Κβαντική Μηχανική I.

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(Non-relativistic) Quantum Mechanics in a Nutshell

1 Basic Mathematics

Linear complex space: A set (of complex "vectors") V is called a linear complex space if a commutative addition and multiplication by a complex number is defined. The elements of V should not be confused with ordinary vectors in real space.

Hilbert space: Consider a linear complex space H, with an inner product, $(\, , \,)$. The inner product is a function that maps $H \times H \to C$ with the following properties:

1. $(x, y) = (y, x)^*$
2. Linearity: $(x, \lambda_1 y_1 + \lambda_2 y_2) = \lambda_1 (x, y_1) + \lambda_2 (x, y_2)$, $\lambda_i \in C$.
3. The inner product is positive definite: $(x, x) \geq 0$. It is equal to zero only if the vector x is the zero vector. The norm of a vector is defined as $||x|| \equiv +\sqrt{(x, x)}$.

If H is complete (every sequence of vectors that converges, it converges to an element of H), then it is called a Hilbert space.

Basis: A set of vectors is called a basis, if any vector of the Hilbert space can be written as a linear combination of the basis vectors. Any such basis can be made orthonormal (basis elements have norm 1 and are mutually orthogonal) by the Gram-Schmidt procedure.

Linear functionals. A linear functional f is a map from a vector space H to the complex numbers, $f : H \to C$.

There is a one-to-one map between vectors and linear functionals. To each vector a in a vector space we associate the linear functional $f_a \equiv (a,)$ using the inner product.
We call the linear functional f_a the linear functional dual to the vector a.

Dirac notation: Vectors $x \in H$ are denoted by kets: $|x\rangle$.

Linear functional dual to a vector $|x\rangle$ are denoted by bras $\langle x|$

The action of linear functional $\langle x|$ on a vector $|y\rangle$ is given by the inner product $\langle x|y\rangle$ (as discussed above).

Linear Operators in a Hilbert space: A linear operator A is a linear map from $H \to H$: $A|x\rangle = |y\rangle$.

Linearity implies that

$$A(\lambda_1|a\rangle + \lambda_2|b\rangle) = \lambda_1 A|a\rangle + \lambda_2 A|b\rangle \ \ , \ \ \lambda_i \in C$$

The hermitial adjoint $A^\dagger$ of an operator A is also an operator defined as

$$\langle x|A^\dagger|y\rangle = \langle y|A|x\rangle^*$$

We call an operator A a hermitian operator if it satisfies $A = A^\dagger$.

We call an operator U a unitary operator if it satisfies $UU^\dagger = 1$.

Dirac representation of operators We define the symbol $|a\rangle\langle b|$ associated to two vectors a, b to act on vectors $x\rangle$ of the Hilbert space as

$$|a\rangle\langle b| \ |x>= |a\rangle \ \langle b|x>= \langle b|x> \ \ |a\rangle$$

and since it is a complex number ($\langle b|x>$) times a vector ($|a\rangle$) it is therefore a vector. As $|a\rangle\langle b|$ maps a vector to a vector, it is an operator in the Hilbert space.

If $|n\rangle$ are the eigenstates of an operator A and A_n are the related eigenvalues then

$$A = \sum_n A_n |n\rangle\langle n|$$

The spectrum of operators. Any vector $|x\rangle \in H$ satisfying

$$A|x\rangle = a|x\rangle \ \ , \ \ a \in C$$

is called an eigenvector of A with eigenvalue a. The eigenvalues of hermitian operators are real numbers and their eigenfunctions form a basis of the Hilbert space.

Sometimes eigenvalues can be degenerate when there is a non-trivial subspace of vectors with the same eigenvalue. The number of linearly independent vectors with the same eigenvalue is the degeneracy of that eigenvalue. The set of all eigenvalues of A is called the spectrum of A.

The spectrum can be discrete or continuous or both. Let $|n, r\rangle$ be the states of the discrete spectrum of a hermitian operator (r is an index that distinguishes degenerate states) and $|\nu, \rho\rangle$, the states in the continuous spectrum (ρ is an index that distinguishes degenerate states).

We can always choose the degenerate basis so that it is orthonormal in the indices r, ρ.

$$\langle n, r|n', r'\rangle = \delta_{n,n'}\delta_{r,r'} \ \ , \ \ \langle n, r|\nu', \rho'\rangle = 0 \ \ , \ \ \langle \nu, \rho|\nu', \rho'\rangle = \delta(\nu - \nu')\delta(\rho - \rho')$$

The commutator $[A, B]$ and anticommutator $\{A, B\}$ of two operators A, B are defined as

$$[A, B] \equiv AB - BA \ \ , \ \ \{A, B\} \equiv AB - BA$$

The matric representation of vectors and operators

Consider an orthonormal basis $|n\rangle$, based on the eigenstates of a hermitian operator A, ($\langle m|n\rangle = \delta_{m,n}$).

Consider an arbitrary vector $|u\rangle$ in the Hilbert space. The inner products with the basis vectors $a_n = \langle n|u\rangle$ give a row of numbers that are the "coordinates" of the vector $u\rangle$ in the basis $|n\rangle$.

The inner products $\langle u|n\rangle = a_n^*$ are the adjoint vector coordinates.

For any operator B, the complex numbers $B_{mn} \equiv \langle m|B|n\rangle$ form the matrix representation of B in the basis $|n\rangle$. The row number is m and the column number is n.

If you use as a basis the eigenstates of A then in this basis its matrix representation is by a diagonal matrix.

(a) The Hermitian adjoint of an operator is represented by the Hermitian adjoint matrix of the matrix representation of the original operator

$$\langle m|B^\dagger|n\rangle = \langle n|B|m\rangle^*$$

(b) Algebraic relations between vectors and operators survive the passage to the matrix representation. Ex: if an operator A satisfies $A^2 = A$, then its matrix representation $A_{mn} \equiv \langle m|A|n\rangle$ satisfies the matrix relation, $\sum_r A_{mr}A_{rn} = A_{mn}$

(c) The trace of any operator is written as $Tr[B] = \sum_n B_{nn}$ and is independent of the basis used to compute it.

Two different orthonormal bases $|a\rangle$, $|m\rangle$ are related by a unitary transformation

$$|m\rangle = \sum_a U_{a,m}|a\rangle \quad , \quad |a\rangle = U^*_{a,n}|n\rangle \quad , \quad UU^\dagger = U^\dagger U = 1$$

The matrix representations of a given operator when we change basis are related by a similarity transformation

$$B_{mn} = U^\dagger_{ma} B_{ab} U_{bn}$$

If $|\psi\rangle$ is the state vector of a quantum mechanical system at a given time, and $|\vec{r}\rangle$ are the eigenstates of the position operators with eigenvalues $\vec{r}$, then $\langle\vec{r}|\psi\rangle \equiv \psi(\vec{r})$ is the probability amplitude for the system to have position $\vec{r}$. This is the wavefunction of the system in the position representation. The scalar product of two states can be written as

$$\langle\phi|\psi\rangle = \int d^3\vec{r}\ \langle\phi|\vec{r}\rangle\langle\vec{r}|\psi\rangle = \int d^3\vec{r}\ \phi^*(\vec{r})\psi(\vec{r})$$

2 Axioms of quantum mechanics

Axiom 1. At a given time $t = t_0$ the state of a quantum system is characterized by a vector (ket) $|\psi(t_0)\rangle \in \mathcal{H}$, with $\mathcal{H}$ a Hilbert space[1]

[1] Hilbert space=infinite dimensional, separable complex vector space with a positive definite inner product.

There is a special hermitian linear operator, $\hat{H}$ acting on $\mathcal{H}$, the hamiltonian. It controls the evolution of a quantum system in time by following equation

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle \tag{1}$$

known as the Schrödinger equation.

Corrolary: The linear combination of two states is a state of the system.

Axiom 2. To any observable O, there corresponds a hermitian operator $\hat{O}$ that acts linearly on $\mathcal{H}$.

Axiom 3. Any observation (measurement) of the observable O on a quantum system gives as a result one of the eigenvalues of $\hat{O}$. The eigenvalues of a hermitian operator are real, and its eigenvectors form a basis in $\mathcal{H}$.

Let λ_n, $|\psi_n\rangle$, $n = 1, 2, \cdots$, be the (discrete) eigenvalues[2] and (orthonormal) eigenvectors of $\hat{O}$

$$\hat{O}\ |\psi_n\rangle = \lambda_n|\psi_n\rangle \ \ , \ \ \langle\psi_n|\psi_m\rangle = \delta_{m,n} \tag{2}$$

A generic state $|\phi\rangle$ of the quantum system can be expanded in the elements of the $|\psi_n\rangle$ basis as

$$|\phi\rangle = \sum_{n=1}^{\infty} c_n\ |\psi_n\rangle \ \ , \ \ c_n = \langle\psi_n|\phi\rangle \tag{3}$$

For an hermitian operator $\hat{A}$ with a continuous spectrum we have similar formulae,

$$\hat{A}\ |\psi_a\rangle = a|\psi_a\rangle \ \ , \ \ \langle\psi_a|\psi_b\rangle = \delta(a-b) \tag{4}$$

A generic state $|\phi\rangle$ of the quantum system can be expanded in the elements of the $|\psi_a\rangle$ basis as

$$|\phi\rangle = \int c(a)\ |\psi_a\rangle\ da \ \ , \ \ c(a) = \langle\psi_a|\phi\rangle \tag{5}$$

Axiom 4.

If the state $|\phi\rangle$ is normalized, ($\langle\phi|\phi\rangle = 1$), then the probability of measuring a non-degenerate eigenvalue λ_n in the state $|\phi\rangle$ is

$$p_n = |c_n|^2 = |\langle\psi_n|\phi\rangle|^2 \tag{6}$$

The sum of all probabilities is one

$$\sum_{n=1}^{\infty} P_n = \sum_{n=1}^{\infty} |\langle\psi_n|\phi\rangle|^2 = \sum_{n=1}^{\infty}\langle\psi_n|\phi\rangle^*\ \langle\psi_n|\phi\rangle \sum_{n=1}^{\infty}\langle\phi|\psi_n\rangle\ \langle\psi_n|\phi\rangle = \langle\phi|\phi\rangle = 1 \tag{7}$$

[2] There are respective formulae for continuous eigenvalues. $\hat{O}|psi_\lambda\rangle = \lambda|psi_\lambda\rangle$ with λ continuous

where we used the completeness relation

$$\sum_{n=1}^{\infty} |\psi_n\rangle \, \langle\psi_n| = 1 \tag{8}$$

Degenerate eigenvalues: If the eigenvalue λ_n is m-fold degenerate, let $|\psi_n^i\rangle$, $i = 1, 2, \cdots, m$ be an orthonormal basis in this degenerate subspace

$$\hat{O}|\psi_n^i\rangle = \lambda_n|\psi_n^i\rangle, \quad \forall i \ , \ \langle\psi_n^i|\psi_n^j\rangle = \delta_{i,j} \tag{9}$$

Then the probability of measuring the eigenvalue λ_n in the state $|\phi\rangle$ is

$$p_n = \sum_{i=1}^{m} |\langle\psi_n^i|\phi\rangle|^2 \tag{10}$$

If the spectrum is continuous, the probability of measuring a value between a and $a + da$ is

$$p(a)da = |\langle\psi_a|\phi\rangle|^2 \, da \tag{11}$$

Corrolary: If $|\phi\rangle$ is normalized, then $e^{i\theta}|\phi\rangle$ (with constant θ) is also normalized, and gives exactly the same probabilities. Note however that relative phases matter: $|\phi_1\rangle + |\phi_2\rangle$ and $|\phi_1\rangle + e^{i\theta}|\phi_2\rangle$ give in general different probabilities.

Axiom 5. Measurement. If a quantum system is in a normalized state $|\psi\rangle$ and at a give time a measurement of the observable O provides one of its eigenvalues λ_n, then automatically the system jumps from $|\psi\rangle$ to

$$|\psi\rangle' = \frac{P_n|\psi\rangle}{\langle\psi|P_n|\psi\rangle} = |\psi_n\rangle \ \ , \ \ P_n = |\psi_n\rangle\langle\psi_n| \tag{12}$$

The state is projected on $|\psi_n\rangle$ by the projection operator P_n, ($P_n^2 = P_n$).

If the eigenvalue λ_n is degenerate, the state $|\psi\rangle$ is projected to an arbitrary vector in the degenerate subspace. The measurement process is NOT described by the Schrödinger equation.

Axiom 6. The Pauli principle. Identical particles with integer spin, must obey Bose statistics: their total wavefunction is symmetric under their exchange. Identical particles with half-integer spin, must obey Fermi statistics: their total wavefunction is anti-symmetric under their exchange.

3 Dynamics

The state of a quantum system $|\psi\rangle$ described by a Hamiltonian operator H is evolving in time by the Schrödinger equation

$$i\hbar\frac{d}{dt}|\psi\rangle = H|\psi\rangle$$

When a measurement process on a system is made, this evolution is temporarily interrupted and the system jumps to the appropriate eigenstate. The solution to this equation, when $\frac{\partial H}{\partial t} = 0$ can be formally written as

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}H(t-t_0)}\ |\psi(t_0)\rangle$$

where the time evolution operator $U(t, t_0) = e^{-\frac{i}{\hbar}H(t-t_0)}$ is unitary. To solve this equation we must find the energy eigenstates $|E\rangle$ of the system

$$H|E\rangle = E|E\rangle$$

The general solution is written as

$$|\psi(t)\rangle = \sum_E c(E)\ e^{-\frac{i}{\hbar}Et}\ |E\rangle$$

where the sum is over the complete basis of eigenstates.