Lecture 6. Quantum operators and quantum states

Physical meaning of operators, states, uncertainty relations, mean values. States: Fock, coherent, mixed states. Examples of such states.

In quantum mechanics, physical observables (coordinate, momentum, angular momentum, energy,…) are described using operators, their eigenvalues and eigenstates. A physical system can be in one of possible quantum states. A state can be pure or mixed. We will start from the operators, but before we will introduce the so-called Dirac's notation.

1. Dirac's notation.

A pure state is described by a state vector: $|\Psi\rangle$. This is so-called Dirac's notation (a 'ket' vector; there is also a 'bra' vector, the Hermitian conjugated one, $\langle\Psi| \equiv (|\Psi\rangle)^+ \equiv (|\Psi^*\rangle)^T$.)

Originally, in quantum mechanics they spoke of wavefunctions, or probability amplitudes to have a certain observable x, $\Psi(x)$. But any function can be viewed as a vector (Fig.1):

$$\Psi(x) \equiv \{\Psi(x_1); \Psi(x_2); \ldots . \Psi(x_n)\} \rightarrow |\Psi\rangle$$

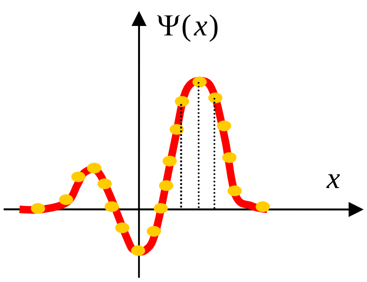

Fig.1

This was a very smart idea by Paul Dirac, to represent wavefunctions by vectors and to use operator algebra. Then, an operator acts on a state vector and a new vector emerges:

$$\hat{A}|\Psi\rangle = |\Phi\rangle.$$

An operator can be represented as a matrix if some basis of vectors is used.

Two vectors can be multiplied in two different ways; inner product (scalar product) gives a number,

$\langle\Phi\|\Psi\rangle \equiv K, \quad \langle\Psi\|\Psi\rangle = 1$ (state vectors are normalized),

but outer product gives a matrix, or an operator:

$|\Psi\rangle\langle\Phi| \equiv \hat{O}, \quad |\Psi\rangle\langle\Psi| \equiv \hat{\Pi}$ (a projector): $\hat{\Pi}|\Phi\rangle = |\Psi\rangle\langle\Psi\|\Phi\rangle \equiv K|\Psi\rangle$,

$\hat{\Pi}^2 = |\Psi\rangle\langle\Psi\|\Psi\rangle\langle\Psi| = |\Psi\rangle\langle\Psi| = \hat{\Pi}.$

The mean value of an operator is in quantum optics calculated by 'sandwiching' this operator between a state (ket) and its conjugate:

$$\langle A\rangle = \langle\Psi|\hat{A}|\Psi\rangle.$$

The same way one can find the second moment $\langle A^2\rangle = \langle\Psi|\hat{A}^2|\Psi\rangle$ and the variance

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

2. Operators and their eigenstates.

At the last lecture, we wrote the Hamiltonian of the field in the form

$$\hat{H} = \hbar\sum_k \omega_k (\hat{a}_k^+ \hat{a}_k + \frac{1}{2}) \equiv \hbar\sum_k \omega_k (\hat{N}_k + \frac{1}{2}).$$

Thus, we defined *the photon-number operator* $\hat{N} = \hat{a}^+\hat{a}$. (Further on, we address just one mode, unless it is explicitly mentioned.) Clearly, it is a Hermitian operator, i.e., it is invariant under Hermitian conjugation, $\hat{A}^+ = \hat{A}$.

Any Hermitian operator has real eigenvalues (real *spectrum of eigenvalues*), forming a complete orthonormal set, and it corresponds to a real (measurable) observable. Accordingly, $\hat{N}$ has real eigenvalues and eigenstates:

$$\hat{N}|N\rangle = N|N\rangle. \qquad (1)$$

Let us now find $\hat{N}a^+|N\rangle$. (Further on, we will omit hats of a, a^+.) Because

$$\hat{N}a^+ = a^+aa^+ = a^+(1+a^+a) = a^+(1+\hat{N}),$$
$$\hat{N}a^+|N\rangle = a^+(1+\hat{N})|N\rangle = (1+N)a^+|N\rangle.$$

This means that if $|N\rangle$ is an eigenstate of the photon-number operator, $a^+|N\rangle$ is also an eigenstate of the same operator, with the eigenvalue $N+1$. Then we can write, up to an unknown factor,

$$a^+|N\rangle \sim |N+1\rangle,$$
$$a^+|N\rangle = g|N+1\rangle.$$

This factor can be found from normalization: we take the square of the norm,

$$\langle N|aa^+|N\rangle = \langle N+1|g^*g|N+1\rangle = |g|^2,$$
$$N+1 = |g|^2.$$

So we obtain the equation

$$a^+|N\rangle = \sqrt{N+1}|N+1\rangle. \qquad (2)$$

(We omitted the phase of g here because the eigenvalues should be real.)
Similar consideration shows that

$$a|N\rangle = \sqrt{N}|N-1\rangle. \qquad (3)$$

Equations (2,3) are called *ladder equations*, and they show why a, a^+ are called photon annihilation and creation operators.
Hence, we introduced *number, or energy, or Fock states*. One of these states is the vacuum, $|0\rangle$, $\hat{N}|0\rangle = 0|0\rangle$. Clearly, the photon number (energy) does not fluctuate in Fock states.
A Fock state can then be written as

$$|N\rangle = \frac{(a^+)^N}{\sqrt{N!}}|0\rangle.$$

Note that photon-number states form a complete orthonormal set; accordingly, any other state can be written as an expansion over photon-number states.

Photon creation and annihilation operators are examples of non-Hermitian operators: $a^+ \neq a$ (for these operators usually the hats are omitted). Being non-Hermitian, they do not correspond to measurable observables.
Let us now consider their eigenstates, *the coherent states*. They will be defined as

$$a|\alpha\rangle = \alpha|\alpha\rangle,$$
$$\langle\alpha|a^+ = \alpha^*\langle\alpha|. \qquad (4)$$

The eigenvalues do not have to be real, as the operators are not Hermitian.
For the same reason, the states do not necessarily form an orthonormal set. In fact, they are normalized (we define them so) but not orthogonal, and their set is complete, in fact, over-complete.
It is useful to write the expansion of a coherent state over Fock states (the latter form a complete set):

$$|\alpha\rangle = \sum_{N=0} c_N|N\rangle,$$

Then act on it from the left by a; we obtain

$$\alpha|\alpha\rangle = \sum_{N=0} c_N a|N\rangle = \sum_{N=0} c_N \sqrt{N}|N-1\rangle = \sum_{N=1} c_N \sqrt{N}|N-1\rangle = \sum_{N'=0} c_{N'+1}\sqrt{N'+1}|N'\rangle,$$

so we obtain the recurrent relation

$$\alpha c_N = c_{N+1}\sqrt{N+1}, \quad c_{N+1} = \alpha \frac{c_N}{\sqrt{N+1}}.$$

From this, $c_N = \alpha^N \frac{c_0}{\sqrt{N!}}$, and c_0 will be obtained from normalization:

$$|\alpha\rangle = c_0 \sum_{N=0} \frac{\alpha^N}{\sqrt{N!}}|N\rangle,$$

$$|c_0|^{-2} = \sum_{N=0} \frac{|\alpha|^{2N}}{N!} = e^{|\alpha|^2}.$$

We finally obtain

$$|\alpha\rangle = e^{-|\alpha|^2/2} \sum_{N=0} \frac{\alpha^N}{\sqrt{N!}}|N\rangle. \quad (5)$$

The vacuum state is part of both coherent and Fock sets: $|0\rangle$.

In a coherent state, the number of photons can be found from (5), but also simply by using the properties (4), so that

$$\langle\alpha|\hat{N}|\alpha\rangle = \langle\alpha|a^+a|\alpha\rangle = |\alpha|^2.$$

Let us also find the variance of the photon number for the coherent state.

$$\Delta\hat{N}^2 = \langle\alpha|a^+aa^+a|\alpha\rangle - \langle\alpha|a^+a|\alpha\rangle^2 = |\alpha|^4 + |\alpha|^2 - |\alpha|^4 = |\alpha|^2 = \langle\hat{N}\rangle.$$

For a coherent state the photon-number variance is equal to the mean value: Poissonian statistics.

Position and momentum operators were introduced at the last lecture in connection with these operators. They are proportional to the Hermitian and anti-Hermitian parts, respectively:

$$\hat{q} \equiv \sqrt{\frac{\hbar}{2\omega}}(a + a^+), \quad \hat{p} \equiv \sqrt{\frac{\hbar\omega}{2}}\frac{a - a^+}{i}.$$

It is convenient to introduce dimensionless operators similar to position and momentum.

Quadratures (dimensionless), the Hermitian and anti-Hermitian parts of a^+, a:

$$\hat{x}_1 \equiv \frac{a + a^+}{2}, \quad \hat{x}_2 \equiv \frac{a - a^+}{2i}.$$

They will correspond to measurable quantities.

We also learned at the previous lecture that photon creation and annihilation operators, as well as the quadratures, *do not commute*:

$$[a, a^+] = 1, \ [\hat{q}, \hat{p}] = i\hbar, \ [\hat{x}_1, \hat{x}_2] = \frac{i}{2}.$$

Uncertainty relation. Whenever two operators do not commute, the product of their uncertainties (standard deviations) cannot be less than some value determined by the commutator:

$[\hat{A}, \hat{B}] \neq 0$,

$\Delta A \equiv \sqrt{Var(A)} \equiv \sqrt{\langle (\hat{A} - \langle \hat{A} \rangle)^2 \rangle}$, then

$$\Delta A \Delta B \geq \frac{1}{2} \left| \langle [\hat{A}, \hat{B}] \rangle \right|. \quad (6)$$

Physically, there are different interpretations:

(1) These values cannot be measured accurately at once.

(2) Measurement of one of them disturbs the other one (Heisenberg's microscope).

(3) One cannot even introduce a joint probability distribution $P(A, B)$. Any such attempts will be punished. (In the next lectures, we will see how it happens!)

3. Normally ordered correlation functions.

It is also important to consider the *normally ordered* combination, where all daggered operators stand first:

$$:\hat{N}^2 :\equiv (a^+)^2 a^2 \neq \hat{N}^2 \equiv aa^+aa^+.$$

In general,

$$:\hat{N}^m :\equiv (a^+)^m a^m.$$

And any functional depending on photon creation and annihilation operators can be written as a sum of normally ordered operators using commutation relations:

$$: f(a, a^+) :$$

For example, $: aa^+a^2 := a^+a^3$ (we applied the operation of normal ordering) but

$$aa^+a^2 = (a^+a + 1)a^2 = a^+a^3 + a^2$$

(we applied the commutation relations and wrote the function as a normally-ordered sum).

It is instructive to consider a factorial combination (recall the factorial moments!)

$$\hat{N}(\hat{N} - 1)...(\hat{N} - k + 1)$$

Because $[\hat{N}, (a^+)^k] = [a^+a, (a^+)^k] = a^+[a, (a^+)^k] = k(a^+)^k$ and $[a^k, \hat{N}] = ka^k$,

$$:\hat{N}^k := (a^+)^k a^k = (a^+)^{k-1} \hat{N} a^{k-1} = \hat{N}(a^+)^{k-1} a^{k-1} - (k-1)(a^+)^{k-1} a^{k-1} = (\hat{N} - k + 1)(a^+)^{k-1} a^{k-1} =$$

$$= (\hat{N} - k + 1)(\hat{N} - k + 2)(a^+)^{k-2} \hat{N} a^{k-2} = ... = (\hat{N} - k + 1)(\hat{N} - k + 2)...(\hat{N} - 1)\hat{N}.$$

We have shown that the factorial combination of operators is equal to the normally-ordered power:

$$\hat{N}(\hat{N} - 1)...(\hat{N} - k + 1) =: \hat{N}^k :.$$

Then the same equality will be valid for the mean values:

$$\langle \hat{N}(\hat{N} - 1)...(\hat{N} - k + 1) \rangle = \langle : \hat{N}^k : \rangle.$$

But the left-hand part is the Glauber's (intensity) kth-order CF, hence the quantum definition for this value is

$$G^{(k)} = \langle \hat{N}(\hat{N} - 1)...(\hat{N} - k + 1) \rangle = \langle : \hat{N}^k : \rangle.$$

The normalized kth-order CF is, accordingly,

$$g^{(k)} \equiv \frac{\langle : \hat{N}^k : \rangle}{\langle \hat{N} \rangle^k}. \quad (10)$$

This is how it should be calculated in quantum mechanics, and the difference between classical and quantum definitions is in normal ordering.

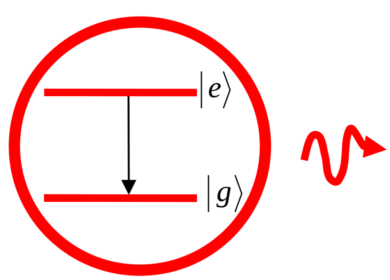

Fig.3

4. Mixed states.

It is not always that a state can be described by a wavefunction (state vector). Most often, we deal with mixed states, which are, in essence, classical mixtures of pure states. In other words, with a probability p_1 the system is in pure state $|\psi_1\rangle$, with a probability p_2 it is in pure state $|\psi_2\rangle$, etc. For a pure state, the density matrix is just a projector: $\hat{\rho}_i = |\psi_i\rangle\langle\psi_i|$. Then, the whole density matrix is

$$\hat{\rho} = \sum_i p_i \hat{\rho}_i = \sum_i p_i |\psi_i\rangle\langle\psi_i|, \sum_i p_i = 1.$$

An atom (described as a two-level system, quantum mechanically, as in Lecture 4) emits light into a single radiation mode. The situation is shown in Fig.3. This time we consider this radiation mode as a quantum system, a harmonic oscillator (Lecture 5). It can be populated with some number of photons. If initially the atom is in excited state $|e\rangle$ and there are no photons in the radiation mode, the state of the joint system is a superposition:

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\{|e\rangle|0\rangle + |g\rangle|1\rangle\}.$$

Here, $|N\rangle$ is the Fock state of the field mode.

The total state cannot be written as a product of the atom state and the field state, i.e., it is entangled – this is the definition of an entangled state. Then the state of the radiation mode alone will be given by the density matrix, obtained by taking partial trace over the atom variables:

itted by a single atom or

density matrix,

$$|\Psi\rangle\langle\Psi| = \frac{1}{2}\{|e\rangle|0\rangle + |g\rangle|1\rangle\}\{\langle e|\langle 0| + \langle g|\langle 1|\} = \frac{1}{2}\{|e\rangle|0\rangle\langle 0|\langle e| + |g\rangle|1\rangle\langle 0|\langle e| + |g\rangle|1\rangle\langle 1|\langle g| + |e\rangle|0\rangle\langle 1|\langle g|\}$$

And then we take the partial trace over the atom states, i.e., we ignore the atom states but leave the terms where they are the same:

$$\rho = \frac{1}{2}\{|e\rangle|0\rangle\langle 0|\langle e| + |g\rangle|1\rangle\langle 1|\langle g|\} = \frac{1}{2}\{|0\rangle\langle 0| + |1\rangle\langle 1|\}.$$

Hence the radiation mode will be in a mixture of Fock states $|0\rangle$ and $|1\rangle$ with ½ probabilities.

Another, very well known example of a mixed state is a thermal (chaotic, Gaussian) state, which we discussed classically in Lecture 3. Quantum mechanically, it is described by the density matrix, which is diagonal in the Fock-state representation. In other words, similar to the previous case, the density matrix is given by a sum of projectors:

$$\rho_{th} = p_0|0\rangle\langle 0| + p_1|1\rangle\langle 1| + p_2|2\rangle\langle 2| + ...,$$

$$p_n \equiv \rho_{thnn} = \frac{1}{1+\langle N\rangle}\left(\frac{\langle N\rangle}{\langle N\rangle+1}\right)^n \equiv \frac{\langle N\rangle^n}{(\langle N\rangle+1)^{n+1}}.$$

This probability distribution is just the discrete-valued analog of the one we obtained classically,

$$p_{th}(I) = \frac{1}{\langle I\rangle}\exp\{-\frac{I}{\langle I\rangle}\}.$$

5. Physical examples of all these states.

A coherent state is emitted by a laser. At the same time, a laser below the threshold emits *a thermal state*. But in reality, even a laser above threshold emits a coherent state up to a phase factor. In any laser, intensity (photon-number) fluctuations are suppressed, but the phase fluctuations are still there; in fact, if they were absent the laser would have an infinitely narrow spectrum. So what happens in reality is the drift of the phase, which can be described by a mixture of coherent states with different phases:

$$\rho_{laser} = p_0 |\alpha e^{i\varphi_0}\rangle\langle \alpha e^{-i\varphi_0}| + p_1 |\alpha e^{i\varphi_1}\rangle\langle \alpha e^{-i\varphi_1}| + p_2 |\alpha e^{i\varphi_2}\rangle\langle \alpha e^{-i\varphi_2}| + \ldots$$

Fock states are already much more 'exotic'; an example is a single-photon state, emitted by a single atom or molecule/ion/quantum dot etc., which will be considered in Lecture 12. Another example is a two-photon state emitted (in superposition with the vacuum) via, for instance, spontaneous parametric down-conversion. This will be also a subject of a whole Lecture 11.

Photon subtraction. It is interesting that the action of the photon annihilation operator can be observed in experiment (Fig.4). For this, a beamsplitter is placed into the beam, reflecting very little (say, 0.1% of intensity). Then if the single-photon detector 'clicks', it means that a photon was subtracted from the beam. This was, for instance, one can make an odd-photon-number state from an even-photon-number state. And how to obtain the latter, will be described in Lecture 11.

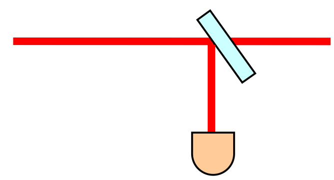

Fig.4

As we will see further, there are some states that can be described classically (thermal, for instance) but some (Fock) cannot. And the coherent state is at the boundary: it has some classical and some nonclassical features.

6. Pictorial description of the states.

It is possible to show different states on the phase plane (q, p or, better, quadratures, x_1, x_2). Fig.5 shows schematically the mean values of the quadratures and their uncertainties for thermal, Fock, and coherent states.

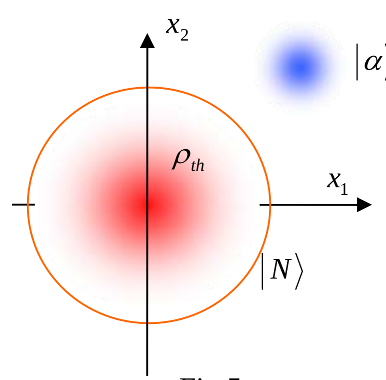

Fig.5

Here the Fock state is shown as a circle, because one can find that

$$\hat{x}_1^{\,2} + \hat{x}_2^{\,2} = \frac{1}{4}\left[a^2 + (a^+)^2 + a^+a + aa^+ - a^2 - (a^+)^2 + a^+a + aa^+\right] = 2\hat{N} + 1.$$

Accordingly, a thermal state is just a mixture of all Fock states.
But this is just an idea of hoe the states look. Of course it is, strictly speaking, impossible to show the joint probability distributions for the quadratures, or, in fact, any non-commuting variables. One can formally introduce such distributions – they are called quasi-probabilities (Glauber-Sudarshan function P, Wigner function W and Husimi function Q) and will be discussed in detail later. But the price for introducing them is that they turn out to be not quite 'proper' probabilities: they can take negative values or have singularities.

Home task:
Find the mean value and the variance of position and momentum in a coherent state.

Books:

1. Mandel & Wolf, Optical coherence and quantum optics, Sec. 10.4, 11.
2. Klyshko, Physical foundations of quantum electronics, Sec. 7.5