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Quantum Mechanics Summary

The following definitions and concepts set up the basic mathematical language used in quantum mechanics, the postulates on which quantum theory is based, and some of the fundamental ideas and principles of the theory.

Physical Motivation

1. Quantum theory has its origins in the empirical fact that physical systems can be observed to exhibit the following behaviour:
   (a) Outcomes of experiments repeated under identical conditions vary in an irreducibly random fashion.
   (b) Physical systems prepared in a given inital state can be observed in a final state in a way that exhibits interference behaviour if the intermediate state of the system between initial preparation and final observation is *not* observed. This interference vanishes if the intermediate state of the system *is* observed.
2. This kind of behaviour can be described in the mathematical language of vectors:
   (a) From part 1a, let $P(\phi|\psi)$ be the (conditional) probability of observing, in an experiment, a system to be in the state $|\phi\rangle$ given that it was prepared in a state $|\psi\rangle$ where ψ and ϕ are lists of information that can be used to specify the states of the system. Then, from part 1b, the presence of interference can be understood if this probability is the square of a probability amplitude $\langle\phi|\psi\rangle$, i.e.

   $$P(\phi|\psi) = |\langle\phi|\psi\rangle|^2$$

   where

   $$\langle\phi|\psi\rangle = \sum_n \langle\phi|n\rangle\langle n|\psi\rangle$$

   and where the n label *all* the possible *mutually exclusive* intermediate states of the system.
   (b) The probability $P(\phi|\psi)$ is then

   $$P(\phi|\psi) = \sum_n P(\phi|n)P(n|\psi) + 2\mathrm{Re}\sum_{\substack{n,m \\ n\neq m}}(\langle\phi|n\rangle\langle n|\psi\rangle)^*\langle\phi|m\rangle\langle m|\psi\rangle$$

   where the cross terms give rise to the interference effects. Observation of the intermediate state reduces this to the standard result of the theory of probability:

   $$P(\phi|\psi) = \sum_n P(\phi|n)P(n|\psi).$$

(c) The ‘cancellation’ of common terms then gives

$$|\psi\rangle = \sum_n |n\rangle\langle n|\psi\rangle$$

which leads to the interpretation of $|\psi\rangle$ and the $|n\rangle$’s as vectors belonging to a complex inner product vector space or state space with the probability amplitudes $\langle n|\psi\rangle$ as the ‘weighting’ of the intermediate states $|n\rangle$.

(d) The probability interpretation along with the ‘mutual exclusivity’ of the intermediate states leads to the orthonormality condition

$$\langle n|m\rangle = \delta_{nm}$$

(e) The states $|n\rangle$ exhaustively cover all the possible intermediate states and so constitute a *complete* orthonormal set of basis states for the state space of the system.

Mathematical Background

The mathematical background is initiated by what is effectively a postulate, so as to motivate the mathematical language used. The postulates themselves are considered in detail later.

1. Every physical state of a quantum system is represented by a symbol known as a *ket* written $|\ldots\rangle$ where $\ldots$ is a label specifying the physical information known about the state. An arbitrary state is written $|\psi\rangle$, or $|\phi\rangle$ and so on.

2. Linear combinations or superpositions of such states define other possible states of the system i.e. every linear superposition of two or more kets $|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle, \ldots,$ is also a state of the quantum system. Thus the ket $|\psi\rangle$ given by

   $$|\psi\rangle = c_1|\phi_1\rangle + c_2|\phi_2\rangle + c_3|\phi_3\rangle + \ldots$$

   also represents a physical state of the system for all complex numbers $c_1, c_2, c_3, \ldots$.

3. If a state of the system is represented by a ket $|\psi\rangle$, then the same physical state is represented by the ket $c|\psi\rangle$ where c is any non-zero complex number.

4. The set of all kets describing a given physical system forms a complex vector space (or Hilbert space) $\mathcal{H}$ also known as the state space or ket space for the system. A ket is thus a vector belonging to $\mathcal{H}$. A ket is also referred to as a state vector, ket vector, or sometimes just state.

5. A set of vectors $|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle, \ldots$ is said to be complete if every state of the quantum system can be represented as a linear superposition of the $|\phi_i\rangle$’s i.e. for any state $|\psi\rangle$ we can write

   $$|\psi\rangle = \sum_i c_i|\phi_i\rangle.$$

   The set of vectors $|\phi_i\rangle$, $i = 1, 2, \ldots$ are said to *span* the vector space.

6. A basis for the state space $\mathcal{H}$ is a complete set of *linearly independent* vectors that span all of $\mathcal{H}$.

7. The number of basis states making up a complete set of basis states for a state space $\mathcal{H}$ is the dimension of the state space. This can be either finite or infinite. In the latter case, the basis states can be denumerable (i.e. discrete) or non-denumerable (i.e. continuous).

8. In quantum mechanics, a state space of infinite dimension is assumed to be *separable*, i.e. that there always exists a denumerable set of basis states.

Inner Product

The following definitions and properties define the inner product of vectors belonging to a state space $\mathcal{H}$, and its representation in terms of bra vectors.

1. If $|\phi\rangle$ and $|\psi\rangle$ are any two vectors belonging to $\mathcal{H}$, then the inner product of these two vectors is a rule that maps the pair of vectors $|\phi\rangle, |\psi\rangle$ into a complex number, written $(|\phi\rangle, |\psi\rangle)$ with the properties

    (a) $(|\phi\rangle, |\psi\rangle) = c$, a complex number;

    (b) $(|\phi\rangle, c_1|\psi_1\rangle + c_2|\psi_2\rangle) = c_1(|\phi\rangle, |\psi_1\rangle) + c_2(|\phi\rangle, |\psi_2\rangle)$ where c_1 and c_2 are complex numbers;

    (c) $(|\psi\rangle, |\psi\rangle) \geq 0$. If $(|\psi\rangle, |\psi\rangle)=0$ then $|\psi\rangle = 0$, the zero vector.

    (d) The quantity $\sqrt{(|\psi\rangle, |\psi\rangle)}$ is known as the *length* or *norm* of $|\psi\rangle$.

    (e) A state $|\phi\rangle$ is normalized, or normalized to unity, if $(|\phi\rangle, |\phi\rangle) = 1$. Two states $|\phi\rangle$ and $|\psi\rangle$ are orthogonal if $(|\phi\rangle, |\psi\rangle) = 0$.

2. The inner product $(|\psi\rangle, |\phi\rangle)$ defines, for all states $|\psi\rangle$, the set of functions (or linear functionals) $(|\psi\rangle, \ )$. The linear functional $(|\psi\rangle, \ )$ maps any ket vector $|\phi\rangle$ into the complex number given by the inner product $(|\psi\rangle, |\phi\rangle)$.

    (a) The set of all linear functionals $(|\psi\rangle, \ )$ forms a complex vector space $\mathcal{H}^*$, the dual space of $\mathcal{H}$.

    (b) The linear functional $(|\psi\rangle, \ )$ is written $\langle\psi|$ and is known as a bra vector.

    (c) To each ket vector $|\psi\rangle$ there corresponds a bra vector $\langle\psi|$ such that if $|\phi_1\rangle \to \langle\phi_1|$ and $|\phi_2\rangle \to \langle\phi_2|$ then
    $$c_1|\phi_1\rangle + c_2|\phi_2\rangle \to c_1^*\langle\phi_1| + c_2^*\langle\phi_2|.$$

    (d) In terms of the bra vector notation, the inner product is written
    $$(|\psi\rangle, |\phi\rangle) = \langle\psi|\phi\rangle.$$

3. A Hilbert space is a vector space on which there is defined an inner product and for which certain convergence criteria need to be satisfied, namely that every Cauchy sequence of vectors belonging to the vector space must converge to a vector that also belongs to the space, the convergence being defined in terms of the inner product. (A condition required in order to be able, for instance, to define the derivatives of state vectors).

Operations on States

1. *Operators*: State vectors can be transformed into other state vectors by the action of operators. The effect of an operator $\hat{A}$ acting on a state vector $|\psi\rangle$ is to change the state of the system to a new state $|\phi\rangle = \hat{A}|\psi\rangle$. An operator is fully characterized when its effect on every state of the state space is known.

2. *Linear Operators*: An operator $\hat{A}$ is linear if it has the property
$$\hat{A}(c_1|\psi_1\rangle + c_2|\psi_2\rangle) = c_1\hat{A}|\psi_1\rangle + c_2\hat{A}|\psi_2\rangle$$
for all complex numbers c_1 and c_2 and all states $|\psi_1\rangle$ and $|\psi_2\rangle$.

3. *Sum of Two Operators*: The sum $\hat{A}+\hat{B}$ of two operators $\hat{A}$ and $\hat{B}$ is defined by

$$(\hat{A}+\hat{B})|\psi\rangle = \hat{A}|\psi\rangle + \hat{B}|\psi\rangle$$

for all states $|\psi\rangle$.

4. *Product of Two Operators*: The product $\hat{A}\hat{B}$ of two operators $\hat{A}$ and $\hat{B}$ is defined by

$$(\hat{A}\hat{B})|\psi\rangle = \hat{A}(\hat{B}|\psi\rangle)$$

for all states $|\psi\rangle$.

5. *The Zero Operator*: The zero operator $\hat{0}$ is such that $\hat{0}|\psi\rangle = 0$, the zero vector, for all $|\psi\rangle$.

6. *The Unit Operator*: The unit operator $\hat{1}$ is such that $\hat{1}|\psi\rangle = |\psi\rangle$ for all $|\psi\rangle$.

7. *Projection Operators*: An operator $\hat{P}$ with the property $\hat{P}^2 = \hat{P}$ is known as a projection operator.

8. *Commutator*: The commutator of two operators $\hat{A}$ and $\hat{B}$ is defined by

$$[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}.$$

9. *Equality of Operators*: Two operators $\hat{A}$ and $\hat{B}$ are equal if $\hat{A}|\psi\rangle = \hat{B}|\psi\rangle$ for all states $|\psi\rangle$.

10. *Action of Operator on Bra Vectors*: The expression $\langle\psi|\hat{A}$ is defined to be such that

$$(\langle\psi|\hat{A})|\phi\rangle = \langle\psi(\hat{A}|\phi\rangle)$$

for all $|\phi\rangle$.

11. *Adjoint of an Operator*: The adjoint (or Hermitean conjugate) $\hat{A}^\dagger$ of an operator $\hat{A}$ is defined such that if $\hat{A}|\psi\rangle = |\phi\rangle$ then $\langle\psi|\hat{A}^\dagger = \langle\phi|$.

12. *Self Adjoint or Hermitean Operators*: If $\hat{A} = \hat{A}^\dagger$ then the operator $\hat{A}$ is *self adjoint* or *Hermitean*. [Note that mathematically speaking, these two terms do not mean quite the same thing, but in quantum mechanics, the distinction is not usually made].

13. *Ket-Bra Notation for Operators*: An expression of the general form

$$\hat{A} = \sum_i c_i|\phi_i\rangle\langle\psi_i|$$

with the rules of manipulation

   (a) $|\phi\rangle(c_1\langle\psi_1| + c_2\langle\psi_2|) = c_1|\phi\rangle\langle\psi_1| + c_2|\phi\rangle\langle\psi_2|$
   (b) $\hat{A}|\chi\rangle = \sum_i c_i|\phi_i\rangle\langle\psi_i|\chi\rangle$
   (c) $\langle\chi|\hat{A} = \sum_i c_i\langle\chi|\phi_i\rangle\langle\psi_i|$

is a linear operator. With this notation it then follows that:

   (a) The Hermitean conjugate of the operator $\hat{A}$ is:

$$\hat{A}^\dagger = \sum_i |\psi_i\rangle\langle\phi_i|.$$

   (b) Any projection operator $\hat{P}$ can be expressed in the form $\hat{P} = |\psi\rangle\langle\psi|$ where $|\psi\rangle$ is normalized to unity.

14. *Eigenvalues and Eigenvectors*: A vector is an eigenvector, eigenket, or eigenstate of an operator $\hat{A}$ if $\hat{A}|\psi\rangle = a|\psi\rangle$ where a is in general a complex number known as the eigenvalue belonging to the eigenvector $|\psi\rangle$. The usual notation is to identify the eigenvector by its eigenvalue i.e. in this case $|\psi\rangle$ becomes $|a\rangle$.

15. *Discrete and Continuous Eigenvalues*: An operator $\hat{A}$ may have discrete eigenvalues a_1, a_2, $a_3, \ldots$, or a continuous set of eigenvectors, e. g. $\alpha_1 < a < \alpha_2$ or both. The set of eigenvalues is known as the *spectrum* of the operator.

16. *Degeneracy*: If two or more distinct eigenvectors have the same eigenvalue, the eigenvalue is said to be *degenerate*.

17. *Properties of Hermitean operators*: If $\hat{A}$ is Hermitean then:

    (a) All eigenvalues of $\hat{A}$ are real, and eigenvectors belonging to different eigenvalues are orthogonal.

    (b) For *discrete* eigenvalues, the associated eigenvectors of an Hermitean operator, $\hat{A}$ say, can be normalized to unity so that $\langle a_i|a_j\rangle = \delta_{ij}$. For *continuous* eigenvalues, the associated eigenvectors can be delta function normalized i. e. $\langle a|a'\rangle = \delta(a - a')$. In either case the eigenvectors are said to be *orthonormal*.

    (c) The eigenstates of a Hermitean operator form a complete set.

    (d) The operator $\hat{A}$ can be expanded (spectral decomposition) as:

    $$\hat{A} = \sum_i a_i|a_i\rangle\langle a_i| + \int_{\mathcal{A}} a|a\rangle\langle a|da.$$

18. *Eigenvectors of Commuting Operators*: If two Hermitean operators $\hat{A}$ and $\hat{B}$ commute, then they have in common a complete set of eigenvectors $|ab\rangle$ such that $\hat{A}|ab\rangle = a|ab\rangle$ and $\hat{B}|ab\rangle = b|ab\rangle$.

19. *The Inverse of an Operator*: An operator $\hat{A}$ has an inverse if there exists an operator $\hat{B}$ such that $\hat{A}\hat{B} = \hat{B}\hat{A} = \hat{1}$. Usually write $\hat{B} = \hat{A}^{-1}$.

20. *Unitary Operator*: An operator $\hat{A}$ is unitary if $\hat{A}^\dagger = \hat{A}^{-1}$.

State Space for Combined Systems

1. If a system is made up of two parts S_1 and S_2, each of which can be considered as a system on its own, and the state spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ of the respective systems are spanned by the complete sets of states $|\psi_1\rangle$, $|\psi_2\rangle$, $|\psi_2\rangle$, ..., and $|\phi_1\rangle$, $|\phi_2\rangle$, $|\phi_2\rangle$, ..., then every state of the combined system can be expressed in the form

    $$|\Psi\rangle = c_1|\psi_1\rangle \otimes |\phi_1\rangle + c_2|\psi_2\rangle \otimes |\phi_2\rangle + \ldots$$

    where the tensor product state $|\psi_i\rangle \otimes |\phi_i\rangle$ represents the state of the combined system in which the system S_1 is in state $|\psi_1\rangle$ and system S_2 in state $|\phi_2\rangle$. In other words, the set of states $|\psi_i\rangle \otimes |\phi_i\rangle$, $i = 1, 2, \ldots$ span the tensor product Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$, the state space of the combined system. The notation $|\psi_i\rangle \otimes |\phi_i\rangle$ is usually replaced by the simpler notation $|\psi_i\rangle|\phi_i\rangle$.

2. The product states $|\psi\rangle|\phi\rangle$ have the properties

    (a) $|\psi\rangle(c_1|\phi_1\rangle + c_2|\phi_2\rangle) = c_1|\psi\rangle|\phi_1\rangle + c_2|\psi\rangle|\phi_2\rangle$.

(b) $(c_1|\psi_1\rangle + c_2|\psi_2\rangle)|\phi\rangle = c_1|\psi_1\rangle|\phi\rangle + c_2|\psi_2\rangle|\phi\rangle$.

(c) The bra vector corresponding to the ket vector $|\psi\rangle|\phi\rangle$ is $\langle\phi|\langle\psi|$ [note the reversal of order of the factors].

(d) $(\langle\phi_1|\langle\psi_1|)(|\psi_2\rangle|\phi_2\rangle) = \langle\phi_1|\phi_2\rangle\langle\psi_1|\psi_2\rangle$.

3. If $\hat{A}_1$ is an operator acting on states of S_1 and $\hat{A}_2$ an operator acting on states of S_2 then an operator acting on states of the combined system, written $\hat{A}_1 \otimes \hat{A}_2$, can be defined with the properties

   (a) $(\hat{A}_1 \otimes \hat{A}_2)|\psi\rangle|\phi\rangle = \hat{A}_1|\psi\rangle \otimes \hat{A}_2|\phi\rangle$.

   (b) $\hat{A}_1 + \hat{A}_2 \equiv \hat{A}_1 \otimes \hat{1}_2 + \hat{1}_1 \otimes \hat{A}_2$.

   (c) With the simpler notation $\hat{A}_1 \otimes \hat{A}_2 \equiv \hat{A}_1\hat{A}_2$, it then also follows that $[\hat{A}_1,\mathrm{A}_2] = 0$.

The above definitions can be readily generalized for systems made up of more than two subsystems.

Basic Postulates and Concepts of Quantum Mechanics

1. Every state of a physical system is represented by a vector, and conversely, each linear superposition of vectors is representative of a possible state of the system. The set of all state vectors describing a given physical system forms a complex vector space (or Hilbert space) also known as the state space for the system. If a state of the system is represented by a vector $|\psi\rangle$, then the same state is represented by the vector $c|\psi\rangle$ where c is any non-zero complex number.

2. To each physically measurable property (called an "observable") of a physical system there corresponds a Hermitean operator (also called an "observable") whose eigenvalues are the possible results of measurements of the corresponding observable. Conversely, any Hermitean operator is understood as representing a possible measureable property of the system.

3. The eigenvectors of each observable associated with a physical system is assumed to form a complete set so that any state of the system can be expressed as a linear superposition of the eigenvectors of any observable of the system.

4. The orthonormal eigenvectors $|a_i\rangle$ (discrete eigenvalues) and $|a\rangle$ (continuous eigenvalues) of any observable are assumed to satisfy the closure or completeness relation

$$\sum_i |a_i\rangle\langle a_i| + \int_{\mathcal{A}} |a\rangle\langle a|da = \hat{1}.$$

5. *Probability Interpretation*:

   (a) Only those states that have finite norm (and hence can be normalized to unity) can represent possible physical states of a system. (However, certain states of infinite norm can be said to represent a possible physical state of a system under certain circumstances.)

   (b) If the two states $|\phi\rangle$ and $|\psi\rangle$ are both normalized to unity, i.e. $\langle\phi|\phi\rangle = \langle\psi|\psi\rangle = 1$, then:

      (i) The inner product $\langle\phi|\psi\rangle$ is the probability amplitude of observing the system to be in the state $|\phi\rangle$ given that it is in the state $|\psi\rangle$.

(ii) The probability of observing the system to be in the state $|\phi\rangle$ given that it is in the state $|\psi\rangle$ is $|\langle\phi|\psi\rangle|^2$.

(c) In the linear superposition of a state $|\psi\rangle$ in terms of the eigenvectors of the observable $\hat{A}$:

$$|\psi\rangle = \sum_i |a_i\rangle\langle a_i|\psi\rangle + \int_{\mathcal{A}} |a\rangle\langle a|\psi\rangle da$$

the quantity $|\langle a_i|\psi\rangle|^2$ is the probability of obtaining the (discrete) result a_i in a measurement of $\hat{A}$ and $|\langle a|\psi\rangle|^2 da$ is the probability of obtaining a result in the range a to $a + da$ for the continuous set of eigenvalues, provided $\langle\psi|\psi\rangle = 1$.

6. *Expectation Value of Observable:* The expectation or mean or average value of the results of observing $\hat{A}$ for a large number of identical systems all in the state $|\psi\rangle$ is $\langle\psi|\hat{A}|\psi\rangle$ if $\langle\psi|\psi\rangle = 1$.

7. *Uncertainty*: The uncertainty or variance ΔA in the results of measurements of an observable $\hat{A}$ on a large number of identical systems all in the state $|\psi\rangle$ is given by:

$$(\Delta A)^2 = \langle\psi|(\hat{A} - \langle\hat{A}\rangle)^2|\psi\rangle = \langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2$$

provided $\langle\psi|\psi\rangle = 1$.

8. *Change of State by Measurement*: If as a result of a measurement of an observable $\hat{A}$, the result a is obtained, then immediately after the measurement, the system is in an eigenstate of $\hat{A}$ with eigenvalue a. (This is the simplest possible assumption concerning the change of state by measurement).

9. If two observables $\hat{A}$ and $\hat{B}$ do not commute, then measurements of $\hat{A}$ and $\hat{B}$ interfere in the sense that alternate measurements of $\hat{A}$ and $\hat{B}$ will yield randomly varying results. Observables $\hat{A}$ and $\hat{B}$ cannot simultaneously have precisely defined values, and the observables are said to be *incompatible*.

10. If two observables $\hat{A}$ and $\hat{B}$ do commute, then there exists states of the system for which these observables simultaneously have precisely defined values. These are the common eigenstates $|ab\rangle$. The observables are then said to be *compatible*.

11. *The Heisenberg Uncertainty Relation*: The uncertainties ΔA and ΔB in two observables for a system in a state $|\psi\rangle$ are related by the inequality

$$\Delta A \Delta B \geq \tfrac{1}{2}|\langle[\hat{A}, \hat{B}]\rangle|.$$

12. *Complete Set of Commuting Observables*: A complete set of commuting observables $\hat{A}$, $\hat{B}$, $\hat{C}, \ldots$ are a set of observables that represent the maximum number of physical observables of a system that simultaneously can have precisely defined values. Their common eigenvectors $|abcd\ldots\rangle$ are completely and uniquely characterized by their eigenvalues $a, b, c, \ldots$, i.e. no two eigenvectors have identical sets of eigenvalues.

13. If $\hat{A}$ is an observable for a quantum system with *discrete* eigenvalues then states and operators of the system can be *represented* in terms of their components with respect to the eigenstates of $\hat{A}$ as basis vectors in the following manner:

(a) The ket vector $|\psi\rangle$ is represented by a column vector of components

$$|\psi\rangle \doteq \begin{pmatrix} \langle a_1|\psi\rangle \\ \langle a_2|\psi\rangle \\ \langle a_3|\psi\rangle \\ \langle a_1|\psi\rangle \end{pmatrix}$$

(b) The bra vector is represented by the row vector of components $\langle\psi|a_i\rangle$

$$\langle\psi| \doteq \begin{pmatrix}\langle\psi|a_1\rangle & \langle\psi|a_2\rangle & \langle\psi|a_3\rangle & \ldots\end{pmatrix}$$

(c) The operator $\hat{B}$ is represented by a matrix with components $\langle a_i|\hat{B}|a_j\rangle$

$$\hat{B} \doteq \begin{pmatrix}\langle a_1|\hat{B}|a_1\rangle & \langle a_1|\hat{B}|a_2\rangle & \langle a_1|\hat{B}|a_3\rangle & \ldots\\ \langle a_2|\hat{B}|a_1\rangle & \langle a_2|\hat{B}|a_2\rangle & \langle a_2|\hat{B}|a_3\rangle & \ldots\\ \langle a_3|\hat{B}|a_1\rangle & \langle a_3|\hat{B}|a_2\rangle & \langle a_3|\hat{B}|a_3\rangle & \ldots\\ \vdots & \vdots & \vdots & \ldots\end{pmatrix}$$

Note the use of the symbol "$\doteq$" rather than "$=$" to indicate that the vectors (or operators) are *represented* by the corresponding column or row vectors, or matrix.

Relations between abstract vectors and operators can then be *represented* as equations in terms of row and column vectors and square matrices.

14. If $\hat{A}$ is an observable with continuous eigenvalues, then a representation in terms of column or row vectors and matrices is no longer explicity possible. Nevertheless, vectors and operators can still be represented in terms of their components. If $\hat{A}$ is an observable for a quantum system with *continuous* eigenvalues then:

(a) The components of the ket vector $|\psi\rangle$ with respect to the basis states $|a\rangle$ are $\langle a|\psi\rangle = \psi(a)$. The quantity $\psi(a)$ is known as the wave function of the state $|\psi\rangle$ in the $\hat{A}$-representation.

(b) The components of the bra vector $\langle\psi|$ are $\langle\psi|a\rangle = \psi^*(a)$.

(c) The components of the operator $\hat{B}$ are given by $\langle a|\hat{B}|a'\rangle$. Note that, in general, these components will be Dirac delta functions or its derivatives.

15. *Infinitesimal time evolution of a quantum system*: If a quantum system is in the state $|\psi(t)\rangle$ at time t, the state of the system an infinitesimal time interval later is assumed to be given by

$$|\psi(t+dt)\rangle = (\hat{1} - i\hat{\Omega}(t)dt)|\psi(t)\rangle$$

where $\hat{\Omega}$ is a (linear) Hermitean operator which may also be time dependent.

16. *The Hamiltonian*: Typically, $\hat{\Omega}$ is written as $\hat{H}/\hbar$ where $\hat{H}$ is known as the *Hamiltonian* of the system, and $\hbar$ is Planck's constant.

17. *The time evolution operator*:

(a) Over the finite time interval (t_0, t)

$$|\psi(t)\rangle = \hat{U}(t, t_0)|\psi(t_0)\rangle$$

where $\hat{U}(t, t_0)$ is a *unitary* operator known as the time evolution, or time development operator.

(b) If the Hamiltonian is time independent, then

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

If the Hamiltonain is time dependent, there is in general no closed form expression for the time evolution operator.

18. *The Schrödinger equation*: In general, the time dependent state vector $|\psi(t)\rangle$ satisfies the equation

$$\hat{H}(t)|\psi(t)\rangle = i\hbar\frac{d|\psi(t)\rangle}{dt}.$$

19. *Stationary states*: If the Hamiltonian $\hat{H}$ is independent of time, then the time dependence of the eigenstates $|E\rangle$ of $\hat{H}$, where

$$\hat{H}|E\rangle = E|E\rangle$$

takes the form

$$|E(t)\rangle = e^{-iEt/\hbar}|E\rangle.$$

so that the probability for the outcome of the measurement of any observable

$$|\langle a|E(t)\rangle|^2 = |\langle a|E\rangle|^2$$

is independent of time.

20. *Conserved quantities*: The observable $\hat{O}$ is said to be conserved if its expectation value $\langle\hat{O}(t)\rangle = \langle\psi(t)|\hat{O}|\psi(t)\rangle$, or

$$\frac{d\langle\hat{O}(t)\rangle}{dt} = \frac{i}{\hbar}\langle[\hat{H},\hat{O}]\rangle = 0$$

for all initial states $|\psi(t_0)\rangle$.

21. *The infinitesimal displacement operator*: In one dimension, if a quantum system is in the eigenstate $|x\rangle$ of the position operator $\hat{x}$, then the state of the system after undergoing an infinitesimal displacement dx is

$$|x + dx\rangle = (\hat{1} + i\hat{K}dx)|x\rangle$$

where $\hat{K}$ is a (linear) Hermitean operator.

22. *The momentum operator*: Typically, $\hat{K}$ is written as $\hat{p}/\hbar$ where $\hat{p}$ is known as the *momentum* operator of the system.

23. *The displacement operator*: If a quantum system in the state $|\psi\rangle$ undergoes a finite displacement a, the state of the system after the displacement is $\hat{D}(a)|\psi\rangle$ where

$$\hat{D}(a) = e^{i\hat{p}a/\hbar}$$

is a *unitary operator*.

24. *Symmetries*: An operation performed on a system (as represented by a unitary operator $\hat{S}$ say) is a symmetry operation if the evolution of the system is unaffected by the operation.

    (a) This is to be understood in the sense that

    $$\hat{S}^{-1}\hat{U}(t,t_0)\hat{S}|\psi\rangle = \hat{U}(t,t_0)|\psi\rangle$$

    i.e. performing the operation ($\hat{S}$), allowing the system to evolve ($\hat{U}(t,t_0)$), and then reversing the operation ($\hat{S}^{-1}$) produces the same outcome as not performing the operation at all, for all states $|\psi\rangle$ of the system.

    (b) As a consequence, the operation represented by the unitary operator $\hat{S}$ is a symmetry operation if

    $$[\hat{S},\hat{H}] = 0$$

    where $\hat{H}$ is the Hamiltonian of the system.

25. *Symmetries and Conservation Laws*: Associated with each symmetry of a quantum system is a conserved observable. In particular, if the space displacement operator $\hat{S} = \hat{D}(a)$ is a symmetry operation, then the conserved quantity is the momentum $\hat{p}$.

26. *Canonical commutation relations*: From the definition of the space displacement operator it follows that
$$[\hat{x}, \hat{p}] = i\hbar$$
or, more generally
$$[\hat{x}, f(\hat{p})] = i\hbar \frac{df(\hat{p})}{d\hat{p}}.$$

27. *Canonical quantization*: The quantum description of a classical physical system can be constructed by demanding that

    (a) All symmetry properties of the classical system also be symmetries of the quantum system.

    (b) The conserved quantities of the quantum system be identified, up to a constant of proportionality, as the Hermitean operators (observables) of the corresponding classically conserved quantities.

    which results in the rules:

    (a) Replace, in the classical Hamiltonian, all generalized positions and momenta p_i and q_i, $i = 1, 2, \ldots$, by Hermitean operators $\hat{p}_i$ and $\hat{q}_i$.

    (b) The classical Hamiltonian $H(q, p)$ becomes the quantum Hamiltonian $\hat{H}(\hat{q}, \hat{p})$.

    (c) The quantum operators $\hat{p}_i$ and $\hat{q}_i$ are required to satisfy the commutation rules
$$[\hat{q}_i, \hat{p}_j] = i\hbar\delta_{ij}$$
$$[\hat{q}_i, \hat{q}_j] = [\hat{p}_i, \hat{p}_j] = 0.$$

28. *The position representation*: This representation is defined in terms of the eigenstates of the position operator $\hat{x}$ (in one dimension). This operator has continuous eigenvalues, so that:

    (a) The wave function of the ket vector in the position representation is $\langle x|\psi\rangle = \psi(x)$.

    (b) The position operator in the position representation is
$$\langle x|\hat{x}|x'\rangle = \delta(x - x')$$

    (c) The momentum operator in the position representation is
$$\langle x|\hat{p}|x'\rangle = -i\hbar \frac{\partial\delta(x - x')}{\partial x'}$$
    or, in a form often more convenient
$$\langle x|\hat{p}|\psi\rangle = -i\hbar \frac{d\psi(x)}{dx}$$

29. *Schrödinger equation in the position representation*: The Schrödinger equation for a particle with Hamiltonian
$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}, t)$$
is, in the position representation
$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x, t)}{\partial x^2} + V(x, t)\Psi(x, t) = i\hbar\frac{\partial\Psi(x, t)}{\partial t}$$
otherwise known as the *Schrödinger wave equation*.

Updated: 1st August 2005 at 4:26pm.