a_1, a_2, \dots) \quad (1.136)$$

- We ofte write a linear combination of two (or more) vectors as

$$|a\alpha + b\beta\rangle \equiv a|\alpha\rangle + b|\beta\rangle \quad (1.137)$$

Def. The **inner product** of two vectors $|\alpha\rangle$ and $|\beta\rangle$ is a complex number, which we write as $\langle\alpha|\beta\rangle$, with the following properties

$$\langle\beta|\alpha\rangle = \langle\alpha|\beta\rangle^* \quad \Rightarrow \quad \langle\alpha|\alpha\rangle \in \mathbb{R} \quad (1.138)$$

$$\langle\alpha|\alpha\rangle \geq 0 \quad \text{and} \quad \langle\alpha|\alpha\rangle = 0 \quad \Leftrightarrow \quad |\alpha\rangle = |0\rangle \quad (1.139)$$

$$\langle\alpha|b\beta + c\gamma\rangle = b\langle\alpha|\beta\rangle + c\langle\alpha|\gamma\rangle, \quad \langle a\alpha + b\beta|\gamma\rangle = a^*\langle\alpha|\gamma\rangle + b^*\langle\beta|\gamma\rangle \quad (1.140)$$

- (i) The inner product is linear wrt the second factor, and antilinear wrt the first factor
- (ii) The inner product satisfies the **Schwarz inequality**

$$|\langle\alpha|\beta\rangle|^2 \leq \langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \quad (1.141)$$

- (iii) The angle between $|\alpha\rangle$ and $|\beta\rangle$ is

$$\cos \theta = \sqrt{\frac{\langle\alpha|\beta\rangle\langle\beta|\alpha\rangle}{\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle}} \quad (1.142)$$

Def. A vector space with an inner product is called an **inner product space**.

Def. We refer to $|\alpha| \equiv \sqrt{\langle \alpha | \alpha \rangle}$ as the **norm** or length of the vector.

A **normalised** vector has unit norm.

The inner product satisfies the **triangle inequality**

$$|\alpha + \beta| \leq |\alpha| + |\beta| \quad (1.143)$$

the norm of $|\alpha\rangle + |\beta\rangle$ is less than or equal to the sum of norms of these vectors, and, therefore, an inner product space is closed under vector addition.

Def. We refer to an inner product space which admits a finite or countable basis as a **Hilbert space**.

All infinite-dimensional (separable) Hilbert spaces are isomorphic to each other.

Def. We say that two vectors are **orthogonal** or perpendicular if their inner product vanishes.

Def. A set of mutually orthogonal normalised basis vectors

$$\langle e_i | e_j \rangle = \delta_{ij} \quad (1.144)$$

is called an **orthonormal** basis. Any basis in a Hilbert space can be converted to orthonormal by using the **Gram-Schmidt procedure**.

Given an orthonormal basis of a Hilbert space and vectors

$$|\alpha\rangle = \sum_i a_i |e_i\rangle, \quad |\beta\rangle = \sum_i b_i |e_i\rangle \quad (1.145)$$

- their inner product is

$$\langle\alpha|\beta\rangle = a_1^* b_1 + a_2^* b_2 + \cdots = \sum_i a_i^* b_i \quad (1.146)$$

- the norm squared is

$$\langle\alpha|\alpha\rangle = |a_1|^2 + |a_2|^2 + \cdots = \sum_i |a_i|^2 \quad (1.147)$$

- the components are

$$a_i = \langle e_i | \alpha \rangle \quad \Rightarrow \quad |\alpha\rangle = \sum_i |e_i\rangle \langle e_i | \alpha \rangle \quad (1.148)$$

- Representing $\langle\alpha|$ and $|\beta\rangle$ as (finite or semi-infinite) row and column, respectively

$$\langle\alpha| \leftrightarrow (a_1^*, a_2^*, \dots), \quad |\beta\rangle \leftrightarrow \begin{pmatrix} b_1 \\ b_2 \\ \vdots \end{pmatrix} \quad (1.149)$$

we identify the given basis $|e_i\rangle$ of a Hilbert space with the canonical basis $|i\rangle$ of a column vector space, and the inner product with the dot product.

- The Hilbert space becomes isomorphic to the column vector space.

Hilbert space of square-integrable functions

Let $|i\rangle, i = 1, 2, \dots$, be any orthonormal basis of an infinite-dim Hilbert space \mathcal{H} .

- Any $|\alpha\rangle \in \mathcal{H}$ can be decomposed as

$$|\alpha\rangle = \sum_{i=1}^{\infty} a_i |i\rangle, \quad a_i = \langle i|\alpha\rangle, \quad \sum_{i=1}^{\infty} |a_i|^2 < \infty \quad (1.150)$$

and be identified with a semi-infinite column.

- In QM it is important to identify a vector in \mathcal{H} with a square-integrable function that is with a complex-valued function $\alpha(x)$ on an interval $[a, b]$ such that

$$\int_a^b dx |\alpha(x)|^2 < \infty \quad (1.151)$$

- To this end let us first relabel the basis $|i\rangle$ as follows

$$|e_k\rangle \equiv |2k\rangle, \quad |e_{1-k}\rangle \equiv |2k-1\rangle, \quad k = 1, 2, \dots, \infty \quad (1.152)$$

The basis vectors $|e_n\rangle$ are labeled by an arbitrary integer $n \in \mathbb{Z}$.

- With respect to this basis $|\alpha\rangle$ has the decomposition

$$|\alpha\rangle = \sum_{n=-\infty}^{\infty} c_n |e_n\rangle, \quad c_n = \langle e_n|\alpha\rangle, \quad \sum_{n=-\infty}^{\infty} |c_n|^2 < \infty \quad (1.153)$$

- Let the components c_n of $|\alpha\rangle$ be the Fourier coefficients of a function $\alpha(x)$ defined on an interval $[a, b]$.
- The function is given by the Fourier series

$$\alpha(x) = \frac{1}{\sqrt{L}} \sum_{n=-\infty}^{\infty} c_n \exp\left(\frac{2\pi}{L} i n x\right), \quad L \equiv b - a \quad (1.154)$$

- This is the square-integrable function that represents the vector $|\alpha\rangle$.
- Let $\beta(x)$ be the function which represents another vector $|\beta\rangle = \sum_n d_n |e_n\rangle$ in \mathcal{H} .
- The inner product is expressed in terms of $\alpha(x)$ and $\beta(x)$ as

$$\langle\alpha|\beta\rangle = \int_a^b dx \alpha^*(x) \beta(x) \quad (1.155)$$

Indeed,

$$\begin{aligned} \int_a^b dx \alpha^*(x) \beta(x) &= \int_a^b dx \frac{1}{\sqrt{L}} \sum_{k=-\infty}^{\infty} c_k^* \exp\left(-\frac{2\pi}{L} i k x\right) \frac{1}{\sqrt{L}} \sum_{n=-\infty}^{\infty} d_n \exp\left(\frac{2\pi}{L} i n x\right) \\ &= \sum_{k,n=-\infty}^{\infty} c_k^* d_n \frac{1}{L} \int_a^b dx \exp\left(\frac{2\pi}{L} i (n - k) x\right) = \sum_{k,n=-\infty}^{\infty} c_k^* d_n \delta_{n-k,0} \\ &= \sum_{n=-\infty}^{\infty} c_n^* d_n = \langle\alpha|\beta\rangle \end{aligned} \quad (1.156)$$

- The Hilbert space of square-integrable functions defined on an interval $[a, b]$ is denoted by $L^2([a, b])$.
- Let us rewrite the vector $|\alpha\rangle$ in terms of the function $\alpha(x)$.

(i) By using

$$c_n = \frac{1}{\sqrt{L}} \int_a^b dx \alpha(x) \exp\left(-\frac{2\pi}{L} i n x\right) \quad (1.157)$$

we get

$$\begin{aligned} |\alpha\rangle &= \sum_{n=-\infty}^{\infty} c_n |e_n\rangle = \sum_{n=-\infty}^{\infty} \frac{1}{\sqrt{L}} \int_a^b dx \alpha(x) \exp\left(-\frac{2\pi}{L} i n x\right) |e_n\rangle \\ &= \int_a^b dx \alpha(x) \left(\sum_{n=-\infty}^{\infty} \frac{1}{\sqrt{L}} \exp\left(-\frac{2\pi}{L} i n x\right) |e_n\rangle \right) \end{aligned} \quad (1.158)$$

(ii) Introducing the kets

$$|x\rangle \equiv \sum_{n=-\infty}^{\infty} \frac{1}{\sqrt{L}} \exp\left(-\frac{2\pi}{L} i n x\right) |e_n\rangle \quad (1.159)$$

we get the following representation of the vector $|\alpha\rangle$

$$|\alpha\rangle = \int_a^b dx \alpha(x) |x\rangle \quad (1.160)$$

- We can think about $|x\rangle$ as basis kets labeled by the continuous label x .
- However, these basis kets are not normalisable. Indeed,

$$\begin{aligned}\langle x|x'\rangle &= \sum_{k=-\infty}^{\infty} \frac{1}{\sqrt{L}} \exp\left(\frac{2\pi}{L} i k x\right) \langle e_k| \sum_{n=-\infty}^{\infty} \frac{1}{\sqrt{L}} \exp\left(-\frac{2\pi}{L} i n x'\right) |e_n\rangle \\ &= \sum_{n=-\infty}^{\infty} \frac{1}{L} \exp\left(\frac{2\pi}{L} i n (x - x')\right) = \delta_L(x - x')\end{aligned}\quad (1.161)$$

where $\delta_L(x)$ is the periodic Dirac's delta function with period L .

- We say that the kets $|x\rangle$ are δ -function normalised.
- The completeness relation $\sum_n |e_n\rangle\langle e_n| = I$ for basis kets $|x\rangle$ takes the form

$$\int_a^b dx |x\rangle\langle x| = I \quad (1.162)$$

- Thus, one can also write

$$|\alpha\rangle = \int_a^b dx |x\rangle\langle x|\alpha\rangle, \quad \alpha(x) = \langle x|\alpha\rangle \quad (1.163)$$

which shows that the function $\alpha(x)$ can be thought of as the x -component of the vector $|\alpha\rangle$ expanded over the basis kets $|x\rangle$.

- The representation (1.160) of vectors in the Hilbert space \mathcal{H}

$$|\alpha\rangle = \int_a^b dx \alpha(x) |x\rangle \quad (1.164)$$

together with the normalisation condition (1.161)

$$\langle x|x'\rangle = \delta_L(x - x') \quad (1.165)$$

- (i) makes no reference to the countable basis $|i\rangle$ or $|e_n\rangle$, and can be used as another definition of a (separable) Hilbert space.
- (ii) makes clear that the interval $[a, b]$ does not have to be finite, and one can consider square-integrable functions on the whole line \mathbb{R} or on a semi-line.
- (iii) A countable basis can then be introduced by using a complete set of orthonormal functions, i.e. such a set that any other function in Hilbert space can be expressed as a linear combinations of the functions from the set

$$\alpha(x) = \sum_{n=1}^{\infty} c_n a_n(x), \quad \int dx a_n^*(x) a_m(x) = \delta_{nm} \quad (1.166)$$

- (iv) The corresponding countable orthonormal basis is then given by

$$|e_n\rangle = \int dx a_n(x) |x\rangle \quad (1.167)$$

- In QM if the continuous label x is the coordinate of a particle then $\alpha(x)$ is called the wave function of a particle in the coordinate representation, and usually denoted by $\psi(x)$.

Linear operators

An operator or a transformation \hat{T} takes each vector in a vector space \mathcal{V} and maps (transforms) it into some other vector

$$|\alpha\rangle \mapsto |\tilde{\alpha}\rangle = \hat{T}|\alpha\rangle \quad (1.168)$$

(i) The operator is linear if the following condition is satisfied

$$\hat{T}(a|\alpha\rangle + b|\beta\rangle) = a(\hat{T}|\alpha\rangle) + b(\hat{T}|\beta\rangle) \quad (1.169)$$

for any vectors $|\alpha\rangle, |\beta\rangle$ and any scalars a, b .

(ii) Vectors obtained this way may belong to a different vector space.

We consider the case where they belong to the original one.

(iii) The **sum** of two operators $\hat{S} + \hat{T}$ and the product of an operator and a scalar $a\hat{T}$ are defined in the natural way

$$(\hat{S} + \hat{T})|\alpha\rangle = \hat{S}|\alpha\rangle + \hat{T}|\alpha\rangle, \quad (a\hat{T})|\alpha\rangle = a(\hat{T}|\alpha\rangle) \quad (1.170)$$

The operator addition and multiplication by scalars make the set of all linear operators a vector space.

- (iv) The **product** $\hat{S}\hat{T}$ of two operators is the net effect of performing them in succession – first \hat{T} , then \hat{S}

$$|\tilde{\alpha}\rangle = \hat{T}|\alpha\rangle, \quad |\tilde{\tilde{\alpha}}\rangle = \hat{S}|\tilde{\alpha}\rangle = \hat{S}(\hat{T}|\alpha\rangle) = \hat{S}\hat{T}|\alpha\rangle \quad (1.171)$$

- (v) Clearly, the product is associative, and since the identity operator, $\hat{I}|\alpha\rangle = |\alpha\rangle$ for all $|\alpha\rangle$, is linear, the vector space of linear operators is a unital associative algebra over \mathbb{C} denoted by $\text{End}(\mathcal{V})$.

- (vi) The **commutator** $[\hat{S}, \hat{T}]$ of two operators is $[\hat{S}, \hat{T}] = \hat{S}\hat{T} - \hat{T}\hat{S}$.

- (vii) The eigenvectors and eigenvalues of an operator are defined in the same way as for matrices

$$\hat{T}|\alpha\rangle = \lambda|\alpha\rangle \quad (1.172)$$

- (viii) The set of all the eigenvalues of \hat{T} is called its spectrum.

If operators act in an inner product space we can define adjoint, hermitian and unitary operators by using the corresponding properties of matrices acting in a ket vector space

- The hermitian conjugate or adjoint of an operator \hat{T} is the operator \hat{T}^\dagger satisfying

$$\langle \alpha | \hat{T}^\dagger | \beta \rangle = \langle \hat{T} \alpha | \beta \rangle = \langle \beta | \hat{T} | \alpha \rangle^* \quad (1.173)$$

for all $|\alpha\rangle$ and $|\beta\rangle$ from the domains of \hat{T} and \hat{T}^\dagger , respectively.

- An operator is called hermitian (or self-adjoint) if $\hat{H}^\dagger = \hat{H}$, and anti-hermitian (or skew-hermitian) if $\hat{A}^\dagger = -\hat{A}$. For any hermitian operator \hat{T} and any vector $|\alpha\rangle$

$$\langle \alpha | \hat{T} | \alpha \rangle \in \mathbb{R} \quad (1.174)$$

In QM observables are represented by hermitian operators, and $\langle \alpha | \hat{T} | \alpha \rangle \in \mathbb{R}$ with a unit vector $|\alpha\rangle$ is called **the expectation value** of the operator \hat{T} in the state $|\alpha\rangle$.

- An operator is called unitary if both the operator and its adjoint preserve the inner product

$$\begin{aligned} \langle \hat{U} \alpha | \hat{U} \beta \rangle &= \langle \hat{U}^\dagger \hat{U} \alpha | \beta \rangle = \langle \alpha | \hat{U}^\dagger \hat{U} | \beta \rangle = \langle \alpha | \beta \rangle &\Rightarrow \hat{U}^\dagger \hat{U} &= \hat{I} \\ \langle \hat{U}^\dagger \alpha | \hat{U}^\dagger \beta \rangle &= \langle \hat{U} \hat{U}^\dagger \alpha | \beta \rangle = \langle \alpha | \hat{U} \hat{U}^\dagger | \beta \rangle = \langle \alpha | \beta \rangle &\Rightarrow \hat{U} \hat{U}^\dagger &= \hat{I} \end{aligned} \quad (1.175)$$

for all $|\alpha\rangle$ and $|\beta\rangle$.

- The inverse \hat{T}^{-1} of an operator \hat{T} is defined as

$$\hat{T}^{-1}\hat{T} = \hat{I} \quad \text{and} \quad \hat{T}\hat{T}^{-1} = \hat{I} \quad (1.176)$$

- The inverse of a unitary operator is equal to its hermitian conjugate

$$\hat{U}^{-1} = \hat{U}^\dagger \quad \Leftrightarrow \quad \hat{U}^\dagger \hat{U} = \hat{U} \hat{U}^\dagger = \hat{I} \quad (1.177)$$

Because of the linearity to know how \hat{T} acts on any vector it is sufficient to know how it acts on basis vectors.

(i) Indeed, if

$$\hat{T}|e_j\rangle = \sum_i T_{ij}|e_i\rangle \quad (1.178)$$

then

$$\hat{T}|\alpha\rangle = \hat{T} \sum_j a_j |e_j\rangle = \sum_j a_j \hat{T}|e_j\rangle = \sum_j a_j \sum_i T_{ij} |e_i\rangle = \sum_i \tilde{a}_i |e_i\rangle = |\tilde{\alpha}\rangle \quad (1.179)$$

Therefore,

$$\tilde{a}_i = \sum_j T_{ij} a_j \quad (1.180)$$

(ii) The **matrix elements** T_{ij} in this basis uniquely characterise the linear operator \hat{T} .

(iii) If the basis is orthonormal then

$$T_{ij} = \langle e_i | \hat{T} | e_j \rangle \quad (1.181)$$

(iv) We can combine T_{ij} in a (finite or semi-infinite) matrix

$$T = \begin{pmatrix} T_{11} & T_{12} & \dots \\ T_{21} & T_{22} & \dots \\ \vdots & \vdots & \ddots \end{pmatrix} \quad (1.182)$$

(v) If the vector space is n -dim linear operators reduce to matrices.

(vi) The sum and the scalar product of operators correspond to the usual matrix rules.

(vii) The product of two operators $\hat{R} = \hat{S}\hat{T}$ is represented by the product of the matrices S and T

$$\tilde{a}_i = \sum_j S_{ij} \tilde{a}_j = \sum_j S_{ij} \left(\sum_k T_{jk} a_k \right) = \sum_k \left(\sum_j S_{ij} T_{jk} \right) a_k = \sum_k R_{ik} a_k, \quad R = ST \quad (1.183)$$

Let us find how matrix elements of an operator \hat{T} in two different bases are related.

- Let $|e_i\rangle$ and $|\epsilon_i\rangle$ be two orthonormal bases
- Let the unitary operator \hat{U} maps one basis to another: $|\epsilon_i\rangle = \hat{U}|e_i\rangle$
- Let T_{ij}^e and T_{ij}^ϵ be matrix elements of \hat{T} in the bases $|e_i\rangle$ and $|\epsilon_i\rangle$, respectively.

- Then,

$$T_{ij}^\epsilon = \langle \epsilon_i | \hat{T} | \epsilon_j \rangle = \langle e_i | \hat{U}^\dagger \hat{T} \hat{U} | e_j \rangle = \sum_{k,l} \langle e_i | \hat{U}^\dagger | e_k \rangle \langle e_k | \hat{T} | e_l \rangle \langle e_l | \hat{U} | e_j \rangle = \sum_{k,l} U_{ik}^{\dagger,e} T_{kl}^e U_{lj}^e \quad (1.184)$$

- Thus, the matrices T^ϵ , T^e representing \hat{T} and constructed as in (1.182) are similar, and are related through a unitary matrix U^e

$$T^\epsilon = U^{\dagger,e} T^e U^e \quad (1.185)$$

- This relation allows us to define the trace and the determinant of an operator
 - The trace of an operator is the sum of its diagonal elements in any orthonormal basis

$$\text{tr } \hat{T} = \sum_{i=1}^n T_{ii}^e \quad (1.186)$$

- The determinant of an operator is equal to the determinant of the matrix of its elements in any orthonormal basis

$$\det \hat{T} = \det T^e \quad (1.187)$$

- Both the trace and the determinant are independent of a choice of basis.

- The relation (1.185)

$$T^\epsilon = U^{\dagger,e} T^e U^e \quad (1.188)$$

shows that two operators \hat{T}_1 and \hat{T}_2 such that $\hat{T}_2 = \hat{U} \hat{T}_1 \hat{U}^\dagger$ for some unitary operator \hat{U} have essentially the same properties, in particular

- the same eigenvalues
 - their eigenvectors are related by \hat{U} .
- These operators are called **unitary equivalent**.

Hilbert space with δ -function normalised basis

If a Hilbert space is infinite-dimensional, and basis kets are δ -function normalised then a discrete index i is replaced by a continuous index x , and the summation over i by the integration over x .

For example,

$$\hat{T}|y\rangle = \int dx T_{xy}|x\rangle, \quad T_{xy} \equiv T(x, y) = \langle x|\hat{T}|y\rangle \quad (1.189)$$

$$|\tilde{\alpha}\rangle = \hat{T}|\alpha\rangle = \int dy \alpha(y) \hat{T}|y\rangle = \int dy \alpha(y) \int dx T(x, y)|x\rangle = \int dx \left(\int dy T(x, y)\alpha(y) \right) |x\rangle \quad (1.190)$$

and herefore

$$\tilde{\alpha}(x) = \int dy T(x, y)\alpha(y) \quad (1.191)$$

Thus, \hat{T} is represented by a (generalised) function $T(x, y)$ of two real variables in such a basis.

Operators \hat{X} and \hat{D} in $L^2(\mathbb{R})$

Consider the Hilbert space $L^2(\mathbb{R})$, and define the coordinate operator

$$\hat{X}|\alpha\rangle \equiv \int dx \, x \, \alpha(x) |x\rangle \quad (1.192)$$

that multiplies $\alpha(x)$ by x , and the derivative operator \hat{D}

$$\hat{D}|\alpha\rangle \equiv \int dx \, \frac{d\alpha(x)}{dx} |x\rangle \quad (1.193)$$

that differentiate $\alpha(x)$ with respect to x .

- It is clear from (1.191) that they can be represented by

$$X(x, y) = x \delta(x - y), \quad D(x, y) = \frac{d}{dx} \delta(x - y) \quad (1.194)$$

but it is easier to use their definitions (1.192) and (1.194).

- Let us find their adjoint operators

$$\langle\alpha|\hat{X}|\beta\rangle = \langle\alpha|\hat{X}\beta\rangle = \int dx \, \alpha^*(x) x \beta(x) = \int dx \, (x \alpha(x))^* \beta(x) = \langle\hat{X}\alpha|\beta\rangle \quad (1.195)$$

$$\langle\alpha|\hat{D}|\beta\rangle = \langle\alpha|\hat{D}\beta\rangle = \int dx \, \alpha^*(x) \frac{d\beta(x)}{dx} = - \int dx \, \frac{d\alpha^*(x)}{dx} \beta(x) = -\langle\hat{D}\alpha|\beta\rangle \quad (1.196)$$

- Thus, \hat{X} is hermitian, $\hat{X}^\dagger = \hat{X}$, while \hat{D} is anti-hermitian, $\hat{D}^\dagger = -\hat{D}$.
- Let us now compute the action of $\hat{X}\hat{D}$ and $\hat{D}\hat{X}$ on $|\alpha\rangle$

$$\begin{aligned}
\hat{X}\hat{D}|\alpha\rangle &= \hat{X} \int dx \frac{d\alpha(x)}{dx} |x\rangle = \int dx x \frac{d\alpha(x)}{dx} |x\rangle \\
\hat{D}\hat{X}|\alpha\rangle &= \hat{D} \int dx x \alpha(x) |x\rangle = \int dx \frac{d}{dx} (x \alpha(x)) |x\rangle \\
&= \int dx x \frac{d\alpha(x)}{dx} |x\rangle + \int dx \alpha(x) |x\rangle = \hat{X}\hat{D}|\alpha\rangle + |\alpha\rangle
\end{aligned} \tag{1.197}$$

- Thus,

$$[\hat{X}, \hat{D}] = -\hat{I} \tag{1.198}$$

- Define the hermitian operator

$$\hat{P} = -i \hbar \hat{D} \tag{1.199}$$

- The operators \hat{X} and \hat{P} satisfy the Heisenberg algebra relation

$$[\hat{X}, \hat{P}] = i \hbar \hat{I} \tag{1.200}$$

- This is a representation of the Heisenberg algebra by linear operators acting in the Hilbert space of square-integrable functions on the real line.
- The representation by the creation \hat{a}^\dagger and annihilation \hat{a} operators acting in the space of semi-infinite columns can be used to find how \hat{a}^\dagger and \hat{a} are realised on the space $L^2(\mathbb{R})$, and which square-integrable functions correspond to the eigenstates of the number operator \hat{N} .

Let us analyse eigenvectors of the hermitian operators \hat{X} and $\hat{K} \equiv -i\hat{D}$.

- Denote an eigenvalue of \hat{X} by x , and the corresponding eigenvector by $|\alpha_x\rangle$

$$\hat{X}|\alpha_x\rangle = x|\alpha_x\rangle \quad \Rightarrow \quad \int dy y \alpha_x(y) |y\rangle = \int dy x \alpha_x(y) |y\rangle \quad \Rightarrow \quad y\alpha_x(y) = x\alpha_x(y) \quad \forall y \quad (1.201)$$

(i) The only solution (up to a constant factor) to this equation is

$$\alpha_x(y) = \delta(x - y) \quad \Rightarrow \quad |\alpha_x\rangle = \int dy \delta(x - y) |y\rangle = |x\rangle \quad (1.202)$$

- (ii) The ket $|x\rangle$ is an eigenvector of \hat{X} with eigenvalue x , and, as we have discussed, they are δ -function normalised.
- (iii) Since x can take any real value, the spectrum of \hat{X} is continuous.

- Denote an eigenvalue of \hat{K} by k , and the corresponding eigenvector by $|\alpha_k\rangle$

$$\begin{aligned}\hat{K}|\alpha_k\rangle = k|\alpha_k\rangle \quad \Rightarrow \quad -i \int dx \frac{d\alpha_k(x)}{dx} |x\rangle &= \int dx k \alpha_k(x) |x\rangle \quad \Rightarrow \\ -i \frac{d\alpha_k(x)}{dx} &= k\alpha_k(x) \quad \forall y\end{aligned}\tag{1.203}$$

(i) The general solution to this equation is

$$\alpha_k(x) = C e^{ikx} \tag{1.204}$$

(ii) There are no normalisable solutions but if we choose k real and $C = 1/\sqrt{2\pi}$ then we get δ -function normalised eigenvectors

$$\alpha_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}, \quad |k\rangle \equiv |\alpha_k\rangle = \int dx \frac{1}{\sqrt{2\pi}} e^{ikx} |x\rangle, \quad \langle x|k\rangle = \frac{1}{\sqrt{2\pi}} e^{ikx} \tag{1.205}$$

$$\begin{aligned}\langle k|k'\rangle &= \int dx \frac{1}{\sqrt{2\pi}} e^{-ikx} \langle x| \int dx' \frac{1}{\sqrt{2\pi}} e^{ik'x'} |x'\rangle = \int dx dx' \frac{1}{2\pi} e^{-ikx + ik'x'} \delta(x - x') \\ &= \int dx \frac{1}{2\pi} e^{-i(k-k')x} = \delta(k - k')\end{aligned}\tag{1.206}$$

(iii) It is easy to check that the eigenkets $|k\rangle$ satisfy the completeness relation

$$\int dk |k\rangle \langle k| = \hat{I} \quad (1.207)$$

Indeed,

$$\begin{aligned} \int dk |k\rangle \langle k| \alpha \rangle &= \int dk |k\rangle \langle k| \int dx \alpha(x) |x\rangle = \int dk dx |k\rangle \alpha(x) \langle k|x\rangle \\ &= \int dk dx \int dx' \frac{1}{\sqrt{2\pi}} e^{ikx'} |x'\rangle \alpha(x) \frac{1}{\sqrt{2\pi}} e^{-ikx} \\ &= \int dx dx' \alpha(x) |x'\rangle \int dk \frac{1}{2\pi} e^{ik(x'-x)} = \int dx dx' \alpha(x) |x'\rangle \delta(x - x') \\ &= \int dx \alpha(x) |x\rangle = |\alpha\rangle \end{aligned} \quad (1.208)$$

(iv) Thus, any vector can be expanded over the eigenkets of $\hat{K} = -i\hat{D}$

$$|\alpha\rangle = \int dk \alpha(k) |k\rangle, \quad \alpha(k) = \langle k|\alpha\rangle = \int dx \alpha(x) \frac{1}{\sqrt{2\pi}} e^{-ikx} \quad (1.209)$$

(v) Thus, $\alpha(k)$ and $\alpha(x)$ are related to each other by Fourier transform, and we can also say that the Fourier transform is the unitary transformation that relates the \hat{X} and \hat{K} bases.

A hermitian operator in an infinite dimensional Hilbert space may have

- no normalisable eigenvectors but then it has a continuous spectrum and δ -function normalised eigenvectors.
- the total spectrum which is the union of the discrete and continuous spectra, i.e. it may have both normalisable eigenvectors with isolated eigenvalues and δ -function normalised eigenvectors with eigenvalues taking values in an interval.

The spectral decomposition of \hat{H} involves the summation over the discrete spectrum and integration over the continuous one.

\hat{X} and \hat{K} are defined by their action on vectors expanded over the \hat{X} basis, i.e. over eigenkets of \hat{X} .

Let us see how the operators act on vectors expanded over the \hat{K} basis.

- \hat{K} just multiplies $\alpha(k)$ by k .

- \hat{X} acts as

$$\begin{aligned}
 \hat{X}|\alpha\rangle &= \int dk \alpha(k) \hat{X}|k\rangle = \int dk \alpha(k) \hat{X} \left(\int dx |x\rangle \langle x| \right) |k\rangle = \int dk dx \alpha(k) \hat{X}|x\rangle \langle x|k\rangle \\
 &= \int dk dx \alpha(k) x |x\rangle \frac{1}{\sqrt{2\pi}} e^{ikx} = \int dk dx \alpha(k) |x\rangle \frac{1}{i} \frac{d}{dk} \frac{1}{\sqrt{2\pi}} e^{ikx} \\
 &= \int dk dx i \frac{d}{dk} \alpha(k) |x\rangle \frac{1}{\sqrt{2\pi}} e^{ikx} = \int dk i \frac{d}{dk} \alpha(k) |k\rangle
 \end{aligned}
 \tag{1.210}$$

- In the \hat{K} basis \hat{X} becomes the derivative operator multiplied by i .

- To summarise,

(i) in the \hat{X} basis the operators \hat{X} and \hat{K} act on functions of x as x and $-i d/dx$

(ii) in the \hat{K} basis they act on functions of k as $i d/dk$ and k .

(iii) Operators with such a reciprocity are said to be **conjugate** to each other.

If we would consider functions on a finite interval from $L^2([a, b])$ then the derivative operator \hat{D} would not be in general anti-hermitian because the integration by parts would produce the boundary contribution

$$\alpha^*(b)\beta(b) - \alpha^*(a)\beta(a) \quad (1.211)$$

- If we restrict the space of functions to those which vanish at $x = a, b$ then \hat{D} is anti-hermitian on this space.
- The boundary contribution also vanishes for functions satisfying twisted boundary conditions

$$\alpha(b) = e^{i\nu} \alpha(a) \quad \forall |\alpha\rangle \in L^2([a, b]), \quad \nu \in \mathbb{R} \quad (1.212)$$

- However, the coordinate operator \hat{X} is not defined on this space.
- A well-defined operator in this case would be for example $\exp(\frac{i\nu}{b-a}\hat{X})$, and $\nu = 2\pi$ would describe periodic functions.

Tensor product of Hilbert spaces and operators

- A mathematically precise definition of the tensor product of two abstract vector spaces is complicated.
- For our purposes we only need Hilbert spaces, and we can use a much simpler but equivalent definition.

Def. Let \mathcal{H}_1 and \mathcal{H}_2 be Hilbert spaces with orthonormal bases $|e_i\rangle$ and $|\epsilon_a\rangle$, respectively. The tensor product of \mathcal{H}_1 and \mathcal{H}_2 is the Hilbert space denoted by $\mathcal{H}_1 \otimes \mathcal{H}_2$ with the orthonormal basis $|e_i \epsilon_a\rangle$

$$\langle e_i \epsilon_a | e_j \epsilon_b \rangle = \delta_{ij} \delta_{ab} \quad (1.213)$$

Obviously, $\mathcal{H}_1 \otimes \mathcal{H}_2$ and $\mathcal{H}_2 \otimes \mathcal{H}_1$ are isomorphic by the identification $|e_i \epsilon_a\rangle \leftrightarrow |\epsilon_a e_i\rangle$.

- **Def.** The tensor product of two vectors $|\alpha\rangle = \sum_i a_i |e_i\rangle \in \mathcal{H}_1$ and $|\beta\rangle = \sum_a b_a |\epsilon_a\rangle \in \mathcal{H}_2$ is the following vector

$$|\alpha\rangle \otimes |\beta\rangle = \sum_{i,a} a_i b_a |e_i \epsilon_a\rangle, \quad |\alpha\rangle \otimes |\beta\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2 \quad (1.214)$$

In particular,

$$|e_i\rangle \otimes |\epsilon_a\rangle = |e_i \epsilon_a\rangle \quad (1.215)$$

The tensor product of two vectors can be considered as a bilinear map from $\mathcal{H}_1 \times \mathcal{H}_2$ into $\mathcal{H}_1 \otimes \mathcal{H}_2$.

- **Def.** Let \hat{S} and \hat{T} be linear operators acting in Hilbert spaces \mathcal{H}_1 and \mathcal{H}_2 , respectively. The tensor product of the two operators is a linear operator denoted by $\hat{S} \otimes \hat{T}$ which acts in $\mathcal{H}_1 \otimes \mathcal{H}_2$ as follows

$$\hat{S} \otimes \hat{T} |e_i \epsilon_a\rangle = \hat{S} |e_i\rangle \otimes \hat{T} |\epsilon_a\rangle \quad (1.216)$$

- The same definitions can be used to define the tensor product of any two vector spaces with finite or countable bases. All one has to do is to drop the requirement of orthonormality.
- With these definitions everything we have discussed in section 1.2 applies to the abstract Hilbert spaces.
- We can also use δ -function normalised bases.

For example,

- (i) the tensor product of $\mathbb{C}^2 \otimes L^2(\mathbb{R})$ can be identified with the space of 2-dimensional columns with components being square-integrable functions on \mathbb{R} ,
- (ii) $L^2(\mathbb{R}) \otimes L^2(\mathbb{R})$ with the space of square-integrable functions on \mathbb{R}^2 .