NITheCS Mini-School - October 2022
Preliminaries

Laure Gouba
Email: laure.gouba@gmail.com

October 12, 2022

1 Bracket notations

When using a vector $\vec{v}$ to represent a quantum state, the Dirac notation in which a "ket" (ket $|v\rangle$) denotes a column vector in a complex vector space is used. It is a notation commonly used in quantum mechanics and does not change the nature of the vectors at all.

$$\vec{v}\begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix} \leftrightarrow |v\rangle = \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix} \tag{1}$$

The "bra" ($\langle v|$) denotes the conjugate transpose

$$\langle v| = (|v\rangle)^\dagger = (v_1^\star, v_2^\star, \dots v_n^\star), \quad ||v||_2 = \sqrt{\langle v|v\rangle} = \sqrt{\sum_{i=i}^{n} |v_i|^2}. \tag{2}$$

Given two vectors $|v\rangle$ and $|w\rangle$, the inner product is denoted

$$\langle v|w\rangle = |v\rangle \cdot |w\rangle = \sum_{i=1}^{n} v_i^\star w_i. \tag{3}$$

The complex conjugate of a bracket is as

$$\overline{\langle v|w\rangle} = \langle w|v\rangle. \tag{4}$$

The braket notation was introduced by Paul Dirac in 1939 and is also known as the Dirac notation.

2 Hilbert space

A vector space with a well defined inner product is called a Hilbert space. The term Hilbert space is often reserved for an infinite-dimensional inner product space having the property that it is complete or closed. However, nowadays the term Hibert space is often used in a way that includes finite-dimensional spaces, which automatically satisfy the condition of completeness.

3 State vector

A quantum state is any possible state in which a quantum mechanical system can be, means the collection of all relevant physical properties of a quantum system (position, momentum spin, polarisation). Two states are said to be exclusive if the fact of being in one of the states with certainty implies that there are no chances whatsoever of being in any of the other states.

- The state of a physical system is represented by a vector $|\psi\rangle$ in a Hilbert space $\mathcal{H}$.
- The space of states $\mathcal{H}$ depends on the particular physical system under consideration. As already said, in general dim $\mathcal{H} = \infty$, but specific aspects of a given system may be described by infinite-dimensional vector spaces. It is part of the theory to specify the physical informations necessary to characterize a "state" of the system.
- In quantum mechanics, two vectors $|\psi\rangle$ and $c|\psi\rangle$, where c is any nonzero complex number have exactly the same physical significance.
- The superposition principle expresses the fact that if $|\psi_1\rangle$ and $|\psi_2\rangle$ corresponds to two physical states, the vector $|\psi_1\rangle + |\psi_2\rangle$ corresponds to another physical state, which has "something" to do with both $|\psi_1\rangle$ and $|\psi_2\rangle$.
- The physical state corresponds not to a particular vector in the Hilbert space, but to the ray, or one-dimensional subspace, defined by the collection of all the complex multiples of a particular vector.
- One can always choose c in such a way that the $|\psi\rangle$. corresponding to a particular physical situation is normalized, $\langle\psi|\psi\rangle = 1$ or $||\psi|| = 1$, where the norm $||\psi|| = 1$, where the norm $||\psi||$ of a state $|\psi\rangle$ is the positive square root of $||\psi||^2 = \langle\psi|\psi\rangle$.
- Normalized vectors can always be multiplied by a phase factor, a complex number of the form $e^{i\phi}$ where ϕ is real, without changing the normalization or the physical interpretation, so normalization itself does not single out a singe vector representing a particular physical state of affairs.

4 Operators

Operators are linear maps of the Hilbert space $\mathcal{H}$ onto itself. If L is an operator, then for any $|\psi\rangle$ in $\mathcal{H}$, $L|\psi\rangle \in \mathcal{H}$.

- Linearity means that

$$L(a|\psi\rangle + b|\phi\rangle) = aL|\psi\rangle + bL|\phi\rangle \tag{5}$$

  for any pair $|\psi\rangle$ and $|\phi\rangle$, and any two complex numbers a and b.

- The product $L_1 L_2$ of two operators L_1 and L_2 is defined by

$$(L_1 L_2)|\psi\rangle = L_1(L_2|\psi\rangle) = L_1 L_2|\psi\rangle. \tag{6}$$

- In general $L_1 L_2 \neq L_2 L_1$.
- Example of a simplest operator is called "dyad": $|\psi\rangle\langle\phi|$. Let's check the action of this dyad on a vector $|\chi\rangle$: $(|\psi\rangle\langle\phi|)\chi\rangle = (\langle\phi|\chi\rangle)|\psi\rangle$.
- The identity operator $\mathbb{I}$ is such that $\mathbb{I}|\psi\rangle = |\psi\rangle$.
- Completeness relation:

$$\mathbb{I} = \sum_j |j\rangle\langle j|, \tag{7}$$

  where $|j\rangle$ are elements of an orthonormal basis. A useful application of the completeness relation is that

$$|\psi\rangle = (\sum_j |j\rangle\langle j|)|\psi\rangle = \sum |j\rangle\langle j|\psi\rangle = \sum_j \langle j|\psi\rangle|j\rangle. \tag{8}$$

4.1 Normal operators

A normal operator N on a Hilbert space $\mathcal{H}$ is one that commutes with its adjoint, $NN^\dagger = N^\dagger N$.

- Normal operators have the property that they can be diagonalized using orthogonal basis, that is

$$N = \sum_j \alpha_j |\psi_j\rangle\langle\psi_j|, \tag{9}$$

  where the basis vectors ψ_j are eigenvectors of N and the numbers (real or complex) are the eigenvalues.
- The matrix of N in this basis is diagonal that is

$$\langle\psi_i|N|\psi_j\rangle = \alpha_i \delta_{ij}. \tag{10}$$

- The equation (9) is often referred to spectral resolution or spectral form of the operator N.

4.2 Hermitian operators

A Hermitian operator or self-adjoint operator L is defined by the property that $L = L^\dagger$, so it is a normal operator.

- The eigenvalues α_j of an Hermitian operator are real numbers.
- The terms " Hermitian" and "self-adjoint" mean the same thing for a finite-dimensional Hilbert space, the distinction is important for infinite -dimensional spaces.
- Hermitian operators in quantum mechanics are used to represent physical variables, quantities such as energy, momentum, angular momentum, position...
- The operator representing the energy is the Hamiltonian H.

- If a quantum system is in the state $|\psi\rangle$, the physical variable corresponding to the operator L has a well-defined value if and only if $|\psi\rangle$ is an eigenvector of L, $L|\psi\rangle = \alpha|\psi\rangle$, where α, necessarily is a real number since $L^\dagger = L$, is the value of the physical variable in this state.

- If $|\psi\rangle$ is not an eigenstate of L, then in this state the physical quantities L is undefined, or meaningless in the sense that quantum theorycan assign it no meaning.

- There have been many attempts to assign a physical meaning to L when a quantum system is in a state which is not an eigenstate of L. All such attempts to make what is called a "hidden variable " theory have been uncessful.

4.3 Projectors

A projector, short of "orthogonal projection operator", is a Hermitian operator $P = P^\dagger$ which is idempotent in the sense that $P^2 = P$. Equivalently it is a Hermitian operator whose eigenvalues are either 0 or 1.

- There is always a basis which depends on the projector in which its matrix is diagonal with only 0 or 1 on the diagonal. Conversely, such a matrix always represents a projector.

- There is a one to one correspondence between a projector P and the subspace $\mathcal{P}$ of the Hilbert space that it projects onto.

- The subspace $\mathcal{P}$ consists of all the kets $|\psi\rangle$ such that $P|\psi\rangle = |\psi\rangle$.

- The term "projector" is used because such an operator "projects" a vector in a perpendicular manner onto a subspace.

- Both of the identity $\mathbb{R}$ and the zero operator 0 which maps every ket onto the zero ket are projectors.

- A more interesting example is the dyad $|\psi\rangle\langle\psi|$ for a normalized ($|||\psi\rangle|| = 1$) state $|\psi\rangle$.

- If ψ is not normalized (and not zero), the corresponding operator is

$$P = \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle}. \tag{11}$$

- If $|\psi\rangle$ and $|\phi\rangle$ are two normalized states orthogonal to each other, $\langle\psi|\phi\rangle = 0$, then the sum $|\psi\rangle\langle\psi| + |\phi\rangle\langle\phi|$ of the corresponding dyads is also a projector.

The physical significance of projectors is that they represent physical properties of a quantum system that can be either true or false.

- The property P corresponding to a projector P is true if the physical state $|\psi\rangle$ of the system is an eigenstate of P with eigenvalue 1, and false if it is an eigenstate with eigenvalue 0.

- If $|\psi\rangle$ is not an eigenstate of P, then the corresponding property is undefined (meaningless) for this state.

4.4 Positive operators

The positive operators form another important class of Hermitian operators, they are defined that for every $|\psi\rangle$

$$\langle\psi|L|\psi\rangle \geq 0. \tag{12}$$

Positive operators arise in quantum mechanics in various contexts, but one of the most important is when dealing with probabilities, which are inherent positive quantities.

4.5 Unitary operators

A unitary operator U has the property that

$$U^\dagger U = \mathbb{I} = UU^\dagger. \tag{13}$$

- Since U commutes with its adjoint, it is a normal operator ($UU^\dagger = U^\dagger U$), the difference is the condition equal to unit that implies that all the eigenvalues of U are complex numbers of magnetude 1., they lie in the unit circle in the complex plane.
- In quantum mechanics unitary operators are used to change from one orthogonal basis to another, to represent symmetries, such as rotational symmetry, and to describe some aspects of the dynamics or time development of a quantum system.

5 Observables

The observables are the physical quantities that can be measured on a system: position, momentum, kinetic energy, angular momentum, etc. Observables $\mathcal{O}$ are represented by linear operators and the linear operators L which correspond to observables are Hermitian and admits basis of eigenvectors

- The observables are Hermitian (more precisely, self-adjoint) linear operators acting on the Hilbert space.
- Not every self adjoint operator corresponds to a physically meaningful observable.
- Not all physical observables are associated with non-trivial self-adjoint operators.
- A quantum state can be an eigenvector of an observable in which case it is called an eigenstate, and the associated eigenvalue corresponds to the value of the observable in that eigenstate.
- Example: if for a quantum state $|\psi\rangle$ and an observable $\mathcal{O}$, we have $\mathcal{O}|\psi\rangle = \lambda|\psi\rangle$, then $|\psi\rangle$ and λ are eigenvector and eigenvalue of $\mathcal{O}$ respectively.
- The possible results of the measure of an observable $\mathcal{O}$ are real numbers $\{\lambda_1, \lambda_2, \ldots\}$. The λ_i's are called the eigenvalues of the observable $\mathcal{O}$.

- λ_i is said to be non-degenerate eigenvalue if there exists a unique eigenstate with eigenvalue λ_i. The observable $\mathcal{O}$ is said to be non-degenerate if all its eigenvalues are non-degenerate.
- Let $\mathcal{O}$ be a non-degenerate observable and $|\psi_i\rangle$ its eigenvectors. Let's choose $\langle\psi_i|\psi_i\rangle = 1$ then $\{|\psi_i\rangle\}$ is a orthonormal basis of the Hilbert space $\mathcal{H}$.
- Let $\mathcal{O}$ be a degenerate observable and let $\mathcal{H}_{\lambda_i}$, the space of eigenvectors of $\mathcal{O}$ with eigenvalues λ_i:
  - The space $\mathcal{H}_{\lambda_i}$ is called the eigenspace associated to λ_i.
  - Its dimension is called the degeneracy of the eigenvalue λ_i.
  - The eigenspaces $\mathcal{H}_{\lambda_i}$ and $\mathcal{H}_{\lambda_j}$ corresponding to different eigenvalues $i \neq j$ are orthogonal.
  - $\mathcal{H} = \oplus_i \mathcal{H}_{\lambda_i}$
- Remark: When two observables have enough simultaneous eigenvectors to form a basis, they are said to be compatible.
- Theorem: If $[L_1, L_2] = 0$, L_1 and L_2 are compatible.
- The average of the results obtained by measuring $\mathcal{O}$ on $|\psi\rangle$ is

$$\langle\psi|L|\psi\rangle = \sum_i \lambda_i \langle\psi_{\lambda_i}|\psi_{\lambda_i}\rangle. \tag{14}$$