# 4.2: States, State Vectors, and Linear Operators

The basic notion of the general formulation of quantum mechanics is the quantum state of a system. [4] To get some gut feeling of this notion, if a quantum state $\alpha$ of a particle may be adequately described by wave mechanics, this description is given by the corresponding wavefunction $\Psi_\alpha(\mathbf{r}, t)$. Note, however, a quantum state as such is not a mathematical object, [5] and can participate in mathematical formulas only as a "label" - e.g., the index of the wavefunction $\Psi_\alpha$. On the other hand, such wavefunction is not a state, but a mathematical object (a complex function of space and time) giving a quantitative description of the state - just as the classical radius vector $\mathbf{r}_\alpha$ and velocity $\mathbf{v}_\alpha$ as real functions of time are mathematical objects describing the motion of the particle in its classical description - see Fig. 3. Similarly, in the Dirac formalism, a certain quantum state $\alpha$ is described by either of two mathematical objects, called the state vectors: the ket-vector $|\alpha\rangle$ and bra-vector $\langle\alpha|$, [6] whose relationship is close to that between the wavefunction $\Psi_\alpha$ and its complex conjugate $\Psi_\alpha{}^*$.

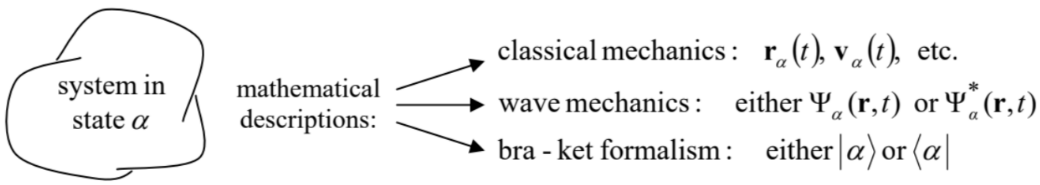


Fig. 4.3. Physical state of a system and its descriptions.

One should be cautious with the term "vector" here. The usual geometric vectors, such as $\mathbf{r}$ and $\mathbf{v}$, are defined in the usual geometric (say, Euclidean) space. In contrast, the bra- and ket-vectors are defined in a more abstract Hilbert space - the full set of its possible bra- and ket-vectors of a given system. [7] So, despite certain similarities with the geometric vectors, the bra- and ket-vectors are different mathematical objects, and we need to define the rules of their handling. The primary rules are essentially postulates and are justified only by the correct description of all experimental observations of the rule corollaries. While there is a general consensus among physicists what the corollaries are, there are many possible ways to carve from them the basic postulate sets. Just as in Sec. 1.2, I will not try too hard to beat the number of the postulates to the smallest possible minimum, trying instead to keep their physical meaning transparent.(i) Ket-vectors. Let us start with ket-vectors - sometimes called just kets for short. Their most important property is the linear superposition. Namely, if several ket-vectors $|\alpha_j\rangle$ describe possible states of a quantum system, numbered by the index $j$, then any linear combination (superposition)

$$|\alpha\rangle = \sum_j c_j |\alpha_j\rangle \tag{4.2.1}$$

where $c_j$ are any (possibly complex) $c$-numbers, also describes a possible state of the same system. [8] Actually, since ket-vectors are new mathematical objects, the exact meaning of the right-hand side of Eq. (6) becomes clear only after we have postulated the following rules of summation of these vectors,

$$|\alpha_j\rangle + |\alpha_{j'}\rangle = |\alpha_{j'}\rangle + |\alpha_j\rangle, \tag{4.2.2}$$

and their multiplication by an arbitrary $c$-number:

$$c|\alpha_j\rangle = |\alpha_j\rangle c. \tag{4.2.3}$$

Note that in the set of wave mechanics postulates, the statements parallel to Eqs. (7) and (8) were unnecessary, because the wavefunctions are the usual (albeit complex) functions of space and time, and we know from the usual algebra that such relations are indeed valid.

As evident from Eq. (6), the complex coefficient $c_j$ may be interpreted as the "weight" of the state $\alpha_j$ in the linear superposition $\alpha$. One important particular case is $c_j = 0$, showing that the state $\alpha_j$ does not participate in the superposition $\alpha$. The corresponding term of the sum (6), i.e. the product

$$\text{Null-state vector} \qquad 0|\alpha_j\rangle, \tag{4.2.4}$$

has a special name: the null-state vector. (It is important to avoid confusion between the null-state corresponding to vector (9), and the ground state of the system, which is frequently denoted by ketvector $|0\rangle$. In some sense, the null-state does not exist at all, while the ground state not only does exist but frequently is the most important quantum state of the system.)

(ii) Bra-vectors and inner products. Bra-vectors $\langle\alpha|$, which obey the rules similar to Eqs. (7) and (8), are not new, independent objects: a ket-vector $|\alpha\rangle$ and the corresponding bra-vector $\langle\alpha|$ describe the same state. In other words, there is a unique dual correspondence between $|\alpha\rangle$ and $\langle\alpha|$,[9] very similar (though not identical) to that between a wavefunction $\Psi$ and its complex conjugate $\Psi^*$. The correspondence between these vectors is described by the following rule: if a ket-vector of a linear superposition is described by Eq. (6), then the corresponding bra-vector is

$$\langle\alpha|=\sum_j c_j^*\langle\alpha_j|=\sum_j\langle\alpha_j|c_j^*. \tag{4.2.5}$$

The mathematical convenience of using two types of vectors rather than just one becomes clear from the notion of their inner product (due to its second, shorthand form, also called the short bracket):

$$(\langle\beta|)(|\alpha\rangle)\equiv\langle\beta\mid\alpha\rangle, \tag{4.2.6}$$

which is a scalar $c$-number, in a certain but limited analogy with the scalar product of the usual geometric vectors. (For one difference, the product (11) may be a complex number.)

The main property of the inner product is its linearity with respect to any of its component vectors. For example, if a linear superposition $\alpha$ is described by the ket-vector (6), then

$$\langle\beta\mid\alpha\rangle=\sum_j c_j\langle\beta\mid\alpha_j\rangle \tag{4.2.7}$$

while if Eq. (10) is true, then

$$\langle\alpha\mid\beta\rangle=\sum_j c_j^*\langle\alpha_j\mid\beta\rangle. \tag{4.2.8}$$

In plain English, $c$-number factors may be moved either into or out of the inner products.

The second key property of the inner product is

$$\langle\alpha\mid\beta\rangle=\langle\beta\mid\alpha\rangle^* \tag{4.2.9}$$

It is compatible with Eq. (10); indeed, the complex conjugation of both parts of Eq. (12) gives:

$$\langle\beta\mid\alpha\rangle^*=\sum_j c_j^*\langle\beta\mid\alpha_j\rangle^*=\sum_j c_j^*\langle\alpha_j\mid\beta\rangle=\langle\alpha\mid\beta\rangle. \tag{4.2.10}$$

Finally, one more rule: the inner product of the bra- and ket-vectors describing the same state (called the norm squared) is real and non-negative,

$$\|\alpha\|^2\equiv\langle\alpha\mid\alpha\rangle\geq 0 \tag{4.2.11}$$

In order to give the reader some feeling about the meaning of this rule: we will see below that if some state $\alpha$ may be described by the wavefunction $\Psi_\alpha(\mathbf{r},t)$, then

$$\langle\alpha\mid\alpha\rangle=\int\Psi_\alpha^*\Psi_\alpha d^3r\geq 0. \tag{4.2.12}$$

Hence the role of the bra- and ket-vectors of the same state is very similar to that of complex-conjugate pairs of its wavefunctions.

(iii) Operators. One more key notion of the Dirac formalism is quantum-mechanical linear operators. Just as for the operators discussed in wave mechanics, the function of an operator is to "generate" of one state from another: if $|\alpha\rangle$ is a possible ket of the system, and $\hat{A}$ is a legitimate [10] operator, then the following combination,

$$\hat{A}|\alpha\rangle, \tag{4.2.13}$$

is also a ket-vector describing a possible state of the system, i.e. a ket-vector in the same Hilbert space as the initial vector $|\alpha\rangle$. An alternative formulation of the same rule is the following clarification of the notion of the Hilbert space: for the given set of linear operators of a system, its Hilbert state includes all vectors that may be obtained from each other using the operations of the type (18). In this context, let me note that the operator set, and hence the Hilbert space of a system, usually (if not always) implies its certain approximate model. For example, if the coupling of orbital degrees of freedom of a particle to its spin may be ignored (as it may be for a non-relativistic particle in the absence of an external magnetic field), we may describe the dynamics of the particle using spin operators only. In this case, the set of all possible spin vectors of the particle forms a Hilbert space separate from that of the orbital-state vectors of that particle.

As the adjective "linear" in the operator definition implies, the main rules governing the operators is their linearity with respect to both any superposition of vectors:

$$\hat{A}\left(\sum_j c_j \left|\alpha_j\right\rangle\right)=\sum_j c_j \hat{A}\left|\alpha_j\right\rangle, \tag{4.2.14}$$

and any superposition of operators:

$$\left(\sum_j c_j \hat{A}_j\right)|\alpha\rangle=\sum_j c_j \hat{A}_j|\alpha\rangle \tag{4.2.15}$$

These rules are evidently similar to Eqs. (1.53)-(1.54) of wave mechanics.

The above rules imply that an operator "acts" on the ket-vector on its right; however, a combination of the type $\langle\alpha|\hat{A}$ is also legitimate and represents a new bra-vector. It is important that, generally, this vector does not represent the same state as the ket-vector (18); instead, the bra-vector isomorphic to the ket-vector (18) is

$$\text{Conjugate operator} \qquad \langle\alpha|\hat{A}^{\dagger}. \tag{4.2.16}$$

This statement serves as the definition of the Hermitian conjugate (also called "Hermitian adjoint") $\hat{A}^{\dagger}$ of the initial operator $\hat{A}$. For an important class of operators, called the Hermitian operators, the conjugation is inconsequential, i.e. for them

$$\hat{A}^{\dagger}=\hat{A} \tag{4.2.17}$$

(This equality, as well as any other operator equation below, means that these operators act similarly on any bra- or ket-vector of the given Hilbert space.) [11]

To proceed further, we need one more additional postulate, sometimes called the associative axiom of multiplication: just as an ordinary product of scalars, any legitimate bra-ket expression, not including explicit summations, does not change from an insertion or removal of a pair of parentheses meaning as usual that the operation inside them has to be performed first. The first two examples of this postulate are given by Eqs. (19) and (20), but the associative axiom is more general and means, for example, that

$$\langle\beta|(\hat{A}|\alpha\rangle)=(\langle\beta|\hat{A})|\alpha\rangle \equiv\langle\beta|\hat{A}|\alpha\rangle, \tag{4.2.18}$$

This last equality serves as the definition of the last form, called the long bracket (evidently, also a scalar), with an operator sandwiched between a bra-vector and a ket-vector. This definition, when combined with the definition of the Hermitian conjugate and Eq. (14), yields an important corollary:

$$\langle\beta|\hat{A}|\alpha\rangle=\langle\beta|(\hat{A}|\alpha\rangle)=\left(\left(\langle\alpha|\hat{A}^{\dagger}\right)|\beta\rangle\right)^*=\left(\left\langle\alpha\left|\hat{A}^{\dagger}\right|\beta\right\rangle\right)^*, \tag{4.2.19}$$

which is most frequently rewritten as

$$\langle\alpha|\hat{A}|\beta\rangle^*=\left\langle\beta\left|\hat{A}^{\dagger}\right|\alpha\right\rangle. \tag{4.2.20}$$

The associative axiom also enables us to comprehend the following definition of one more, outer product of bra- and ket-vectors:

$$|\beta\rangle\langle\alpha|. \tag{4.2.21}$$

In contrast to the inner product (11), which is a scalar, this mathematical construct is an operator. Indeed, the associative axiom allows us to remove parentheses in the following expression:

$$(|\beta\rangle\langle\alpha|)|\gamma\rangle=|\beta\rangle\langle\alpha \mid \gamma\rangle. \tag{4.2.22}$$

But the last short bracket is just a scalar; hence the mathematical object (26), acting on a ket-vector (in this case, $|\gamma\rangle$), gives a new ket-vector, which is the essence of the operator's action. Very similarly,

$$\langle\delta|(|\beta\rangle\langle\alpha|)=\langle\delta \mid \beta\rangle\langle\alpha| \tag{4.2.23}$$

- again a typical operator's action on a bra-vector. So, Eq. (26) defines an operator.

Now let us perform the following calculation. We may use the parentheses' insertion into the bra-ket equality following from Eq. (14),

$$\langle\gamma \mid \alpha\rangle\langle\beta \mid \delta\rangle=(\langle\delta \mid \beta\rangle\langle\alpha \mid \gamma\rangle)^{*} \tag{4.2.24}$$

to transform it to the following form:

$$\langle\gamma|(|\alpha\rangle\langle\beta|)|\delta\rangle=(\langle\delta|(|\beta\rangle\langle\alpha|)|\gamma\rangle)^{*}. \tag{4.2.25}$$

Since this equality should be valid for any state vectors $\langle\gamma$ and $|\beta\rangle$, its comparison with Eq. (25) gives the following operator equality

$$(|\alpha\rangle\langle\beta|)^{\dagger}=|\beta\rangle\langle\alpha|. \tag{4.2.26}$$

This is the conjugate rule for outer products; it reminds the rule (14) for inner products but involves the Hermitian (rather than the usual complex) conjugation.

The associative axiom is also valid for the operator "multiplication":

$$(\hat{A}\hat{B})|\alpha\rangle=\hat{A}(\hat{B}|\alpha\rangle), \quad \langle\beta|(\hat{A}\hat{B})=(\langle\beta|\hat{A})\hat{B}, \tag{4.2.27}$$

showing that the action of an operator product on a state vector is nothing more than the sequential action of its operands. However, we have to be careful with the operator products; generally, they do not commute: $\hat{A}\hat{B}\neq\hat{B}\hat{A}$. This is why the commutator - the operator defined as

$$[\hat{A},\hat{B}]\equiv\hat{A}\hat{B}-\hat{B}\hat{A} \tag{4.2.28}$$

is a non-trivial and very useful notion. Another similar notion is the anticommutator: 12

$$\{\hat{A},\hat{B}\}\equiv\hat{A}\hat{B}+\hat{B}\hat{A} \tag{4.2.29}$$

Finally, the bra-ket formalism broadly uses two special operators. The null-operator $\hat{0}$ is defined by the following relations:

$$\hat{0}|\alpha\rangle\equiv 0|\alpha\rangle, \quad \langle\alpha|\hat{0}\equiv\langle\alpha|0, \tag{4.2.30}$$

where $\alpha$ is an arbitrary state; we may say that the null-operator "kills" any state, turning it into the nullstate. Another useful notion is the identity operator, which is defined by the following action (or rather "inaction" :-) on an arbitrary state vector:

$$\hat{I}|\alpha\rangle\equiv|\alpha\rangle, \quad \langle\alpha|\hat{I}\equiv\langle\alpha|. \tag{4.2.31}$$

These definitions show that the null-operator and the identity operator are Hermitian.

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[4] An attentive reader could notice my smuggling the term "system" instead of "particle", which was used in the previous chapters. Indeed, the bra-ket formalism allows the description of quantum systems much more complex than a single spinless particle that is a typical (though not the only possible) subject of wave mechanics.

[5] As was expressed nicely by Asher Peres, one of the pioneers of the quantum information theory, "quantum phenomena do not occur in the Hilbert space, they occur in a laboratory".

[6] The terms bra and ket were suggested to reflect the fact that the pair $\langle\beta|$ and $|\alpha\rangle$ may be considered as the parts of the combinations like $\langle\beta \mid \alpha\rangle$ (see below), which remind expressions in the usual angle brackets.

[7] I have to confess that this is a bit loose definition; it will be refined soon.

[8] One may express the same statement by saying that the vector $|\alpha\rangle$ belongs to the same Hilbert space as all $|\alpha_j\rangle$.

[9] Mathematicians like to say that the ket- and bra-vectors of the same quantum system are defined in two isomorphic Hilbert spaces.

[10] Here the term "legitimate" means "having a clear sense in the bra-ket formalism". Some examples of "illegitimate" expressions are: $|\alpha\rangle\hat{A}$, $\hat{A}\langle\alpha|$, $|\alpha\rangle|\beta rangle, and\langle\alpha|\langle\beta|$. Note, however, that the last two expressions may be legitimate if $\alpha$ and $\beta$ are states of

different systems, i.e. if their state vectors belong to different Hilbert spaces. We will run into such direct products of the bra- and ket-vectors (sometimes denoted, respectively, as $|\alpha\rangle \otimes |\beta\rangle$ and $\langle\alpha| \otimes \langle\beta|$) in Chapters 6-10.

[11] If we consider $c$-numbers as a particular type of operators (which is legitimate for any Hilbert space), then according to Eqs. (11) and (21), for them the Hermitian conjugation is equivalent to the simple complex conjugation, so that only real $c$-numbers may be considered as a particular type of the Hermitian operators (22).

[12] Another popular notation for the anticommutator (34) is $[\hat{A}, \hat{B}]_+$;it will not be used in these notes.