Chapter 5. Some Exactly Solvable Problems

This describes several simplest but important applications of the bra-ket formalism, notably including a few wave-mechanics problems we have already started to discuss in Chapters 2 and 3.

5.1. Two-level systems

In the course of discussion of the bra-ket formalism in the last chapter, we have already considered several examples of how it works for electron’s spin. We have seen, in particular, that in magnetic field the electron has eigenenergies (4.167), i.e. two energy levels. As will be shown later in the course, such two-energy-level picture is valid not only for electrons and other spin-$\frac{1}{2}$ elementary particles (such as muons and neutrinos), but also may give a good approximation for other important quantum systems. For example, as was already mentioned in Chapter 2, two energy levels are sufficient for an approximate description of dynamics of two weakly coupled quantum wells (Sec. 2.6), and of level anticrossing in the weak-potential approximation of the band theory (Sec. 2.7). Such two-level systems (alternatively called “spin-$\frac{1}{2}$-like” systems) are nowadays the focus of additional attention in the view of prospects of their possible use for information processing and encryption. (In the last context, to be discussed in Sec. 8.5, a two-level system is usually called a qubit.)

This is why before proceeding to other problems, let us summarize in brief what we have already learned about properties and dynamics of two-level systems, in a more convenient language. According to the general Eq. (4.6), a ket-(or bra-) vector of an arbitrary pure (coherent) state $\alpha$ of such a system may be presented, at any instant, as a linear combination of two basis vectors, for example

$$|\alpha\rangle = \alpha_\uparrow |\uparrow\rangle + \alpha_\downarrow |\downarrow\rangle,$$

and hence is completely described by two complex coefficients ($c$-numbers) – say, $\alpha_\uparrow$ and $\alpha_\downarrow$. These two numbers are not completely arbitrary; they are restricted by the normalization condition. If the basis vectors are normalized, then to have the system in some basis state with a 100% probability, we need

$$W_\Sigma = \langle \alpha | \alpha \rangle = \left( \langle \uparrow | \alpha^*_\uparrow \langle \uparrow | + \langle \downarrow | \alpha^*_\downarrow \langle \downarrow | \right) = \alpha^*_\uparrow \alpha_\uparrow + \alpha^*_\downarrow \alpha_\downarrow = |\alpha_\uparrow|^2 + |\alpha_\downarrow|^2 = 1.$$

This requirement is automatically satisfied if we take the moduli of $\alpha_\uparrow$ and $\alpha_\downarrow$ equal to the sine and cosine of the same (real) angle. Thus we can write, for example,

$$\alpha_\uparrow = \cos \frac{\theta}{2} e^{i\gamma}, \quad \alpha_\downarrow = \sin \frac{\theta}{2} e^{i(\gamma+\varphi)}.$$

Moreover, according to the general Eq. (4.125), if we deal with just one system,$^1$ the common phase factor $\exp\{i\gamma\}$ is unimportant for calculation of any expectation values, and we can take $\gamma = 0$, so that Eq. (3) is reduced to

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$^1$ To recall why this condition is crucial, please revisit the beginning of Sec. 2.3. Note also that, in particular, the mutual phase shifts between different qubits are very important for quantum information processing (see Chapter 7 below), so that most discussions of these applications have to start from Eq. (3) rather than Eq. (4).
\[
\alpha_\uparrow = \cos \frac{\theta}{2}, \quad \alpha_\downarrow = \sin \frac{\theta}{2} e^{i\phi}.
\]  

(5.4)

The reason why the argument of sine and cosine functions is usually taken in the form \(\theta/2\), becomes clear from Fig. 1a: Eq. (4) conveniently maps each state \(\alpha\) on a certain representation point of a unit-radius Bloch sphere,\(^2\) with polar angle \(\theta\) and azimuthal angle \(\phi\). In particular, state \(\uparrow\) (with \(\alpha_\uparrow = 1\) and \(\alpha_\downarrow = 0\)) corresponds to the North Pole of the sphere (\(\theta = 0\)), while state \(\downarrow\) (with \(\alpha_\uparrow = 0\) and \(\alpha_\downarrow = 1\)), to its South pole (\(\theta = \pi\)).\(^3\) Similarly, states \(\rightarrow\) and \(\leftarrow\), described by Eqs. (4.122), i.e. having \(\alpha_\uparrow = 1/\sqrt{2}\) and \(\alpha_\downarrow = \pm 1/\sqrt{2}\), correspond to points with \(\theta = \pi/2\) and to, respectively, \(\phi = 0\) and \(\phi = \pi\). Two more special points (denoted in Fig. 1a as \(\otimes\) and \(\otimes\)) are also located on sphere’s equator (at \(\theta = \pi/2\) and \(\phi = \pm \pi/2\)); it is easy to check that they correspond to the eigenstates of matrix \(\sigma_y\) (in the same \(z\)-basis).

In order to understand why such mutually perpendicular location of these three special point pairs on the Bloch sphere is not occasional, let us plug Eqs. (4) into Eqs. (4.131)-(4.133) for the expectation values of spin components. The result is

\[
\langle S_x \rangle = \frac{\hbar}{2} \sin \theta \cos \phi, \quad \langle S_y \rangle = \frac{\hbar}{2} \sin \theta \sin \phi, \quad \langle S_z \rangle = \frac{\hbar}{2} \cos \theta,
\]

(5.5)

showing that the radius-vector of the representation point on the sphere is (after multiplication by \(\hbar/2\)) just the expectation value of the spin vector \(S\).

Fig. 5.1. Bloch sphere: (a) notation, and presentation of spin precession in magnetic fields directed along: (b) axis \(z\), and (c) axis \(x\).

Now let us see how does the representation point moves in various cases. First of all, according to Eqs. (4.157)-(4.158), in the absence of an external field (when the Hamiltonian operator is equal to zero and hence the time-evolution operator is constant) the point does not move at all. Now, if we apply to an electron a magnetic field directed along axis \(z\), then, according to Eqs. (4.202), the Heisenberg operator of \(S_z\) (and hence the expectation value \(\langle S_z \rangle\)) remains constant, while angle \(\phi\) in Eq. (5) evolves

\(^2\) Named after the same F. Bloch who has pioneered the energy band theory that was discussed in Chapters 2-3.

\(^3\) In the quantum information literature, ket-vectors \(\ket{\uparrow}\) and \(\ket{\downarrow}\) of these two states of a qubit are usually denoted as \(\ket{1}\) (“quantum one”) and \(\ket{0}\) (“quantum zero”).
in time as $\Omega t + \text{const}$. This means that the torque-induced precession of the spin in a constant field $\mathbf{B} = n_z \mathbf{B}$ is described by a circular rotation of the representation point about axis $z$ (in Fig. 1b, in the horizontal plane) with the classical precession frequency $\Omega$. This is essentially the classical picture of rotation of the angular momentum vector about the precession axis $z$, with both its length and the $z$-component conserved.\(^4\)

It is straightforward to repeat all calculations of Sec. 4.6 for a field of a different orientation and prove the (virtually evident) result that the representation point performs a similar rotation about the field direction. (Fig. 1c shows such rotation for an $x$-directed field.) Finally, note that it is sufficient to turn off the field to stop the precession instantly. (Since Eq. (4.158) is the first-order differential equation, the representation point has no effective inertia.\(^5\)) Hence changing the direction and magnitude of the external field, it is possible to move spin’s representation point to any position on the Bloch sphere. (In Chapter 6 we will examine another method of manipulating the point position, that is based on external rf field and is more convenient for some two-level systems.)

In the context of quantum information, this means that in the absence of uncontrollable interaction with environment, it is possible to prepare a qubit in any pure quantum state, and then keep it unchanged. From here it is clear that a qubit is very much different from and a classical bistable system used to store single bits of information – such as the voltage state of a usual SRAM cell (a positive-feedback loop of two transistor-based inverters). As Eq. (4) shows, qubit’s state is determined by two independent, continuous parameters $\theta$ and $\phi$, so it may store much more information than one bit. (The difference is even more spectacular in qubit systems, to be discussed in Sec. 8.5.) However, classical bistable systems, due to their nonlinearity, are stable with respect to small perturbations, so that their operation is rather robust with respect to unintentional interaction with their environment. In contrast, qubit’s state may be readily disturbed (i.e. its representation point on the Bloch sphere shifted) by even minor perturbations, and does not have an internal state stabilization mechanism.\(^6\) Due to this reason, qubit-based systems are rather vulnerable to environment-induced drifts, including dephasing and relaxation effects, which will be discussed in Chapter 7.

5.2. Revisiting wave mechanics

In order to use the bra-ket formalism for the description of the “orbital” motion of a particle as a whole, we have to either rewrite or even modify some of its formulas for the case of observables with continuous spectrum of eigenvalues. (One example we already know well are the momentum and kinetic energy of a free particle.) In that case, all the above expressions for states, their bra- and ket-vectors, and eigenvalues, should be stripped of discrete indices, like the index $j$ in the key equation (4.68), which determines eigenstates and eigenvalues of observable $A$. For that, Eq. (4.68) may be rewritten in the form

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\(^4\) Still, it is crucial to appreciate the difference between the expectation values (5), i.e. $c$-numbers, and the actual observables $S_x$, $S_y$, and $S_z$ which are described in quantum mechanics by operators. For example, according to Eq. (4.156), for any position on the Bloch sphere, it is impossible to have exact values of Cartesian components, as it is in the classical picture.

\(^5\) The same is true for the angular momentum $\mathbf{L}$ at the classical torque-induced precession – see, e.g., CM Sec.6.5 and in particular Eq. (6.71).

\(^6\) In this aspect as well, the information processing systems based on qubits are closer to classical analog computers rather than classical digital ones.
\[ \hat{A} |a_\alpha\rangle = A |a_\alpha\rangle. \]  

(5.6)

More essentially, all sums over such continuous eigenstate sets should be replaced by integrals. For example, for a full and orthonormal set of eigenstates (6), the closure relation (4.44) should be replaced with

\[
\int dA |a_\alpha\rangle \langle a_\alpha| = \hat{1},
\]

(5.7)

where the integral should be taken over the whole interval of possible values of observable \( \hat{A} \). Applying this relation to the ket-vector of an arbitrary state \( |\alpha\rangle \) (generally, not an eigenstate of operator \( \hat{A} \)), we get

\[
|\alpha\rangle = \hat{1} |\alpha\rangle = \int dA |a_\alpha\rangle \langle a_\alpha| |\alpha\rangle = \int dA \langle a_\alpha| |\alpha\rangle |a_\alpha\rangle.
\]

(5.8)

This integral replaces sum (4.37) for the representation of an arbitrary ket-vector as an expansion over eigenstates of an operator. For the particular case when \( |\alpha\rangle = |a_\alpha\rangle \), this relation requires

\[
\langle a_\alpha| |a_\alpha\rangle = \delta(A - A');
\]

(5.9)

this formula replaces the orthonormality condition (4.38).

According to Eq. (8), in the continuous case the bra-ket \( \langle a_\alpha| |\alpha\rangle \) still plays the role of the coefficient whose modulus squared determines state \( a_\alpha \)'s probability – see the last form of Eq. (4.120). However, in the continuous spectrum case the probability to find the system exactly in a particular state is infinitesimal. Instead we should speak about the probability density \( w(A) \propto |\langle a_\alpha| |\alpha\rangle|^2 \) to find the observable within a small interval \( dA \) about a certain value \( A \). The coefficient in that relation may be found by making the similar change from summation to integration (without any additional coefficients) in the normalization condition (4.121):

\[
\int dA \langle a_\alpha| |a_\alpha\rangle \langle a_\alpha| |\alpha\rangle = 1.
\]

(5.10)

Since the total probability of the system to be in some state should also equal \( \int w(A) dA \), this means that

\[
w(A) = \langle a_\alpha| |a_\alpha\rangle \langle a_\alpha| |\alpha\rangle = |\langle a_\alpha| |\alpha\rangle|^2.
\]

(5.11)

Now let us see how we can calculate expectation values of continuous observables, i.e. their ensemble averages. If we speak about the same observable \( A \) whose eigenstates are used as the basis (or any compatible observable), everything is simple. Inserting Eq. (11) into the general statistical relation

\[
\langle A \rangle = \int w(A) AdA,
\]

(5.12)

which is just the evident continuous version of Eq. (1.37), we get

\[
\langle A \rangle = \int \langle a_\alpha| A |a_\alpha\rangle \langle a_\alpha| |\alpha\rangle dA.
\]

(5.13)

Presenting this expression as a double integral,

\[
\langle A \rangle = \int dA \int dA' \langle a_\alpha| A |a_\alpha'\rangle \delta(A - A') \langle a_\alpha'| |\alpha\rangle,
\]

(5.14)

\footnote{Notice that in the contrast to the discrete spectrum case, the dimensionality of the bra- and ket-vectors so normalized is different from 1.}
and using the continuous-spectrum version of Eq. (4.98),
\[ \langle a_A | \hat{A} | a_{A'} \rangle = A \delta(A - A'), \] (5.15)
we may write
\[ \langle \hat{A} \rangle = \int dA \int dA' \langle \alpha | a_A \rangle \langle a_A | \hat{A} | a_{A'} \rangle \langle a_{A'} | \alpha \rangle = \langle \alpha | \hat{A} | \alpha \rangle, \] (5.16)
so that Eq. (4.125) remains valid in the continuous-spectrum case without any changes.

The situation is a bit more complicated for the expectation values of operators that do not commute with the base-creating operator, because the matrix of such an operator in that may not be diagonal. We will consider (and overcome :-) this technical difficulty very soon, but otherwise we are ready for the discussion of wave mechanics. (For the notation simplicity I will discuss its 1D version; the generalization to the 2D and 3D cases is straightforward.)

Let us consider what is called the coordinate representation, postulating the (intuitively almost evident) existence of a quantum state basis, whose with ket-vectors will be called \(|x\rangle\), corresponding to a certain, exactly defined value \(x\) of particle’s coordinate. Writing the following evident identity:
\[ x | x \rangle = x | x \rangle, \] (5.17)
and comparing this relation with Eq. (6), we see that they do not contradict each other if we assume that \(x\) in the left-hand part of this equation is considered as the coordinate operator \(\hat{x}\) whose action on a ket-(or bra-) vector is just its multiplication by c-number \(x\). (This looks like a proof, but is actually a separate, independent postulate, no matter how plausible.)

In this coordinate representation, the inner product \(\langle a_A | \alpha(t) \rangle\) becomes \(|x| \alpha(t)\rangle\), and Eq. (11) takes the form
\[ w(x, t) = \langle \alpha(t) | x \rangle \langle x | \alpha(t) \rangle = \langle x | \alpha(t) \rangle^* \langle x | \alpha(t) \rangle. \] (5.18)
Comparing this formula with the basic postulate (1.22) of wave mechanics, we see that they coincide if the Schrödinger’s wavefunction of time-evolving state \(\alpha(t)\) is identified with that bra-ket:\(^8\)
\[ \Psi_\alpha(x, t) = \langle x | \alpha(t) \rangle. \] (5.19)

This key formula provides the connection between the bra-ket formalism and wave mechanics, and should not be too surprising for the (thoughtful :-) reader. Indeed, Eqs. (4.45) shows that any inner product of vectors describing two states is a measure of their coincidence - just as the scalar product of two geometric vectors. (The orthonormality condition (4.38) is a particular manifestation of this fact.) In this language, value (19) of wavefunction \(\Psi_\alpha\) at point \(x\) and moment \(t\) characterizes “how much of a particular coordinate \(x\)” does the state \(\alpha\) contain at that particular instance. (Of course this informal language is too crude to describe the fact that \(\Psi_\alpha(x, t)\) is a complex function, which has not only a modulus, but also a phase.)

\(^8\) I do not quite like expressions like \(\langle x | \Psi \rangle\) used in some papers and even textbooks. Of course, one is free to replace \(\alpha\) with any other letter (\(\Psi\) including) to denote a quantum state, but then it is better not to use the same letter to denote the wavefunction, i.e. an inner product of two state vectors, to avoid confusion.
Let us rewrite the most important formulas of the bra-ket formalism (so far, in the Schrödinger picture) in the wave mechanics notation. In particular, let us use Eq. (19) to calculate the (partial) time derivative of the wavefunction, multiplied by the usual coefficient $i\hbar$:

$$i\hbar \frac{\partial \Psi}{\partial t} = i\hbar \frac{\partial}{\partial t} \langle \alpha(t) \rangle.$$  \hspace{1cm} (5.20)

Since the coordinate operator $\hat{x}$ does not depend on time explicitly, its eigenstates $x$ are stationary, and we can swap the time derivative and the time-independent ket-vector and hence $\langle x \rangle$. Making use of the Schrödinger-picture equations (4.157) and (4.158), and then inserting the identity operator in the continuous form (7) of the closure relation, written for the coordinate eigenstates,

$$\int dx' |x'\rangle \langle x'| = \hat{1},$$  \hspace{1cm} (5.21)

we may continue to develop the right-hand part of Eq. (20) as

$$\langle x | i\hbar \frac{\partial}{\partial t} | \alpha(t) \rangle = \langle x | i\hbar \frac{\partial}{\partial t} \hat{u}(t, t_0) | \alpha(t_0) \rangle = \langle x | \hat{H} \hat{u}(t, t_0) | \alpha(t_0) \rangle = \langle x | \hat{H} | \alpha(t) \rangle = \int dx' \langle x | \hat{H} | x' \rangle \langle x' | \alpha(t) \rangle = \int dx' \langle x | \hat{H} | x' \rangle \Psi_\alpha(x', t).$$ \hspace{1cm} (5.22)

For a general Hamiltonian operator, we have to stop here, because if it does not commute with the coordinate operator, its matrix in the $x$-basis is not diagonal, and integral (22) cannot be worked out explicitly. However, there exists a broad set of space-local operators\(^9\) whose arguments include just one value of the spatial coordinate, for which we can move ket-vector $\langle x \rangle$ to the right\(^10\)

$$\langle x | \hat{A} | x' \rangle \Psi(x', t) = \hat{A} \Psi(x', t) \langle x | x' \rangle = \hat{A} \Psi(x, t) \delta(x-x').$$ \hspace{1cm} (5.23)

where operator $\hat{A}$ in the last two forms should be understood as its coordinate representation that is defined by Eq. (23) - if it is valid for a particular operator. For example, consider the 1D version of operator (1.40),

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + U(\hat{x}, t),$$  \hspace{1cm} (5.24)

which was the basis of all our discussions in Chapter 2. Its potential-energy part commutes with operator $\hat{x}$, so its matrix in the $x$-basis is diagonal, meaning that this part of Hamiltonian (24) is clearly local, with its coordinate representation given merely by the $c$-number function $U(x, t)$. The situation with the kinetic energy, which is a function of momentum operator $\hat{p}_x$, not commuting with $\hat{x}$, is less evident. Let me show that this operator is also local, and in the same shot derive (the 1D version of) Eq. (1.26), if we postulate the commutation relation (2.14):

$$\hat{x} \hat{p}_x - \hat{p}_x \hat{x} = i\hbar \hat{1}.$$ \hspace{1cm} (5.25)

\(^9\) Of all the operators we will encounter in this course, only the statistical operator $\hat{w}$ is substantially non-local – see Sec. 7.2.

\(^10\) In the second equality, I have use Eq. (9) for variable $x$. 

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\(\int dx' \langle x | \hat{H} | x' \rangle \Psi_\alpha(x', t)\)
For that, let us consider the following matrix element, \( \langle x | \hat{\mathbf{x}} \hat{\mathbf{p}}_x - \hat{\mathbf{p}}_x \hat{\mathbf{x}} | x' \rangle \). On one hand, we may use Eq. (25) to write
\[
\langle x | \hat{\mathbf{x}} \hat{\mathbf{p}}_x - \hat{\mathbf{p}}_x \hat{\mathbf{x}} | x' \rangle = \langle x | \hat{\mathbf{p}} | x' \rangle = i\hbar \langle x | x' \rangle = i\hbar \delta(x - x').
\] (5.26)

On the other hand, since \( \hat{\mathbf{x}} | x' \rangle = x' | x' \rangle \) and \( \langle x | \hat{\mathbf{x}} = \langle x | x \rangle \), we can write
\[
\langle x | \hat{\mathbf{x}} \hat{\mathbf{p}}_x - \hat{\mathbf{p}}_x \hat{\mathbf{x}} | x' \rangle = \langle x | x \hat{\mathbf{p}}_x - \hat{\mathbf{p}}_x x | x' \rangle = (x - x')(x | \hat{\mathbf{p}}_x | x').
\] (5.27)

Comparing Eqs. (26) and (27), we may write
\[
\langle x | \hat{\mathbf{p}}_x | x' \rangle = i\hbar \frac{\delta(x - x')}{(x - x')}.
\] (5.28a)

Thus \( \hat{\mathbf{p}}_x \) is a local operator. Since Eq. (28a) may be rewritten as
\[
\langle x | \hat{\mathbf{p}}_x | x' \rangle = -i\hbar \frac{\partial}{\partial x} \delta(x - x'),
\] (5.28b)

its comparison with Eq. (23) shows that the formula used so much in Chapter 2,
\[
\hat{\mathbf{p}}_x = -i\hbar \frac{\partial}{\partial x},
\] (5.29)
is indeed valid, but only for the coordinate representation of the momentum operator. (Later in this section we will see that in an alternative, momentum representation, this operator looks completely differently.)

It is straightforward to show (and virtually evident) that any operator \( f(\hat{\mathbf{p}}) \) is local as well, with its coordinate representation being
\[
f\left( -i\hbar \frac{\partial}{\partial x} \right).
\] (5.30)

In particular, this pertains to the kinetic energy operator in Eq. (24), so that Eq. (20) is reduced to the Schrödinger equation in its familiar wave-mechanics form (1.28), if by \( \hat{H} \) we mean its coordinate representation:
\[
\hat{H} = \frac{1}{2m} \left( -i\hbar \frac{\partial}{\partial x} \right)^2 + U(x,t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U(x,t).
\] (5.31)

Now let us return, as was promised, to operators that do not commute with operator \( \hat{\mathbf{x}} \), and hence do not have to share its continuous spectrum. Inner-multiplying both parts of the general Eq. (4.68) by ket-vector \( \langle x \rangle \), and inserting into the left-hand part the identity operator in form (21), we get
\[
\int dx' \langle x | \hat{\mathbf{A}} | x' \rangle \langle x' | a_j \rangle = A_j \langle x | a_j \rangle,
\] (5.32)

11 The equivalence of the two forms of Eq. (28) may be readily proven, for example, by comparison of their effect on any differentiable function \( f(x, x') \), using its Taylor expansion over argument \( x \) at point \( x' = x \) – a simple but good exercise for the reader.
i.e., using the wavefunction definition (19),
\[ \int dx' \langle x' | \hat{A}(x', t) | x \rangle \Psi_j(x', t) = A_j \Psi_j(x, t). \tag{5.33} \]

If the operator \( \hat{A} \) is space-local, i.e. satisfies Eq. (23), then this result is immediately reduced to
\[ \hat{A}\Psi_j(x, t) = A_j \Psi_j(x, t), \tag{5.34} \]
(where the left-hand part implies the coordinate representation of the operator), even if the operator does not commute with operator \( \hat{x} \).\(^{12}\) The most important case of this coordinate-representation form of the eigenproblem (4.68) is the familiar Eq. (1.60) for eigenvalues \( E_n \) of energy. Hence, the energy spectrum of a system (that, as we know very well from the first chapters of the course, may be discrete) is nothing more than the set of eigenvalues of its Hamiltonian operator – a very important conclusion indeed.

The operator locality also simplifies the expression for its expectation value. Indeed, plugging the completeness relation in the form (21) into the general Eq. (4.125) twice (written in the first case for \( x \) and in the second case for \( x' \)), we get
\[ \langle \hat{A} \rangle = \int dx \int dx' \langle x(t) | \hat{A} | x' \rangle \langle x' | \alpha(t) \rangle = \int dx \int dx' \Psi_a^*(x, t) \hat{A} \Psi_a(x, t) \delta(x - x') = \int \Psi_a^*(x, t) \hat{A} \Psi_a(x, t) dx . \tag{5.35} \]

Now, Eq. (23) reduces this result to just
\[ \langle \hat{A} \rangle = \int dx \int dx' \Psi_a^*(x, t) \hat{A} \Psi_a(x, t) \delta(x - x') = \int \Psi_a^*(x, t) \hat{A} \Psi_a(x, t) dx . \tag{5.36} \]
i.e. to Eq. (1.23), which we had to postulate in Chapter 1.

So, we have essentially derived all basic relations of wave mechanics from the bra-ket formalism, which will also allow us to get some important new results in that area. Before doing that, let us have a look at a pair of very interesting relations, together called the \textit{Ehrenfest theorem}. In order to derive them, let us calculate the following commutator:\(^{13}\)
\[ [\hat{x}, \hat{p}_x^2] = \hat{x} \hat{p}_x \hat{p}_x - \hat{p}_x \hat{x} \hat{p}_x . \tag{5.37} \]

Rewriting Heisenberg’s commutation relation (25) as
\[ \hat{x} \hat{p}_x = \hat{p}_x \hat{x} + i\hbar, \tag{5.38} \]
we can use it twice in the first term of the right-hand part of Eq. (37) to sequentially move the momentum operators to the left:
\[ \hat{x} \hat{p}_x \hat{p}_x = (\hat{p}_x \hat{x} + i\hbar) \hat{p}_x = \hat{p}_x \hat{x} \hat{p}_x + i\hbar \hat{p}_x = \hat{p}_x (\hat{p}_x \hat{x} + i\hbar) + i\hbar \hat{p}_x = \hat{p}_x \hat{p}_x \hat{x} + 2i\hbar \hat{p}_x . \tag{5.39} \]

\(^{12}\) In some systems of quantum mechanics postulates, the Schrödinger equation (1.28) itself is considered as a sort of eigenstate/eigenvalue problem (34) for operator \( i\hbar \partial / \partial t \). Notice that such construct is very close to that of the momentum operator \(-i\hbar \partial / \partial x\), and similar arguments may be given for both expressions, starting from the invariance of the quantum state of a free particle with respect to translations in time and space, respectively.

\(^{13}\) It is not important whether we speak about the Schrödinger or Heisenberg picture here. Indeed, if three operators in the former picture are related as \([ \hat{A}_s, \hat{B}_s \] = \( \hat{C}_s \), then according to Eq. (4.190), in the latter picture
\[ [\hat{A}_n, \hat{B}_n] = [\hat{U} \hat{A}_n \hat{U}^\dagger, \hat{U} \hat{B}_n \hat{U}^\dagger] = \hat{U} \hat{A}_n \hat{U} \hat{U}^\dagger \hat{B}_n \hat{U} - \hat{U} \hat{B}_n \hat{U} \hat{U}^\dagger \hat{A}_n \hat{U} = \hat{U} \hat{A}_n \hat{B}_n \hat{U} = \hat{U} \hat{C}_s \hat{U} = \hat{C}_n . \]
The first term of the result cancels with the second term of Eq. (37), so that the commutator is rather simple:

$$[\hat{x}, \hat{p}_x^2] = 2i\hbar \hat{p}_x.$$  \hspace{1cm} (5.40)

Let us use this equality to calculate the Heisenberg-picture equation of motion for operator $\hat{x}$, applying the general Heisenberg equation (4.199) to the orbital motion, when the Hamiltonian has the form (31), with time-independent potential $U(x)$:\footnote{Since this Hamiltonian is time-independent, we may replace the partial derivative over time $t$ with the full one.}

$$\frac{d\hat{x}}{dt} = \frac{1}{i\hbar} [\hat{x}, \hat{H}] = \frac{1}{i\hbar} \left[ \hat{x}, \frac{\hat{p}_x^2}{2m} + U(\hat{x}) \right].$$  \hspace{1cm} (5.41)

The potential energy operator commutes with the coordinate operator. Thus, the right-hand part of Eq. (41) is proportional to commutator (40):

$$\frac{d\hat{x}}{dt} = \hat{p}_x$$  \hspace{1cm} (5.42)

In that operator equality, we readily recognize the classical relation between particle’s momentum and velocity.

Now let us see what does a similar procedure give for the momentum’s derivative:

$$\frac{d\hat{p}_x}{dt} = \frac{1}{i\hbar} [\hat{p}_x, \hat{H}] = \frac{1}{i\hbar} \left[ \hat{p}_x, \frac{\hat{p}_x^2}{2m} + U(\hat{x}) \right].$$  \hspace{1cm} (5.43)

The kinetic energy operator commutes with the momentum operator, and hence may be dropped from the right-hand part of this equation. In order to calculate the remaining commutator of the momentum and potential energy, let us use the fact that any smooth potential profile may be represented by its Taylor expansion:

$$U(\hat{x}) = \sum_{k=0}^{\infty} \frac{1}{k!} \frac{\partial^k U}{\partial x^k} \hat{x}^k,$$  \hspace{1cm} (5.44)

where the derivatives of $U$ should be understood as $c$-numbers (evaluated at $x = 0$), so that we may write

$$[\hat{p}_x, U(\hat{x})] = \sum_{k=0}^{\infty} \frac{1}{k!} \frac{\partial^k U}{\partial x^k} \left[ \hat{p}_x, \hat{x}^k \right] = \sum_{k=0}^{\infty} \frac{1}{k!} \frac{\partial^k U}{\partial x^k} \left( \hat{p}_x \hat{x}^k - \hat{x}^k \hat{p}_x \right).$$  \hspace{1cm} (5.45)

Applying Eq. (38) $k$ times to the last term in the parentheses, exactly as we did it in Eq. (39), we get

$$[\hat{p}_x, U(\hat{x})] = -\sum_{k=0}^{\infty} \frac{1}{k!} \frac{\partial^k U}{\partial x^k} i\hbar \hat{x}^{k-1} = -i\hbar \sum_{k=1}^{\infty} \frac{1}{(k-1)!} \frac{\partial^k U}{\partial x^k} \hat{x}^{k-1}.$$  \hspace{1cm} (5.46)

But the last sum is just the Taylor expansion of the derivative $\partial U/\partial x$. Indeed,

$$\frac{\partial U}{\partial x} = \sum_{k=1}^{\infty} \frac{1}{k!} \frac{\partial^k U}{\partial x^k} \hat{x}^{k-1} = \sum_{k=0}^{\infty} \frac{1}{k!} \frac{\partial^{k+1} U}{\partial x^{k+1}} \hat{x}^k = \sum_{k=1}^{\infty} \frac{1}{(k-1)!} \frac{\partial^k U}{\partial x^k} \hat{x}^{k-1},$$  \hspace{1cm} (5.47)
where at the last step I have replaced the notation of the summation index from \( k' \) to \( k - 1 \). As a result, Eq. (43) yields:

\[
\frac{d\hat{p}_x}{dt} = -\frac{\partial}{\partial \hat{x}} U(\hat{x}).
\]  

(5.48)

This equation again coincides with the classical equation of motion! Discussing spin dynamics in Sec. 4.6 and 5.1, we have already seen that this is very typical of the Heisenberg picture. Moreover, averaging Eqs. (42) and (48) over the initial state (as Eq. (4.191) prescribes\(^\text{15}\)), we get similar results for the expectation values:\(^\text{16}\)

\[
\frac{d\langle x \rangle}{dt} = \frac{\langle p_x \rangle}{m}, \quad \frac{d\langle p_x \rangle}{dt} = -\langle \frac{\partial U}{\partial \hat{x}} \rangle.
\]  

(5.49)

However, it is important to remember that the equivalence between these quantum-mechanical equations and similar equations of classical mechanics is superficial, and the degree of the similarity between the two mechanics very much depends on the problem. As one extreme, let us consider the case when a particle’s state, at any moment between \( t_0 \) and \( t \), may be accurately represented by one, relatively narrow wave packet. Then we may interpret Eqs. (49) as equations of essentially classical motion for the wave packet’s center, in accordance with the correspondence principle. However, even in this case it is important to remember about the purely quantum mechanical effects of nonvanishing wave packet width and its spreading in time, which were discussed in Sec. 2.2.

In the opposite extreme, Eqs. (49), though valid, may tell almost nothing about system’s dynamics. Maybe the most apparent example is the “leaky” quantum well that was discussed in Sec. 2.5 - see Fig. 2.18 and its discussion. Since both the potential \( U(x) \) and the initial state are symmetric relative to point \( x = 0 \), the right-hand parts of both Eqs. (49) identically equal zero. Of course, the result (that average values of both momentum and coordinate stay equal zero at all times) is correct, but it does not tell us too much about the rich dynamics of the system (the finite lifetime of the metastable state, the formation of two wave packets, their waveform and propagation speed), and about the important insight the solution gives for the quantum measurement theory. Another similar example is the band theory (Sec. 2.7), with its purely quantum effect of the allowed energy bands and forbidden gaps, of which Eq. (49) gives no clue.

To summarize, the Ehrenfest theorem is important as an illustration of the correspondence principle, but its predictive power should not be exaggerated.

Now we are ready to patch some holes left during our studies of wave mechanics in Chapters 1-3. First of all, I have promised you to develop a more balanced view at the monochromatic de Broglie waves (4.1), which would be more respectful to the evident \( r \leftrightarrow p \) symmetry of the coordinate and momentum. Let us do this for the 1D case when the wave may be presented as\(^\text{17}\)

\[^{15}\text{Indeed, acting exactly as at derivation of Eq. (36), for a space-local Heisenberg operator we get}
\]

\[\langle A \rangle(t) = \int \Psi^*(x,t_0)\hat{A}_H(t,t_0)\Psi(x,t_0)dx.\]

\[^{16}\text{The set of equations (49) constitute the Ehrenfest theorem.}\]

\[^{17}\text{From this point on, for the sake of brevity I will drop index } x \text{ in the notation of the momentum – just as it was done in Chapter 2.}\]
\[
\psi_p(x) = a_p \exp\left\{i \frac{px}{\hbar}\right\}, \quad \text{for all } -\infty < x < +\infty.
\] (5.50)

Let us have a good look at this function. Since it satisfies equation (34) for the 1D momentum operator
\[
\hat{p} = -i\hbar \frac{\partial}{\partial x},
\]
\[
\hat{p} \psi_p = p \psi_p, \quad \text{'}
\] (5.51)
\(\psi_p\) is an eigenfunction of the momentum operator. But this means that we can also write Eq. (6) for the corresponding ket-vector:
\[
\hat{p} |p\rangle = p |p\rangle, \quad (5.52)
\]
and according to Eq. (19) the wavefunction may be presented as
\[
\psi_p(x) = \langle x | p \rangle. \quad (5.53)
\]

Expression (53) is quite remarkable in its \(x \leftrightarrow p\) symmetry - which may be pursued further on. Before doing that, however, we have to discuss normalization of such functions. Indeed, in this case, the probability density \(w(x)\) (18) is constant, so that its integral
\[
\int_{-\infty}^{+\infty} w(x) dx = \int_{-\infty}^{+\infty} \psi_p(x) \psi_p^*(x) dx \quad (5.54)
\]
diverges if \(a_p \neq 0\). Earlier in the course, we discussed two ways to avoid this divergence. One is to use a very large but finite integration volume – see Eq. (1.31). Another way to avoid the divergence is to form a wave packet of the type (2.20), possibly of a very large length and very narrow spread of momenta \(p\). Then integral (54) may be required to equal 1 without any conceptual problem.

However, both these methods violate the \(x \leftrightarrow p\) symmetry, and hence are inconvenient for our current purposes. Instead, let us continue to identify the bra- and ket-vectors \(\langle a_A |\) and \(|a_A \rangle\) of the general theory, developed in the beginning of this section, with eigenvectors \(\langle p |\) and \(|p \rangle\) of momentum – just as we have already done in Eq. (52). Then the normalization condition (9) becomes
\[
\langle p | p' \rangle = \delta(p - p'). \quad (5.55)
\]
Inserting the identity operator in the form (21) (with the integration variable \(x'\) replaced by \(x\)) into the left-hand side of this equation, we can translate this normalization rule to the wavefunction language:
\[
\int dx \langle p | x \rangle \langle x | p' \rangle \equiv \int dx \psi_p^*(x) \psi_p(x) = \delta(p - p'). \quad (5.56)
\]
Now using Eq. (50), this requirement turns into the following condition:
\[
a_p a_{p'} \int_{-\infty}^{+\infty} \exp\left\{i \frac{(p - p')x}{\hbar}\right\} dx \equiv |a_p|^2 2\pi \hbar \delta(p - p') = \delta(p - p'), \quad (5.57)
\]
so that, finally, \(a_p = \exp\{i \phi/(2\pi\hbar)^{1/2}\\), where \(\phi\) is an arbitrary (real) phase, and Eq. (50) becomes\(^{18}\)

\[^{18}\] Repeating the calculation for each Cartesian component of a plane monochromatic wave of arbitrary dimensionality \(d\), we get
\[
\psi_p = (2\pi\hbar)^{d/2} \exp\{i(p \cdot r/\hbar + \phi)\}.
\]
As was mentioned above, for finite-length wave packets such normalization is not really necessary. However, frequently it makes sense to keep the pre-exponential coefficient in Eq. (58) even for wave packets, because of the following reason. Let us form a wave packet of the type (2.20), based on wavefunctions (58) - taking $\phi = 0$ for the notation brevity, because it may be incorporated into function $\varphi(p)$:

$$
\psi_p(x) = \frac{1}{(2\pi \hbar)^{1/2}} \exp\left\{i \left( \frac{px}{\hbar} + \phi \right) \right\}, \quad (5.58)
$$

From the mathematical point of view, this is just the equation of a 1D Fourier spatial transform, and its reciprocal is

$$
\varphi(p) \equiv \frac{1}{(2\pi \hbar)^{1/2}} \int \psi(x) \exp\left\{-i \frac{px}{\hbar} \right\} dx. \quad (5.59)
$$

These expressions are completely symmetrical, and present the same wave packet; this is why functions $\psi(x)$ and $\varphi(p)$ are frequently called, respectively, the coordinate ($x$-) and momentum ($p$-) representations of the (same) state of the particle. Using Eqs. (53) and (58), they may be presented in an even more manifestly symmetric form,

$$
\psi(x) = \int \varphi(p) \langle x | p \rangle dp, \quad \varphi(p) = \int \psi(x) \langle p | x \rangle dx, \quad (5.61)
$$

in which the scalar products satisfy the basic postulate (4.14) of the bra-ket formalism:

$$
\langle p | x \rangle = \frac{1}{(2\pi \hbar)^{1/2}} \exp\left\{-i \frac{px}{\hbar} \right\} = \langle x | p \rangle^*. \quad (5.62)
$$

We already know that in the $x$-representation, i.e. in the usual wave mechanics, the coordinate operator $\hat{x}$ is reduced to the multiplication by $x$, and the momentum operator is proportional to a derivative over $x$:

$$
\left. \hat{x} \right|_{\text{in } x} = x, \quad \left. \hat{p} \right|_{\text{in } x} = -i\hbar \frac{\partial}{\partial x}. \quad (5.63)
$$

It is natural to guess that in the $p$-representation, the expressions for operators would be reciprocal:

$$
\left. \hat{x} \right|_{\text{in } p} = i\hbar \frac{\partial}{\partial p}, \quad \left. \hat{p} \right|_{\text{in } p} = p, \quad (5.64)
$$

with the difference in one sign only, due to the opposite signs of the Fourier exponents in Eqs. (59) and (60). The proof of Eqs. (64) is straightforward; for example, acting by the momentum operator to wavefunction (59), we get

$$
\hat{p} \psi(x) = -i\hbar \frac{\partial}{\partial x} \psi(x) = \frac{1}{(2\pi \hbar)^{1/2}} \int \varphi(p) \left\{-i\hbar \frac{\partial}{\partial x} \exp\left\{i \frac{px}{\hbar} \right\} \right\} dp = \frac{1}{(2\pi \hbar)^{1/2}} \int p \varphi(p) \exp\left\{i \frac{px}{\hbar} \right\} dp, \quad (5.65)
$$
and similarly for operator \( \hat{x} \) acting on function \( \varphi(p) \). Hence, the action of the operators (63) on wavefunction \( \psi \) (i.e. state’s \( x \)-representation) gives the same results as the action of operators (64) on function \( \varphi \) (i.e. its \( p \)-representation).

It is interesting to have one more, different look at this coordinate-to-momentum duality. For that, notice that according to Eqs. (4.82)-(4.84), we may consider the bra-ket \( \langle x|p \rangle \) as an element of the (infinite-size) matrix \( U_{xp} \) of the unitary transform from the \( x \)-basis to \( p \)-basis. Now let us derive the operator transform rule that would be a continuous version of Eq. (4.92). Say, we want to calculate a matrix element of some operator in the \( p \)-representation:

\[
\langle p | \hat{A} | p' \rangle. \tag{5.66}
\]

Inserting two identity operators (21) into this bra-ket, and then using Eq. (53) and its complex conjugate, and also Eq. (23) (again, valid only for space-local operators!), we get

\[
\langle p | \hat{A} | p' \rangle = \int dx \int dx' \langle p | x \rangle \langle x | \hat{A} | x' \rangle \langle x' | p' \rangle = \int dx \int dx' \psi^*_p(x) \langle x | \hat{A} | x' \rangle \psi_p(x').
\]

For example, for the momentum operator itself, this relation yields:

\[
\langle p | \hat{p} | p' \rangle = \frac{1}{2\pi\hbar} \int dx \exp \left\{ -i \frac{px}{\hbar} \right\} \delta(x-x') \hat{A} \exp \left\{ i \frac{p'x'}{\hbar} \right\} = \frac{1}{2\pi\hbar} \int dx \exp \left\{ -i \frac{px}{\hbar} \right\} \hat{A} \exp \left\{ i \frac{p'x'}{\hbar} \right\}. \tag{5.67}
\]

Due to Eq. (52), this result is equivalent to the second of Eqs. (64).

A natural question arises: why is the momentum representation used much less frequently than the coordinate representation - i.e., the wave mechanics? The answer is purely practical: besides the special case of the harmonic oscillator (to be revisited in Sec. 4 below), the orbital motion Hamiltonian (31) is not \( x \leftrightarrow p \) symmetric, with the potential energy \( U(x) \) being typically a more complex function than the kinetic energy, which is quadratic in momentum. Because of that, it is easier for problem solution to keep the potential energy operator just a wavefunction multiplier, as it is in the coordinate representation.

The most significant exception of this rule is the motion in a periodic potential, especially in the presence of additional external force \( F(t) \), which may result in the effects discussed in Secs. 2.8 and 2.9 (the Bloch oscillations, Landau-Zener tunneling etc.). Indeed, in this case the dispersion relation \( E_n(q) \), typically rather involved, plays the role of the effective kinetic energy, while the effective potential energy \( U_{ef} = -F(t)x \) in the field of the additional force is a simple function of \( x \). This is why discussions of the listed and more complex issues of the band theory (such as quasiparticle scattering, mobility, diffusion, etc.) in solid state physics theory are most typically based on the momentum representation.

### 5.3. Feynman’s path integrals

As has been already mentioned, even within the realm of wave mechanics, the bra-ket language allows to streamline some calculations that would be very bulky using the notation used in Chapters 1-3. Probably the best example in the famous alternative, path integral formulation of quantum mechanics,
developed in 1948 by R. Feynman.\textsuperscript{19} I will review this important concept - admittedly cutting one math corner for brevity.\textsuperscript{20} (This shortcut will be clearly marked.)

Let us inner-multiply both parts of Eq. (4.157), which is essentially the definition of the time-evolution operator, by the bra-vector of state $x$,

$$ \langle x | \alpha(t) \rangle = \langle x | \hat{u}(t,t_0) | \alpha(t_0) \rangle, $$

(5.69)

insert the identity operator before the ket-vector in the right-hand part, and then use the closure condition in the form of Eq. (21), with $x'$ replaced with $x_0$:

$$ \langle x | \alpha(t) \rangle = \int dx_0 \langle x | \hat{u}(t,t_0) | x_0 \rangle \langle x_0 | \alpha(t_0) \rangle. $$

(5.70)

According to Eq. (19), this equality may be presented as

$$ \Psi_a(x,t) = \int dx_0 \langle x | \hat{u}(t,t_0) | x_0 \rangle \Psi_a(x_0,t_0). $$

(5.71)

Comparing this expression with Eq. (2.44), we see that the bra-ket in this relation is nothing else than the 1D propagator, which was discussed in Sec. 2.2:

$$ \langle x | \hat{u}(t,t_0) | x_0 \rangle = G(x,t;x_0,t_0). $$

(5.72)

As a reminder, we have already calculated the propagator for a free particle – see Eq. (2.49).

Now let us break the time segment $[t_0, t]$ into $N$ (for the time being, not necessarily equal) parts by inserting $(N - 1)$ intermediate points (Fig. 2)

$$ t_0 < t_1 < ... < t_k < ... < t_{N-1} < t, $$

(5.73)

and rewrite the time evolution operator in the form

$$ \hat{u}(t,t_0) = \hat{u}(t,t_{N-1}) \hat{u}(t_{N-1},t_{N-2})...\hat{u}(t_2,t_1) \hat{u}(t_1,t_0), $$

(5.74)

whose correctness is evident from the very definition (4.157) of the operator. Plugging Eq. (74) into Eq. (72), let us insert the identity operator, again in the form (21) but written for $x_k$ rather than $x'$, between each two partial evolution operators including time argument $t_k$. The result is

$$ G(x,t;x_0,t_0) = \int dx_{N-1} \int dx_{N-2} ... \int dx_1 \langle x | \hat{u}(t,t_{N-1}) | x_{N-1} \rangle \langle x_{N-1} | \hat{u}(t_{N-1},t_{N-2}) | x_{N-2} \rangle...\langle x_1 | \hat{u}(t_1,t_0) | x_0 \rangle. $$

(5.75)

\begin{center}
\begin{figure}
\centering
\includegraphics[width=\textwidth]{fig5_2}
\caption{Time partition and coordinate notation at the initial stage of the Feynman’s path integral derivation.}
\end{figure}
\end{center}

\textsuperscript{19} According to Feynman’s memories, his work was motivated by a “mysterious” remark by P. A. M. Dirac in his pioneering 1930 textbook on quantum mechanics.

\textsuperscript{20} For a more thorough discussion of the path-integral approach, see the famous text R. Feynman and A. Hibbs, \textit{Quantum Mechanics and Path Integrals} first published in 1965. (For its latest edition by Dover in 2010, the book was emended by D. Styler.) For a more recent monograph that reviews more applications, see L. Schulman, \textit{Techniques and Applications of Path Integration}, Wiley, 1981.
The physical sense of each integration variable \( x_k \) is the wavefunction’s argument at time \( t_k \) - see Fig. 2. The key Feynman’s breakthrough was the realization that if all intervals are similar and sufficiently small, \( t_k - t_{k-1} = d\tau \to 0 \), all the partial bra-kets participating in Eq. (75) may be readily expressed via Eq. (2.49), even if the particle is not free, but moves in a stationary potential profile \( U(x) \). To show that, let us use either Eq. (4.175) or Eq. (4.181), which, for a small time interval \( d\tau \), give the same result:

\[
\hat{u}(\tau + d\tau, \tau) = \exp \left\{ -\frac{i}{\hbar} \hat{H} d\tau \right\} = \exp \left\{ -\frac{i}{\hbar} \left( \frac{\hat{p}^2}{2m} - d\tau + U(\hat{x}) d\tau \right) \right\}
\]

Generally, an exponent of a sum of two operators may be treated as that of \( c \)-number arguments, and in particular factored into a product of two exponents, only if the operators commute. (Indeed, in this case we can use all the standard algebra for exponents of \( c \)-number arguments.) In our case, this is not so, because operator \( \hat{p} \) does not commute with \( \hat{x} \), and hence with \( U(\hat{x}) \). However, it may be shown\(^\text{21}\) that for an infinitesimal time interval \( d\tau \), the nonvanishing commutator

\[
\left[ \frac{\hat{p}^2}{2m} d\tau, U(\hat{x}) d\tau \right] \neq 0,
\]

proportional to \((d\tau)^2\), is so small that in the first approximation in \( d\tau \) its effects may be ignored. As a result, we may factor the right-hand part in Eq. (76) by writing

\[
\hat{u}(\tau + d\tau, \tau)_{d\tau \to 0} \to \exp \left\{ -\frac{i}{\hbar} \frac{\hat{p}^2}{2m} d\tau \right\} \exp \left\{ -\frac{i}{\hbar} U(\hat{x}) d\tau \right\}
\]

(This approximation is very much similar in spirit to the rectangle-formula approximation for a usual 1D integral, which in also asymptotically impeccable.)

Since the second exponential function in the right-hand part of Eq. (78) commutes with the coordinate operator, we can move it out of each partial bra-ket participating in Eq. (75), with \( U(x) \) turning into a \( c \)-number function:

\[
\langle x_{\tau + d\tau} | \hat{u}(\tau + d\tau, \tau) | x_\tau \rangle = \langle x_{\tau + d\tau} | \exp \left\{ -\frac{i}{\hbar} \frac{\hat{p}^2}{2m} d\tau \right\} | x_\tau \rangle \exp \left\{ -\frac{i}{\hbar} U(x) d\tau \right\}
\]

But the remaining bra-ket is just the propagator of a free particle, and we can use Eq. (2.49) for it:

\[
\langle x_{\tau + d\tau} | \exp \left\{ -\frac{i}{\hbar} \frac{\hat{p}^2}{2m} d\tau \right\} | x_\tau \rangle = \left( \frac{m}{2\pi i\hbar d\tau} \right)^{1/2} \exp \left\{ i \frac{m(dx)^2}{2\hbar d\tau} \right\}
\]

As the result, the full propagator (75) takes the form

\[
G(x,t; x_0,t_0) = \lim_{d\tau \to 0} \int dx_{N-1} \int dx_{N-2} \ldots \int dx_1 \left( \frac{m}{2\pi i\hbar d\tau} \right)^{N/2} \exp \left\{ \sum_{k=1}^{N} \left[ i \frac{m(dx)^2}{2\hbar d\tau} - i \frac{U(x)}{\hbar} d\tau \right] \right\}
\]

\(\text{21}\) A strict proof of this intuitively evident statement would take more space and time than I can afford.
At \( N \to \infty \) and hence \( d\tau \equiv (t - t_0)/N \to 0 \), the sum under the exponent in this expression tends to an integral:

\[
\sum_{k=1}^{N} i \frac{m}{\hbar} \left( \frac{dx}{d\tau} \right)^2 - U(x) \bigg|_{\tau = t_k} d\tau \to i \frac{1}{\hbar} \int \left[ \frac{m}{2} \left( \frac{dx}{d\tau} \right)^2 - U(x) \right] d\tau,
\]

and the expression in square brackets is just the particle’s Lagrangian function \( L \).\(^{22}\)

The integral of the function over time is the classical action \( S \) calculated along a particular “path” \( x(\tau) \).\(^{23}\) As a result, defining the (1D) path integral as

\[
\int (...) D[x(\tau)] \equiv \lim_{N \to \infty} \left( \frac{m}{2\pi\hbar d\tau} \right)^{N/2} \int dx_{N-1} \int dx_{N-2} \ldots \int dx_1 (\ldots),
\]

we can bring our result to a superficially simple form

\[
G(x,t;x_0,t_0) = \int \exp \left[ \frac{i}{\hbar} S[x(\tau)] \right] D[x(\tau)].
\]

The name “path integral” for the mathematical construct (83a) may be readily explained if we keep the number \( N \) of time intervals large but finite, and also approximate each of the enclosed integrals by a sum over \( M \gg 1 \) discrete points along the coordinate axis (Fig. 3a).

Then the path integral is a product of \((N-1)\) sums corresponding to different values of time \( \tau \), each of them with \( M \) terms, each of the terms representing the function under the integral at a particular spatial point. Multiplying those \((N-1)\) sums, we get a sum of \((N-1)M\) terms, each evaluating the function at a specific spatial-temporal point \([x, \tau]\). These terms may be now grouped to represent all possible different continuous classical paths \( x[\tau] \) from the initial point \([x_0,t_0]\) to the finite point \([x,t]\). It is evident that the last interpretation remains true even in the continuous limit \( N, M \to \infty \) – see Fig. 3b.

Why does such representation of the sum have sense? This is because in the classical limit the particle follows just a certain path, corresponding to the minimum of action \( S \).\(^{22}\) Hence, for all close trajectories, the difference \((S - S_{cl})\) is proportional to the square of the deviation from the classical trajectory. Hence, for a quasiclassical motion, with \( S_{cl} \gg \hbar \), there is a substantial bunch of close trajectories, with \((S - S_{cl}) \ll \hbar\), that give similar contributions to the path integral. On the other hand,

\(^{22}\) See, e.g., CM Sec. 2.1.

\(^{23}\) See, e.g., CM Sec. 10.3.
strongly non-classical trajectories, with \((S - S_{cl}) \gg \hbar\), give phases \(S\hbar\) rapidly oscillating from one trajectory to the next one, and their contributions to the path integral are averaged out.\(^{24}\) As a result, for the quasiclassical motion, the propagator’s exponent may be evaluated on the classical path:

\[
G_{\text{cl}} \propto \exp \left\{ \frac{i}{\hbar} S_{\text{cl}} \right\} = \exp \left\{ \frac{i}{\hbar} \int_{t_0}^{t} \left[ \frac{m}{2} \left( \frac{dx}{d\tau} \right)^2 - U(x) \right] d\tau \right\}.
\] (5.84)

The sum of the kinetic and potential energies is the full energy \(E\) of the particle, that remains constant for motion in a stationary potential \(U(x)\), so that we may rewrite the expression under the integral as\(^{25}\)

\[
\left[ \frac{m}{2} \left( \frac{dx}{d\tau} \right)^2 - U(x) \right] d\tau = \left[ m \left( \frac{dx}{d\tau} \right)^2 - E \right] d\tau = m \frac{dx}{d\tau} dx - Ed\tau.
\] (5.85)

With that replacement, Eq. (83b) yields

\[
G_{\text{cl}} \propto \exp \left\{ \frac{i}{\hbar} \int_{x_0}^{x} m \frac{dx}{d\tau} dx \right\} \exp \left\{ -\frac{i}{\hbar} E(t-t_0) \right\} = \exp \left\{ i \int_{x_0}^{x} p(x) dx \right\} \exp \left\{ -\frac{i}{\hbar} E(t-t_0) \right\},
\] (5.86)

where \(p\) is the classical momentum of the particle. But (at least, leaving the pre-exponential factor alone) this is exactly the WKB approximation result that was derived and studied in detail in Chapter 2!

One may question the value of a calculation that yields the results that could be readily obtained from Schrödinger’s wave mechanics. The Feynman’s approach, is indeed not used too often, but it has its merits. First, it has an important philosophical (and hence heuristic) value. Indeed, Eq. (83) may be interpreted by saying that the essence of quantum mechanics is the exploration, by the system, of all possible paths \(x(\tau)\), each of them classical-like in the sense that the particle’s coordinate \(x\) and velocity \(dx/d\tau\) (and hence its momentum) are exactly defined simultaneously at each point. The resulting contributions to the path integral are added up coherently to form the final propagator \(G\), and via it, the final probability \(W \propto |G|^2\) of the particle propagation from \([x_0, t_0]\) to \([x, t]\). Of course, as the scale of action (i.e. of the energy-by-time product) of the motion decreases and becomes comparable to \(\hbar\), more and more paths produce substantial contribution to this sum, and hence to \(W\), ensuring a larger and larger difference between the quantum and classical properties of the system.

Second, the path integral provides a justification for some simple explanations of quantum phenomena. A typical example is the quantum interference effects discussed in Sec. 3.1 – see, e.g., Fig. 3.1 and the corresponding text. At that discussion, we used the Huygens principle to argue that at the two-slit interference, the WKB approximation might be restricted of effects by two paths that pass through different slits, but otherwise consisting of straight-line segments. To have another look at that assumption, let us generalize the path integral to multi-dimensional geometries. Fortunately, the simple structure of Eq. (83b) makes such generalization virtually evident:

\(^{24}\) This fact may be proved by expanding the difference \((S - S_{cl})\) in the Taylor series in path variations (leaving only the leading quadratic terms) and working out the resulting Gaussian integrals. It is interesting that the integration, together with the pre-exponential coefficient in Eq. (83a), gives exactly the pre-exponential factor that we have already found in Sec. 2.4 when refining the WKB approximation.

\(^{25}\) The same trick is often used in analytical classical mechanics – say, for proving the Hamilton principle, and for the derivation of the Hamilton – Jacobi equations (see, e.g. CM Secs. 10.3-4).
where definition (83a) of the path integral should be also modified correspondingly. (I will not go into these technical details.) For the Young-type experiment (Fig. 3.1), where a classical particle could reach the detector only after passing through one of the slits, the classical paths are the straight-line segments shown in Fig. 3.1, and if they are much longer than the de Broglie wavelength, the propagator may be well approximated by the sum of two integrals of $Ld\tau = i\mathbf{p}(\mathbf{r}) \cdot d\mathbf{r}/\hbar$ - as it was done in Sec. 3.1.

Last but not least, the path integral allows simple solutions of some problems that would be hard to get by other methods. As the simplest example, let us consider the problem of tunneling in multi-dimensional space, sketched in Fig. 4 for the 2D case - just for graphics’ simplicity. Here, potential $U(x, y)$ has the “saddle” shape. (Another helpful image is a mountain path between two summits, in Fig. 4 located on the top and at the bottom of the drawing.) A particle of energy $E$ may move classically in the left and right regions with $U(x, y) < E$, but can pass from one of these regions to another one only via the quantum-mechanical tunneling under the pass. Let us calculate the transparency of this tunnel barrier in the WKB approximation, ignoring the possible pre-exponential factor.

![Fig. 5.4. Saddle-type 2D potential profile and the instanton trajectory of a particle of energy $E$ (dashed line, schematically).](image)

According to the evident multi-dimensional generalization Eq. (86), for the classically forbidden region, where $E < U(x, y)$, the contributions to propagator (87) are proportional to

$$\exp\left\{ -\int_{t_0}^{t} \mathbf{k}(\mathbf{r}) \cdot d\mathbf{r} \right\} \exp\left\{ -\frac{i}{\hbar} E(t - t_0) \right\},$$

where the magnitude of vector $\mathbf{k}$ at each point may be calculated just in the 1D case - see, e.g., Eq. (2.97),

$$\frac{\hbar^2 \mathbf{k}^2(\mathbf{r})}{2m} = U(\mathbf{r}) - E,$$

while its direction should be tangential to the path trajectory in space. Now the path integral is actually much simpler than in the classically-allowed region, because the spatial exponents are purely real and there is no complex interference between them. Because of the minus sign in the exponent, the largest
contribution to $G$ evidently comes from the trajectory (or rather a narrow bundle of trajectories) for which the functional

$$\int_{r_0}^{r} \kappa(r') \cdot dr'$$

(5.90)

has the smallest value, and the barrier transmission coefficient may be calculated as

$$T \approx |G|^2 \approx \exp \left\{ -2 \int_{r_0}^{r} \kappa(r') \cdot dr' \right\},$$

(5.91)

where $r$ and $r_0$ are certain points on the opposite classical turning-point surfaces: $U(r) = U(r_0) = E$.\(^{26}\)

Thus the tunneling problem is reduced to finding the trajectory (including points $r$ and $r_0$) that connects the two surfaces and minimizes functional (90). This is of course a well-known problem of the calculus of variations,\(^{27}\) but it is interesting that the path integral provides a simple alternative way of solving it. Let us consider an auxiliary problem of particle’s motion in a potential profile $U_{\text{inv}}(r)$ that is inverted relative to particle’s energy $E$, i.e. is defined by the following equality:

$$U_{\text{inv}}(r) - E \equiv E - U(r).$$

(5.92)

As was discussed above, at fixed energy $E$, the path integral for the WKB motion in the classically allowed region of potential $U_{\text{inv}}(x,y)$ (that coincides with the classically forbidden region of the original problem) is dominated by the classical trajectory corresponding to the minimum of

$$S_{\text{inv}} = \int_{r_0}^{r} p_{\text{inv}}(r') \cdot dr' = \hbar \int_{r_0}^{r} k_{\text{inv}}(r') \cdot dr,$$

(5.93)

where $k_{\text{inv}}$ should be determined from the relation

$$\frac{\hbar^2 k_{\text{inv}}^2(r)}{2m} \equiv E - U_{\text{inv}}(r).$$

(5.94)

But comparing Eqs. (89), (92), and (94), we see that $k_{\text{inv}} = \kappa$ at each point of space! This means that the tunneling path (in the WKB limit) corresponds to the classical (so-called instanton)\(^{28}\) trajectory of the same particle in the inverted potential $U_{\text{inv}}(r)$. If the initial point $r_0$ is fixed, this trajectory may be readily found by the means of classical mechanics. (Note that the initial velocity of the instanton launched from point $r_0$ should be zero, because by the classical turning point definition: $U_{\text{inv}}(r_0) = U(r_0) = E$.) Thus the problem is reduced to a simpler task of maximizing the transparency (91) over the position of $r_0$ on the equipotential surface $U(r_0) = E$. Moreover, for many symmetric potentials, the position of this point may be readily guessed without calculations.

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\(^{26}\) One can argue that the pre-exponential coefficient in Eq. (91) should be close to 1, just like in Eq. (2.117), especially if the potential is smooth in the sense of Eq. (2.107), where $x$ is the coordinate along the trajectory.\(^{27}\)

\(^{27}\) For a concise introduction to the field see, e.g., I. Gelfand and S. Fomin, *Calculus of Variations*, Dover, 2000, or L. Elsgolc, *Calculus of Variations*, Dover, 2007.\(^{28}\)

\(^{28}\) In quantum field theory, the instanton concept may be formulated somewhat differently, and has more complex applications - see, e.g. R. Rajaraman, *Solitons and Instantons*, North Holland, 1987.
Note that besides the calculation of barrier transparency, the instanton trajectory has one more important implication: the so-called traversal time $\tau_t$ of the classical motion along it, in the inverted potential, defined by Eq. (94), plays the role of the most important (though not the only one) time scale of particle’s tunneling under the potential barrier.29

5.4. Revisiting harmonic oscillator

Let us return to the 1D harmonic oscillator, i.e. any system described by Hamiltonian (2.50) with potential energy (2.111):

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega_0^2 \hat{x}^2}{2}. \quad (5.95)$$

In Sec. 2.10 we have used the "brute-force" (wave-mechanics) approach to analyze the eigenfunctions $\psi_n(x)$ and eigenvalues $E_n$ of this Hamiltonian, and found that, unfortunately, that approach required relatively complex math that obscures the physics of these stationary ("Fock") states. Now let us use the bra-ket formalism to make the properties of these states much more transparent, using very simple calculations.

First, introducing normalized (dimensionless) operators of coordinates and momentum:30

$$\hat{\xi} \equiv \frac{\hat{x}}{x_0}, \quad \hat{\zeta} \equiv \frac{\hat{p}}{m\omega_0 x_0}, \quad (5.96)$$

where $x_0 = (\hbar/m\omega_0)^{1/2}$ is the natural coordinate scale ($\sqrt{2}$ the r.m.s. spread of ground-state wavefunction) which was discussed in detail in Sec. 2.10, we can present Hamiltonian (95) in a very simple and symmetric form:

$$\hat{H} = \frac{\hbar \omega_0}{2} (\hat{\xi}^2 + \hat{\zeta}^2). \quad (5.97)$$

Now, let us introduce a new operator

$$\hat{a} \equiv \frac{1}{\sqrt{2}} \left( \hat{\xi} + i \hat{\zeta} \right) = \left( \frac{m\omega_0}{2\hbar} \right)^{1/2} \left( \hat{x} + i \frac{\hat{p}}{m\omega_0} \right). \quad (5.98a)$$

Since both operators $\hat{\xi}$ and $\hat{\zeta}$ correspond to real observables, i.e. have real eigenvalues and hence are Hermitian (self-adjoint), the Hermitian conjugate of operator $\hat{a}$ is simply its complex conjugate:

$$\hat{a}^\dagger = \frac{1}{\sqrt{2}} \left( \hat{\xi} - i \hat{\zeta} \right) = \left( \frac{m\omega_0}{2\hbar} \right)^{1/2} \left( \hat{x} - i \frac{\hat{p}}{m\omega_0} \right). \quad (5.98b)$$

Solving the system of two equations (98) for $\hat{\xi}$ and $\hat{\zeta}$, we may readily get reciprocal relations

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30 This normalization is not really necessary, it just makes the following calculations less bulky - and thus more aesthetically appealing.
\[ \hat{\xi} = \frac{1}{\sqrt{2}} \left( \hat{a} + \hat{a}^\dagger \right), \quad \hat{\zeta} = \frac{1}{\sqrt{2}i} \left( \hat{a} - \hat{a}^\dagger \right). \] (5.99)

Our Hamiltonian (97) includes squares of these operators. Calculating them, we have to be careful to avoid swapping the new operators, because they do not commute. Indeed, for the normalized operators (96), Eq. (2.14) gives

\[ \left[ \hat{\xi}, \hat{\zeta} \right] = \frac{1}{\omega_o^2 m \omega_o} \left[ \hat{x}, \hat{p} \right] = i \hat{l}, \] (5.100)

so that Eqs. (98) yield

\[ \left[ \hat{a}, \hat{a}^\dagger \right] = \frac{1}{2} \left( \left[ \hat{\xi} + i \hat{\zeta} \right] \left[ \hat{\xi} - i \hat{\zeta} \right] \right) = -\frac{i}{2} \left( \left[ \hat{\xi}, \hat{\zeta} \right] - \left[ \hat{\zeta}, \hat{\xi} \right] \right) = \hat{l}. \] (5.101)

With such due caution, Eq. (99) gives

\[ \hat{\xi}^2 = \frac{1}{2} \left( \hat{a}^2 + \hat{a}^\dagger \hat{a} + \hat{a}^\dagger \hat{a} \right), \quad \hat{\zeta}^2 = -\frac{1}{2} \left( \hat{a}^2 + \hat{a}^\dagger \hat{a} - \hat{a}^\dagger \hat{a} + \hat{a} \hat{a}^\dagger \right). \] (5.102)

Plugging these expressions back into Eq. (97), we get

\[ \hat{H} = \frac{\hbar \omega_o}{2} \left( \hat{a} \hat{a}^\dagger + \hat{a}^\dagger \hat{a} \right). \] (5.103)

This expression is elegant enough, but may be recast into an even more convenient form. For that, let us rewrite the commutation relation (100) as

\[ \hat{a} \hat{a}^\dagger = \hat{a}^\dagger \hat{a} + \hat{l}, \] (5.104)

and plug it into Eq. (103). The result is

\[ \hat{H} = \frac{\hbar \omega_o}{2} \left( 2 \hat{a}^\dagger \hat{a} + \hat{l} \right) = \hbar \omega_o \left( \hat{N} + \frac{1}{2} \hat{l} \right), \] (5.105)

where, in the last form, one more (evidently, Hermitian) operator,

\[ \hat{N} = \hat{a}^\dagger \hat{a}, \] (5.106)

has been introduced. Since, according to Eq. (105), operators \( \hat{H} \) and \( \hat{N} \) differ only by the addition of an identity operator and the multiplication by a \( c \)-number, these operators commute. Hence, according to the general arguments of Sec. 4.5, they share the set of stationary (Fock) eigenstates \( n \), and we can write the eigenproblem for the new operator as

\[ \hat{N} | n \rangle = N_n | n \rangle, \] (5.107)

where \( N_n \) are some eigenvalues that, according to Eq. (105), determine also the energy spectrum of the oscillator:

\[ E_n = \hbar \omega_o \left( N_n + \frac{1}{2} \right). \] (5.108)
So far, we know only that all eigenvalues $N_n$ are real, but not much more. In order to calculate them, let us carry out the following calculation - splendid in its simplicity and efficiency. Consider the result of action of operator $\hat{N}$ on the ket-vector $\hat{a}^\dagger |n\rangle$. Using the definition (106) and the associative rule, we may write

$$\hat{N}\left(\hat{a}^\dagger |n\rangle\right) = \left(\hat{a}^\dagger \hat{a}\right)\left(\hat{a}^\dagger |n\rangle\right) = \hat{a}^\dagger \left(\hat{a} \hat{a}^\dagger \right)|n\rangle.$$  \hspace{1cm} (5.109)

Now using the commutation relation (104), and then Eq. (107), we may continue as

$$\hat{a}^\dagger \left(\hat{a} \hat{a}^\dagger \right)|n\rangle = \hat{a}^\dagger \left(\hat{a} \hat{a}^\dagger + \hat{I}\right)|n\rangle = \hat{a}^\dagger \left(\hat{N} + \hat{I}\right)|n\rangle = \hat{a}^\dagger \left(N_n + 1\right)|n\rangle = \left(N_n + 1\right)\left(\hat{a}^\dagger |n\rangle\right).$$  \hspace{1cm} (5.110)

Let us summarize the result of this calculation:

$$\hat{N}\left(\hat{a}^\dagger |n\rangle\right) = \left(N_n + 1\right)\left(\hat{a}^\dagger |n\rangle\right).$$  \hspace{1cm} (5.111)

Performing an absolutely similar calculation with operator $\hat{a}$, we can also get another formula:

$$\hat{N}(\hat{a}|n\rangle) = \left(N_n - 1\right)(\hat{a}|n\rangle).$$  \hspace{1cm} (5.112)

It is time to stop calculations and translate these results into plain English: if $|n\rangle$ is an eigenket of operator $\hat{N}$ with eigenvalue $N_n$, then $\hat{a}^\dagger |n\rangle$ and $\hat{a}|n\rangle$ are also eigenkets of that operator, with eigenvalues $(N_n + 1)$, and $(N_n - 1)$, respectively. This statement may be presented with the ladder diagram shown in Fig. 5.

![Fig. 5.5. Hierarchy (the “ladder diagram”) of eigenstates of a 1D harmonic oscillator. Arrows show the actions of the creation and annihilation operators on the eigenstates.](image)

Operator $\hat{a}^\dagger$ moves the system a step up the ladder, while operator $\hat{a}$ brings it one step down. In other words, the former operator creates a new excitation of the system, while the latter operator kills (“annihilates”) such excitation. This is why $\hat{a}^\dagger$ is called the creation operator, and $\hat{a}$, the annihilation operator. In its turn, according to Eq. (107), operator $\hat{N}$ does not change the state of the system, but “counts” its position on the ladder:

$$\langle n |\hat{N}|n\rangle = \langle n |N_n |n\rangle = N_n.$$  \hspace{1cm} (5.113)

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31 For the electromagnetic field oscillators, such excitations are called photons; for the mechanical wave field oscillators, phonons, etc.
This is why \( \hat{N} \) is called the number operator, in our current context meaning the number of the elementary excitations of the oscillator.

This calculation still needs a completion. Indeed, we still do not know whether the ladder shown in Fig. 5 shows all eigenstates of the oscillator, and what exactly the numbers \( N_n \) are. Fascinating enough, both questions may be answered by exploring a single paradox. Let us start with some state (step of the ladder), and keep going down it, applying operator \( \hat{a} \) again and again. Each time, eigenvalue \( N_n \) is decreased by one, so that eventually it should become negative. However, this cannot happen, because any real eigenstate, including the states presented by kets \(|d\rangle \equiv \hat{a}|n\rangle \) and \(|n\rangle\), should have a positive norm – see Eq. (4.16). Comparing the norms,

\[
\|n\|^2 = \langle n|n\rangle, \quad \|d\|^2 = \langle n|\hat{a}^\dagger a|n\rangle = \langle n|\hat{N}|n\rangle = N_n \langle n|n\rangle,
\]

we see that the both of them cannot be positive simultaneously if \( N_n \) is negative.

The way toward the resolution of this paradox is to notice that the action of the creation and annihilation operators on the stationary states may consist in not only their promotion to the next step of the ladder diagram, but also by their multiplication by some \( c \)-numbers:

\[
\hat{a}|n\rangle = A_n |n-1\rangle, \quad \hat{a}^\dagger |n\rangle = A'_n |n+1\rangle.
\]

(Linear relations (111) and (112) clearly allow that.) Let us calculate coefficients \( A_n \) assuming, for convenience, that all eigenstates, including states \( n \) and \( (n-1) \), are normalized:

\[
\langle n|n\rangle = 1, \quad \langle n-1|n-1\rangle = \langle n|\hat{a}^\dagger \hat{a}|n\rangle = \frac{1}{A_n A^*_n} \langle n|\hat{N}|n\rangle = \frac{N_n}{A_n A^*_n} \langle n|n\rangle = 1.
\]

From here, we get \(|A_n| = (N_n)^{1/2}\), i.e.

\[
\hat{a}|n\rangle = N_n^{1/2} e^{i\varphi_n} |n-1\rangle,
\]

where \( \varphi_n \) is an arbitrary real phase. Now let us consider what happens if all numbers \( N_n \) are integers. (Because of the definition of \( N_n \), given by Eq. (107), it is convenient to call these integers \( n \), i.e. by the same letter as the corresponding eigenstate.) Then when we have come down to state with \( n = 0 \), an attempt to make one more step down gives

\[
\hat{a}|0\rangle = 0|-1\rangle.
\]

But in accordance with Eq. (4.9), the state in the right-hand part of this equation is the “null-state”, i.e. does not exist.\(^{32}\) This gives the (only known :-) resolution of the state ladder paradox: the ladder has the lowest step with \( N_n = n = 0 \).

As a by-product of our discussion, we have obtained a very important relation \( N_n = n \), which means, in particular, that the state ladder includes all eigenstates of the oscillator. Plugging this relation into Eq. (108), we see that the full spectrum of eigenenergies of the harmonic oscillator is described by the simple formula

\[ N_n = n \]

\(^{32}\) Please note again the radical difference between the null-state in the right-hand part of Eq. (118) and the state described by ket-vector \(|0\rangle\) in the left-hand side of that relation. The latter state does exist and, moreover, presents the most important, ground state of the system, with \( n = 0 \) - see Eq. (2.269).
\[ E_n = \hbar \omega_0 \left( n + \frac{1}{2} \right), \quad n = 0, 1, 2\ldots, \]  

(5.119)

which was already discussed in Sec. 2.10. It is rather remarkable that the bra-ket formalism has allowed us to derive it without calculation of the corresponding (rather cumbersome) wavefunctions \( \psi_n(x) \) – see Eqs. (2.279).

Moreover, the formalism may be also used to calculate virtually any bra-ket pertaining to the oscillator, without using \( \psi_n(x) \). In order to illustrate that, let us first calculate \( A'_n \) participating in the latter of relations (115). This can be done absolutely similarly to the above calculation of \( A_n \); otherwise, since we already know that \( |A_n| = (N_n)^{1/2} = n^{1/2} \), we may notice that according to Eqs. (106) and (115), the eigenproblem (107), that in our new notation for \( N_n \) becomes

\[ \hat{N}|n\rangle = n|n\rangle, \]  

(5.120)

may be rewritten as

\[ n|n\rangle = \hat{a}^\dagger \hat{a}|n\rangle = \hat{a}^\dagger A_n |n-1\rangle = A_n A_{n-1} |n\rangle. \]  

(5.121)

Comparing the first and the last form of this equality, we see that \( |A_{n-1}| = n!/|A_n| = n^{1/2} \), i.e. \( A'_n = (n + 1)^{1/2} \exp(i\phi_n) \). Taking all phases \( \phi_n \) and \( \phi_n' \) equal to zero for simplicity, we may reduce Eqs. (115) to their final, standard form\(^{33} \)

\[ \hat{a}^\dagger |n\rangle = (n + 1)^{1/2} |n+1\rangle, \quad \hat{a} |n\rangle = n^{1/2} |n-1\rangle. \]  

(5.122)

Now we can use these formulas to calculate, for example, the matrix elements of operator \( \hat{x} \) in the Fock state basis:

\[ \langle n'|\hat{x}|n\rangle = x_n \langle n'|\hat{\xi}|n\rangle = \frac{x_n}{\sqrt{2}} \langle n'|\left( \hat{a} + \hat{a}^\dagger \right)|n\rangle = \frac{x_0}{\sqrt{2}} \left( \langle n'|\hat{a}|n\rangle + \langle n'|\hat{a}^\dagger|n\rangle \right). \]  

(5.123)

To complete the calculation, we may now use Eqs. (122) and the Fock state orthonormality:

\[ \langle n'|n\rangle = \delta_{n'n}. \]  

(5.124)

The result is

\[ \langle n'|\hat{x}|n\rangle = \frac{x_0}{\sqrt{2}} \left( n^{1/2} \delta_{n,n-1} + (n+1)^{1/2} \delta_{n,n+1} \right) = \left( \frac{\hbar}{2m\omega_0} \right)^{1/2} \left( n^{1/2} \delta_{n,n-1} + (n+1)^{1/2} \delta_{n,n+1} \right) \]  

(5.125)

Acting absolutely similarly, for the momentum bra-kets we get a similar expression:

\[ \langle n'|\hat{p}|n\rangle = i \left( \frac{\hbar m\omega_0}{2} \right)^{1/2} \left( -n^{1/2} \delta_{n,n-1} + (n+1)^{1/2} \delta_{n,n+1} \right). \]  

(5.126)

Hence the matrices of both operators in the Fock-state basis have only two diagonals, adjacent to the main diagonal; all other elements (including the diagonal ones) are zeros.

\(^{33} \) A useful mnemonic rule is that the \( c \)-number coefficient in any of these relations is equal to the square root of the largest number of the two states it relates.
Matrix elements of higher powers of these operators, as well as their products, may be handled similarly, though the higher is the power, the bulkier is the result. For example,\textsuperscript{34}

\[
\langle n'| \hat{x}^2 | n \rangle = \sum_{n''=0}^{\infty} \langle n'| \hat{x} | n'' \rangle \langle n'' | \hat{x} | n \rangle \\
= \frac{x_0^2}{2} \sum_{n''=0}^{\infty} \left( (n'')^{1/2} \delta_{n'',n'-1} + (n'' + 1)^{1/2} \delta_{n'',n'+1} \right) \left( n^{1/2} \delta_{n',n-1} + (n+1)^{1/2} \delta_{n',n+1} \right) \\
= \frac{x_0^2}{2} \left\{ n(n-1) \right\}^{1/2} \delta_{n',n-2} + \left[ (n+1)(n+2) \right]^{1/2} \delta_{n',n+2} + (2n+1)\delta_{n',n} \}.
\]

For applications, the most important of these matrix elements are those on its main diagonal:

\[
\langle x^2 \rangle = \langle n| \hat{x}^2 | n \rangle = \frac{x_0^2}{2} (2n+1).
\]

This expression shows, in particular, that the expectation value of oscillator’s potential energy in \( n \)-th Fock state is

\[
\langle U \rangle = \frac{m\omega_0^2}{2} \langle x^2 \rangle = \frac{\hbar\omega_0}{2} \left( n + \frac{1}{2} \right).
\]

This is exactly \( \frac{1}{2} \) of the total energy (119) of the oscillator. As a sanity check, an absolutely similar calculation of the kinetic energy shows that

\[
\frac{\langle p^2 \rangle}{2m} = \frac{1}{2m} \langle n| \hat{p}^2 | n \rangle = \frac{\hbar\omega_0}{2} \left( n + \frac{1}{2} \right),
\]

i.e. both partial energies equal \( E_n/2 \), just as in a classical oscillator.\textsuperscript{35}

5.5. The Glauber and squeezed states

There is evidently a huge difference between a quantum stationary (Fock) state of the oscillator and its classical state. Indeed, let us write the classical Hamilton equations of motion of the oscillator (using capital letters to distinguish the classical variables from arguments of quantum wavefunctions):

\[
\dot{X} = \frac{P}{m}, \quad \dot{P} = -\frac{\partial U}{\partial X} = -m\omega_0^2 X.
\]

On the “phase plane” with Cartesian coordinates \( x \) and \( p \) (Fig. 6), these equations describe clockwise rotation of the representation point \( \{X(t), P(t)\} \) along an elliptic trajectory starting from the initial point \( \{X(0), P(0)\} \). (The normalization of momentum by \( m\omega_0 \), similar to the one performed by the second of Eqs. (96), makes the trajectory pleasingly circular, with a constant radius equal to oscillation’s amplitude \( A \), reflecting the constant full energy

\textsuperscript{34} The first line of Eq. (127), evidently valid for any time-independent system, is the simplest of the so-called \textit{sum rules}, which will be repeatedly discussed below.

\textsuperscript{35} Still note that operators of the partial (potential and kinetic) energies do \textit{not} commute with either each other or with the full-energy (Hamiltonian) operator, so that the Fock states \( n \) are \textit{not} their eigenstates.
\[
E_c = \frac{m\omega_0^2}{2} A^2, \quad A^2 = [X(t)]^2 + \left[\frac{P(t)}{m\omega_0}\right]^2 = \text{const} = [X(0)]^2 + \left[\frac{P(0)}{m\omega_0}\right]^2,
\]

(5.132)
determined by the initial conditions.\)

For the forthcoming comparison with quantum states, it is convenient to describe this classical solution by the following dimensionless complex variable

\[
\alpha(t) = \frac{1}{\sqrt{2x_0}} \left( X(t) + i \frac{P(t)}{m\omega_0} \right),
\]

(5.133)
which is essentially the standard complex-number representation of system’s position on the 2D phase plane, with \(|\alpha| = A/\sqrt{2x_0}\). With this definition, Eqs. (131) are conveniently merged into one equation,

\[
\dot{\alpha} = -i\omega_0 \alpha,
\]

(5.134)
with an evident, very simple solution

\[
\alpha(t) = \alpha(0)e^{-i\omega_0 t},
\]

(5.135)
where the constant \(\alpha(0)\) may be complex, and is just the (normalized) classical complex amplitude of oscillations.\(^{36}\) This equation describes sinusoidal oscillations of both \(X(t) \propto \text{Re}[\alpha(t)]\) and \(P \propto \text{Im}[\alpha(t)]\), with a phase shift of \(\pi/2\) between them.

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\(^{36}\) See, e.g., CM Chapter 4, especially Eqs. (4.4) and Fig. 4.9 and its discussion.

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Fig. 5.6. Schematic representation of various states of a harmonic oscillator on the phase plane. The bold black point represents a classical state, with the dashed line showing its trajectory. (Very imperfect) classical images of the Fock states with \(n = 0, 1,\) and \(2\) are shown in blue, while the blurred red spot is the (equally schematic) Glauber state’s image. Finally, the magenta elliptical spot is a classical image of a squeezed ground state. Arrows show the direction of states’ evolution in time.

On the other hand, according to the basic Eqs. (4.157)-(4.158), the time dependence of a Fock state, as of a stationary state of the oscillator, is limited to the phase factor \(\exp\{-iE_nt/\hbar\}\) not in observables, but rather in the wavefunction, and a result, gives time-independent expectation values of \(x,\)

\(p,\) or of any function thereof. (Moreover, as Eqs. (125) and (126) show, \(\langle x \rangle = \langle p \rangle = 0.\) Taking into
account Eqs. (129) and (130), the closest (though very imperfect) geometric image\textsuperscript{37} for such a state on the phase plane is a blurred circle of radius $A_n = x_0(2n + 1)^{1/2}$, along which the wavefunction is uniformly spread as a wave – see the blue rings in Fig. 6. For the ground state ($n = 0$), with wavefunction (2.269), a better image is a blurred round spot, of radius $\sim x_0$, at the origin.

However, the Fock states $n$ are not the only possible quantum states of the oscillator: according to the basic Eq. (4.6), a state described by ket-vector

$$\left| \alpha \right\rangle = \sum_{n=0}^{\infty} \alpha_n \left| n \right\rangle$$

(5.136)

with any set of (complex) $c$-numbers $\alpha_n$, is also its legitimate state, subject only to the normalization condition $\langle \alpha | \alpha \rangle = 1$, giving

$$\sum_{n=0}^{\infty} |\alpha_n|^2 = 1.$$  

(5.137)

It is natural to ask: can we select coefficients $\alpha_n$ in such a special way that the state properties would be closer to the classical ones; in particular the expectation values $\langle x \rangle$ and $\langle p \rangle$ of coordinate and momentum would evolve in time just as the classical values $X(t)$ and $P(t)$, while the uncertainties of these observables would be time-independent and the same as in the ground state:

$$\delta x = \frac{x_0}{\sqrt{2}} = \left( \frac{\hbar}{2m\omega_0} \right)^{1/2}, \quad \delta p = \frac{m\omega_0 x_0}{\sqrt{2}} = \left( \frac{\hbar m \omega_0}{2} \right)^{1/2},$$

(5.138)

with the smallest possible value of the uncertainty product, $\delta x \delta p = \hbar/2$.\textsuperscript{38} Let me show that such a Glauber state,\textsuperscript{39} which is schematically represented in Fig. 6 by a blurred red spot around the classical point $\{X(t), P(t)\}$, is indeed possible.

Conceptually the simplest way to find the corresponding coefficients $\alpha_n$ would be to calculate $\langle x \rangle$, $\langle p \rangle$, $\delta x$ and $\delta p$ for an arbitrary set of $\alpha_n$, and then try to optimize these coefficients to reach our goal. However, this problem may be solved much easier using wave mechanics. Indeed, let us consider the following wavefunction

$$\Psi_{\alpha}(x,t) = C_0 \exp \left\{ - \frac{m\omega_0}{2\hbar} \left[ x - X(t) \right]^2 + i \frac{P(t)x}{\hbar} \right\}.$$  

(5.139)

Its comparison with Eqs. (2.16) and (2.269) shows that this is just a Gaussian wave packet with the average momentum $P$ and the coordinate width $\delta x$ given by Eq. (138), but shifted along axis $x$ by $X$.

\textsuperscript{37} I have to confess that such geometric mapping of a quantum state on the phase plane $[x, p]$ is not exactly defined; you may think about colored areas in Fig. 6 as regions of pairs $\{x, p\}$ most probably obtained in measurements. A quantitative definition of such a mapping will be given in Sec. 7.3 using the Wigner function, though, as we will see, even such imaging definition has certain internal contradictions. Still such cartoons may have considerable cognitive/heuristic value, if their limitations are kept in mind.

\textsuperscript{38} In the quantum theory of measurements, Eqs. (138) are frequently referred to as the standard quantum limit.

\textsuperscript{39} Named after R. J. Glauber who studied these states in detail in 1965, though they had been discussed in brief by E. Schrödinger as early as in 1926. Another popular name, “coherent”, for the Glauber states is very misleading, because all the quantum states we have studied so far (including the Fock states) may be presented as coherent (pure) superpositions of the basis states.
Hence, this wavefunction satisfies all the above requirements, and a straightforward (though a bit bulky) differentiation over \( x \) and \( t \) shows it also satisfies oscillator’s Schrödinger equation, provided that that functions \( X(t) \) and \( P(t) \) satisfy classical Eqs. (131).

This fact is true even for a more general situation when the oscillator, initially in its ground state\(^{40}\) comes under effect of a classical force \( F(t) \). (Evidently, for its description it is sufficient to add this function to the right-hand part of the second of Eqs. (131).) Moreover, the electromagnetic radiation formed in “good” (single-mode) lasers is also in the Glauber state. (As will be discussed in Chapter 9, the experimental formation of Fock states \( n \), with the only exception of \( n = 0 \), i.e. the ground state, is much harder.) This is why the Glauber states are so important.

Though Eq. (139) gives the full wave-mechanics description of a Glauber state, there is a substantial place for the bra-ket formalism here too. For example, in order to calculate the corresponding coefficients in expansion (136),

\[
\alpha_n = \langle n | \alpha \rangle = \int dx \langle n | x \rangle \langle x | \alpha \rangle = \int \psi_n^*(x) \psi_\alpha(x) dx , \tag{5.140}
\]

we would need to use not only the simple Eq. (139), but also the Fock state wavefunctions \( \psi_n(x) \), which are not very appealing – see Eq. (2.279). Instead, this calculation may be readily done in the bra-ket formalism, giving us one important byproduct result.

Let us start from expressing the double shift of the ground state (by \( X \) and \( P \)), that has led us to Eq. (139), in the operator language. Forgetting about the \( P \) for a minute, let us find a translation operator \( \hat{T}_X \) that produces the desirable shift of coordinate by \( X \) of an arbitrary wavefunction \( \psi(x) \) – say represented as the standard wave packet (59). Evidently, the result of its action, in the coordinate representation, is

\[
\hat{T}_X \psi(x) = \psi(x - X) = \frac{1}{(2\pi\hbar)^{1/2}} \int \varphi(p) \exp \left\{ -i \frac{p(x - X)}{\hbar} \right\} dp . \tag{5.141}
\]

Hence, the shift may be achieved by the multiplication of each Fourier component of the packet, with momentum \( p \), by \( \exp \left\{ -i \frac{pX}{\hbar} \right\} \). This gives us a hint that the general form of the translation operator, valid in \textit{any} representation, should be

\[
\hat{T}_X = \exp \left\{ -i \frac{\hat{p}X}{\hbar} \right\} . \tag{5.142}
\]

The proof of this formula is provided by the fact that any operator is uniquely determined by the set of its matrix elements in any full and orthogonal basis, in particular the basis of momentum states \( p \). According to Eq. (141), the analog of Eq. (23) for the \( p \)-representation, applied to the translation operator (which is evidently local), is

\[
\langle p | \hat{T}_X | p' \rangle \varphi(p') = \delta(p - p') \exp \left\{ -i \frac{pX}{\hbar} \right\} \varphi(p) , \tag{5.143}
\]

so that operator (142) does exactly the job we need it to.

\(^{40}\) As will be discussed in Chapter 7, the ground state may be readily formed, for example, by providing a weak coupling of the oscillator to a low-temperature \((k_B T \ll h\omega_0)\) environment.
The operator that provides the shift of momentum by \( P \) is absolutely similar - with the opposite sign under the exponent, due to the opposite sign of the exponent in the reciprocal Fourier transform, so that the simultaneous shift by both \( X \) and \( P \) may be achieved by the following translation operator:

\[
\hat{T}_\alpha = \exp\left\{ i \frac{P\hat{x} - \hat{p}X}{\hbar} \right\},
\]

(5.144)

As we already know, for a harmonic oscillator the creation-annihilation operators are more natural, so that we may use Eqs. (96) and (99) to recast Eq. (144) as

\[
\hat{T}_\alpha = \exp\left\{ \alpha\hat{a}^\dagger - \alpha^*\hat{a} \right\}, \quad \text{with} \quad \hat{T}_\alpha^\dagger = \exp\left\{ \alpha^*\hat{a} - \alpha\hat{a}^\dagger \right\},
\]

(5.145)

where the \( c \)-number \( \alpha \) (generally, a function of time) is defined by Eq. (133). Now, according to Eq. (139), we may form the Glauber state’s ket-vector just as

\[
|\alpha\rangle = \hat{T}_\alpha|0\rangle.
\]

(5.146)

This formula looks nice and simple, but making practical calculations (say, calculating expectation values of variables) with the translation operator (144) is not too easy because of its exponent-of-operators form. Fortunately, it turns out that a much simpler representation for the Glauber state is possible. To show this, let us start with the following general (and very useful) property of exponential functions of operators: if

\[
[A, B] = \mu \hat{A},
\]

(5.147)

(where \( \hat{A} \) and \( \hat{B} \) are arbitrary operators, and \( \mu \) is a \( c \)-number), then

\[
\exp\{+\hat{A}\} \hat{B} \exp\{-\hat{A}\} = \hat{B} + \mu \hat{A}.
\]

(5.148)

Let us apply Eqs. (147)-(148) to two cases, both with

\[
\hat{A} = \alpha^*\hat{a} - \alpha\hat{a}^\dagger, \quad \text{so that} \quad \exp\{+\hat{A}\} = \hat{T}_\alpha^\dagger, \quad \exp\{-\hat{A}\} = \hat{T}_\alpha.
\]

(5.149)

First, let us take \( \hat{B} = \hat{I} \), then Eq. (147) is valid with \( \mu = 0 \), and Eq. (148) yields

\[
\hat{T}_\alpha^\dagger \hat{T}_\alpha = \hat{I},
\]

(5.150)

This equality means that the translation operator is unitary – not a big surprise, because if we shift a classical point on the complex phase plane by \((+\alpha)\) and then by \((-\alpha)\), we certainly must come back to the initial position. Relation (150) means merely that this fact is also true for any quantum state as well.

Second, let us take \( \hat{B} = \hat{a} \); in order to verify Eq. (147) and find the corresponding \( \mu \), let us calculate the commutator. Using, at the due stage of calculation, Eq. (104), we get

\[
[\hat{A}, \hat{B}] = [\alpha^*\hat{a} - \alpha\hat{a}^\dagger, \hat{a}] = -\alpha [\hat{a}^\dagger, \hat{a}] = \alpha \hat{a},
\]

(5.151)

\[\text{\footnote{The proof of Eq. (148) may be readily achieved by expanding operator } \hat{f}(\lambda) \equiv \exp\{+\lambda\hat{A}\} \hat{B} \exp\{-\lambda\hat{A}\} \text{ in the Taylor series in the } c \text{-number parameter } \lambda, \text{ and then evaluating the result at } \lambda = 1.}\]
so that in this case $\mu = \alpha$, and Eq. (148) yields
\[ \hat{\tau}_a \hat{a}^\dagger \hat{\tau}_a = \hat{a} + \alpha \hat{a}. \] (5.152)

We have approached the summit of this beautiful calculation. Let us consider operator
\[ \hat{\tau}_a \hat{\tau}_a^\dagger \hat{\tau}_a . \] (5.153)
Using Eq. (150), we may reduce this expression to $\hat{a} \hat{\tau}_a$, while the application of Eq. (151) to the same expression yields $\hat{\tau}_a \hat{a} + \alpha \hat{\tau}_a$. Hence, we get the following operator equality
\[ \hat{a} \hat{\tau}_a = \hat{\tau}_a \hat{a} + \alpha \hat{\tau}_a , \] (5.154)
which may be applied to any state. Now acting by these two operators on the ground state $|0\rangle$ and using the facts that $\hat{a} |0\rangle$ is the null-state, while $\hat{\tau}_a |0\rangle = |\alpha\rangle$, we finally get a very simple and elegant result:42
\[ \hat{a} |\alpha\rangle = \alpha |\alpha\rangle . \] (5.155)

Thus any Glauber state is just one of eigenstates of the annihilation operator, namely the one with the eigenvalue equal to parameter $\alpha$, i.e. to the complex representation (133) of the classical state which is the center of the Glauber state’s distribution.43 This fact makes the calculations of the Glauber state properties much simpler. As the simplest example, let us use Eq. (155) to find $\langle x \rangle$ in the Glauber state:
\[ \langle x \rangle = \langle \alpha | x \rangle = \frac{x_0}{\sqrt{2}} (\alpha \langle \hat{a} + \hat{a}^\dagger | \alpha \rangle) = \frac{x_0}{\sqrt{2}} (\alpha \langle \hat{a} | \alpha \rangle + \alpha \langle \hat{a}^\dagger | \alpha \rangle) . \] (5.156)
In the first term in the parentheses, we can apply Eq. (155) directly, while in the second term, we can use the bra-counterpart of that relation, $\langle \alpha | \hat{a}^\dagger = \langle \alpha | \alpha^*$. Now assuming that the Glauber state is normalized, $\langle \alpha | \alpha \rangle = 1$, and using Eq. (133), we get
\[ \langle x \rangle = \frac{x_0}{\sqrt{2}} (\alpha \langle | \alpha \rangle + \alpha \langle | \alpha \rangle^* ) = \frac{x_0}{\sqrt{2}} (\alpha + \alpha^*) = X , \] (5.157)
Acting absolutely similarly, we may readily extend this sanity check to verify that $\langle p \rangle = P$, and that $\delta x$ and $\delta p$ indeed obey Eq. (138).

As a more thorough sanity check, let us use Eq. (155) to re-calculate Glauber state’s wavefunction (139). Inner-multiplying both sides of that relation by bra-vector $\langle x |$, and using definition (98a) of the annihilation operator, we get

42 It is also rather counter-intuitive. Indeed, according to Eq. (122), the annihilation operator $\hat{a}$, acting on a Fock state $n$, “beats it down” to the lower-energy state $(n - 1)$ – see Eq. (119). However, according to Eq. (155), its action on a Glauber state $\alpha$ does not lead to the state change and hence to an energy decrease! The resolution of this paradox may be achieved via representation of the Glauber state as a series of Fock states – see Eq. (165) below. Operator $\hat{a}$ indeed transfers each Fock component to a lower-energy state, but it also re-weighs each term of the expansion, so that the complete energy of the Glauber state remains constant.

43 Note that the spectrum of eigenvalues $\alpha$ of eigenproblem (155) is continuous – it may be any complex number!
\[
\frac{1}{\sqrt{2x_0}} \langle x \left( \hat{x} + i \frac{\hat{p}}{m\omega_0} \right) \rangle \alpha = \alpha \langle x | \alpha \rangle. \quad (5.158)
\]

Since \( \langle x | \) is the bra-vector of the eigenstate of the Hermitian operator \( \hat{x} \), they may be swapped, with the operator giving its eigenvalue \( x \); acting on that bra-vector by the (local!) operator of momentum, we have to use it in the coordinate representation (63). As a result, we get
\[
\frac{1}{\sqrt{2x_0}} \left( x \langle x | \alpha \rangle + \frac{\hbar}{m\omega_0} \frac{\partial}{\partial x} \langle x | \alpha \rangle \right) = \alpha \langle x | \alpha \rangle. \quad (5.159)
\]

But \( \langle x | \alpha \rangle \) is nothing else than the Glauber state’s wavefunction \( \Psi_\alpha \), so that Eq. (153) gives for it a first-order differential equation
\[
\frac{1}{\sqrt{2x_0}} \left( x \Psi_\alpha + \frac{\hbar}{m\omega_0} \frac{\partial}{\partial x} \Psi_\alpha \right) = \alpha \Psi_\alpha. \quad (5.160)
\]

Chasing \( \Psi_\alpha \) and \( x \) to the opposite sides of the equation, and using definition (133) of parameter \( \alpha \), we may bring this equation to a form
\[
\frac{\partial \Psi_\alpha}{\Psi_\alpha} = \frac{m\omega_0}{\hbar} \left[ -x + \left( X + i \frac{P}{m\omega_0} \right) \right] \frac{\partial x}{\partial x}. \quad (5.161)
\]

Integrating both parts, we return to Eq. (139) that had been derived by wave-mechanics means.

Now that we can use Eq. (155) for finding coefficients \( \alpha_n \) in the expansion (136) of the Glauber state \( \alpha \) in series over the Fock states \( n \). Plugging Eq. (136) into each side of Eq. (155), using the first of Eq. (122) in the left-hand part, and requiring the coefficients at each ket-vector \( |n\rangle \) in both parts to be equal, we get the following recurrence relation for the coefficients:
\[
\alpha_{n+1} = \frac{\alpha}{(n + 1)^{1/2}} \alpha_n. \quad (5.162)
\]

Assuming some value of \( \alpha_0 \), and applying the relation sequentially for \( n = 1, 2, \ldots \), we get
\[
\alpha_n = \frac{\alpha^n}{(n!)^{1/2}} \alpha_0. \quad (5.163)
\]

Now we can find \( \alpha_0 \) from the normalization requirement (137), getting
\[
|\alpha_0|^2 \sum_{n=0}^{\infty} \frac{\alpha^{2n}}{n!} = 1. \quad (5.164)
\]

In this sum, we may readily recognize the Taylor expansion of \( \exp\{ |\alpha|^2 \} \), so that the final result (besides an arbitrary common phase multiplier) is
\[
|\alpha\rangle = \exp \left\{ -\frac{|\alpha|^2}{2} \right\} \sum_{n=0}^{\infty} \frac{\alpha^n}{(n!)^{1/2}} |n\rangle. \quad (5.165)
\]
It means in particular that the probability $W_n = \alpha_n \alpha_n^*$ of finding the system energy on $n$-th energy level (119) obeys the well-known Poisson distribution (Fig. 7):

$$W_n = \frac{(\langle n \rangle)^n}{n!} e^{-\langle n \rangle}, \quad (5.166)$$

where in our particular case

$$\langle n \rangle = |\alpha|^2. \quad (5.167)$$

For applications, perhaps the most important mathematical property of this distribution is

$$\delta n = \langle n \rangle^{1/2}; \quad (5.168)$$

note also that at $\langle n \rangle >> 1$, and hence $\delta n << \langle n \rangle$, the Poisson distribution approaches the Gaussian (“normal”) one.

Now let us discuss the evolution of the Glauber state in time. In the Schrödinger language, it is completely described by dynamics (131) of the $c$-number shifts $\hat{X}(t)$ and $\hat{P}(t)$ participating in wavefunction (139). Note again that, in contrast to the spread of the wave packet of a free particle, discussed in Sec. 2.2, in the harmonic oscillator the Gaussian packet of special width (138) does not spread at all!

An alternative and equivalent way of dynamics description is to use the Heisenberg equation of motion. As Eqs. (42) and (48) tell us, such equations for Heisenberg operators of coordinate and momentum they have to be similar to the classical equation (131):

$$\dot{\hat{x}}_H = \frac{\hat{p}_H}{m}, \quad \dot{\hat{p}}_H = -m\omega_0^2 \hat{x}_H. \quad (5.169)$$

Now using Eqs. (98), for the Heisenberg-picture creation and annihilation operators we get equations

$$\hat{\alpha}_H = -i\omega_0 \hat{\alpha}_H^*, \quad \hat{\alpha}_H^\dagger = +i\omega_0 \hat{\alpha}_H^\dagger, \quad (5.170)$$

that are completely similar for the classical equation (134) for the $c$-number parameter $\alpha$ and its complex conjugate, and hence have the solutions identical to Eq. (135):
\[
\hat{a}_\| (t) = \hat{a}_\| (0)e^{-i\omega_0 t}, \quad \hat{a}_\| (t) = \hat{a}_\| (0)e^{i\omega_0 t}.
\]  
(5.171)

As was discussed in Sec. 4.6, such equations are very convenient because they enable simple calculation of time evolution of observables for any initial state of the oscillator (Fock, Glauber, or any other) using Eq. (4.191). Applied to a Glauber state \(\alpha(0)\), such calculation gives the same results as have already been derived earlier in this section, in particular confirms that the Gaussian wave packet of the special width (138) does not spread in time.

Now let us consider what happens if the initial wave packet is still Gaussian, but has a different width, say \(\Delta x < x_0/\sqrt{2}\). As we already know from Sec. 2.2, the momentum spread \(\Delta \hat{p}\) will be correspondingly larger, still with the smallest uncertainty product: \(\Delta x \Delta \hat{p} = \hbar/2\). Such squeezed ground states, with zero expectation values of \(x\) and \(\hat{p}\), may be generated from the Fock/Glauber ground state:

\[
|\sigma\rangle = \hat{S}_\sigma |0\rangle,
\]  
(5.172a)

using the so-called squeezing operator,

\[
\hat{S}_\sigma = \exp\left\{\frac{1}{2}\left(\sigma^{*} \hat{a}\hat{a} - \sigma \hat{a}^{\dagger}\hat{a}^{\dagger}\right)\right\},
\]  
(5.172b)

which depends on a complex c-number parameter \(\sigma = re^{i\theta}\). Parameter’s modulus \(r\) determines the squeezing degree; it is straightforward to use Eq. (172) for checking that if \(\sigma\) is real (\(\theta = 0, \xi = r\)), then

\[
\Delta x = x_0 e^{-r} = \left(\frac{\hbar}{2m\omega_0}\right)^{1/2} e^{-r}, \quad \Delta \hat{p} = \frac{m\omega_0 x_0}{\sqrt{2}} e^{r} = \left(\frac{\hbar m\omega_0}{2}\right)^{1/2} e^{r}, \quad \text{so that} \quad \Delta x \Delta \hat{p} = \frac{\hbar}{2}.
\]  
(5.173)

On the phase plane (Fig. 6), this state, with \(r > 0\), may be represented by an oval spot squeezed along axis \(x\) (hence the state’s name) and stretched along axis \(\hat{p}\); the same formulas but with \(r < 0\) describe the opposite squeezing. On the other hand, phase \(\theta\) of the squeeze parameter \(\sigma\) determines the angle \(\theta/2\) of oval’s turn about the phase plane origin – see the magenta ellipse in Fig. 6; if \(\theta \neq 0\), Eqs. (173) are valid for variables \(\{x', p'\}\) obtained from \(\{x, p\}\) via clockwise rotation by that angle. For any of such origin-centered squeezed states, time evolution is reduced to an increase of the angle with rate \(\omega_0\), i.e. to the clockwise rotation of the ellipse, without its deformation, with angular velocity \(\omega_0\) – see the magenta arrows in Fig. 6. As a result, uncertainties \(\Delta x\) and \(\Delta \hat{p}\) oscillate in time with double frequency \(2\omega_0\), while their product is constant at its minimal possible value \(\hbar/2\).

Such squeezed ground states have important implications for quantum measurements (see Sec. 7.7 below) and may be formed, for example, by parametric excitation of the oscillator,\(^{44}\) with a parameter modulation depth close to, but still below the threshold of parametric oscillations excitation. Unfortunately, I do have time for a further discussion of this interesting topic,\(^{45}\) but still need to mention

\(^{44}\) For a discussion and classical theory of this effect, see, e.g., CM Sec. 4.5.
a more general class of squeezed states, centered to an arbitrary point \( \{X, P\} \) rather than the origin, that may be formed by an additional action of the displacement operator (144) on the squeezed ground state (172). Calculations similar to those that led us from Eq. (145) to Eq. (155), but now for the product operator \( \hat{a} \hat{a}^\dagger \), rather than bare \( \hat{a} \), show that such a general squeezed state is an eigenstate of the following mixed operator

\[
\hat{b} \equiv \hat{a} \cosh r + \hat{a}^\dagger e^{i\theta} \sinh r ,
\]

with eigenvalue

\[
\beta = \alpha \cosh r + \alpha^* e^{i\theta} \sinh r .
\]

For the particular case \( \alpha = 0 \), Eq. (174b) yields \( \beta = 0 \), i.e. the action of operator (174a) on the squeezed ground state \( \varphi \) with the same \( r \) and \( \theta \) yields the null-state, thus generalizing Eq. (118), which is valid for the “usual” (non-squeezed) ground state.

5.6. Revisiting spherically-symmetric problems

One more blank spot to fill has been left in our study of wave mechanics of spherically-3D symmetric systems in Sec. 3.6. Indeed, while the eigenfunctions describing axially-symmetric 2D systems, and the azimuthal components of those in spherically-symmetric 3D systems, are very simple,

\[
\psi_m = \frac{1}{(2\pi)^{1/2}} e^{im\varphi} , \quad m = 0, \pm 1, \pm 2, ...
\]

the polar components of the eigenfunctions in the latter case (i.e., of spherical harmonics) include the associate Legendre functions \( P_l^m(\cos \theta) \) that may be expressed via elementary functions only indirectly – see Eqs. (3.165) and (3.168). This makes all the calculations less than transparent and, in particular, does not allow a clear insight into the origin of the very simple eigenvalue spectrum – see, e.g., Eq. (3.163). The bra-ket formalism, applied to the angular momentum operator, allows one to get such insight, and also produces a very convenient tool for many calculations involving spherically-symmetric potentials.

Let us start from using the correspondence principle to spell out the quantum-mechanical operator of the orbital angular momentum \( \mathbf{L} \equiv r \times \mathbf{p} \) of a point particle:

\[
\hat{\mathbf{L}} \equiv \hat{\mathbf{r}} \times \hat{\mathbf{p}} = \begin{vmatrix}
\mathbf{n}_x & \mathbf{n}_y & \mathbf{n}_z \\
\hat{x} & \hat{y} & \hat{z} \\
\hat{p}_x & \hat{p}_y & \hat{p}_z
\end{vmatrix} , \quad \text{i.e., } \hat{L}_x \equiv \hat{y} \hat{p}_z - \hat{z} \hat{p}_y , \quad \text{etc.,}
\]

From this definition, we can readily calculate the commutation relations for all Cartesian components of operators \( \hat{\mathbf{L}}, \hat{\mathbf{r}}, \text{ and } \hat{\mathbf{p}} \); for example,

\[
[\hat{L}_x, \hat{y}] = [\hat{y} \hat{p}_z - \hat{z} \hat{p}_y, \hat{y}] = -\hat{z} [\hat{p}_y, \hat{y}] = i\hbar \hat{z} ,
\]

etc. Using the sequential numbering of coordinate axes \( (x = r_1, \text{ etc.}) \), the summary of these calculations may be presented in similar, compact (and beautiful!) forms:
\[
\begin{align*}
\left\{ \hat{L}_j, \hat{r}_j \right\} &= i\hbar \hat{r}_j \epsilon_{jj'}, \\
\left\{ \hat{L}_j, \hat{p}_{jj'} \right\} &= i\hbar \hat{p}_{jj'} \epsilon_{jj'}, \\
\left\{ \hat{L}_j, \hat{L}_{jj'} \right\} &= i\hbar \hat{L}_{jj'} \epsilon_{jj'},
\end{align*}
\]  
(5.178)

where each of indices \( j \) and \( j' \) and \( j'' \) may take values 1, 2, and 3, \( j'' \) is the complementary index of the same set (not equal to either \( j \) or \( j' \)), and \( \epsilon_{jj'} \) is the Levi-Civita symbol (or “permutation symbol”).

Also introducing in the natural way a (scalar!) operator of the observable \( \hat{L}^2 = \left| \mathbf{L} \right|^2 \),

\[
\hat{L}^2 \equiv \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2,
\]  
(5.179)

it is straightforward to check that this operator commutes with each of the Cartesian components:

\[
\left[ \hat{L}^2, \hat{L}_j \right] = 0. 
\]  
(5.180)

This result, at the first sight, may seem to contradict the last of Eqs. (178). Indeed, haven’t we learned in Sec. 4.5 that commuting operators (e.g., \( \hat{L}^2 \) and any of \( \hat{L}_j \)) share their eigenstate sets? If yes, shouldn’t that mean that this set has to be common for all 4 operators? The resolution in this paradox may be found in the condition that was mentioned just after Eq. (4.138), but (sorry!) not sufficiently emphasized there. According to that relation, if an operator has degenerate eigenstates (i.e. if \( A_j = A_{j'} \) even for \( j \neq j' \)), they should not be necessarily shared by another compatible operator. This is exactly the situation with the orbital angular momentum operators, that may be schematically shown at a Venn diagram (Fig. 8): the set of eigenstates of operator \( \hat{L}^2 \) is highly degenerate, and is broader than those of the component operators \( \hat{L}_j \) (that, as will be shown below, are non-degenerate until we consider particle’s spin).

Fig. 5.8. Venn diagram showing (schematically) the partitioning of the set of eigenstates of operator \( \hat{L}^2 \). Each inner sector corresponds to the states shared with one of Cartesian component operators \( \hat{L}_j \), while the outer (shaded) ring presents the eigenstates of \( \hat{L}^2 \) that are not shared with either of \( \hat{L}_j \) - e.g., all linear combinations of eigenstates of different component operators.

---

46 See, e.g., MA Eq. (13.2).
47 The importance of this issue stems from the following fact: it is easy (and is hence left to the reader :-) to use Eqs. (5.178) to prove that operators of all \( L_j \) and of \( \hat{L}^2 \) commute with the Hamiltonian of a particle in the spherically-symmetric potential \( U(r) \), and hence all their eigenstates are the stationary states in such a field.
48 This is just a particular example of Venn diagrams (introduced in the 1880s by J. Venn) that show possible relations (such as intersections, unions, complements, etc.) between various sets of objects, and are a very useful tool in the general set theory.
49 Note that this particular result is consistent with the classical picture of the angular momentum vector: even when its length is fixed, the vector may be oriented in various directions, corresponding to different values of its Cartesian components. However, in the classical picture, all these component may be fixed simultaneously, while in the quantum picture this is not true.
Let us focus on just one of these 3 joint sets of eigenstates – by tradition, of operators $\hat{L}^2$ and $\hat{L}_z$. (This tradition is due to the canonical form of spherical coordinates, in which the polar angle is measured from axis $z$. Indeed, using Eqs. (63), in the coordinate representation we get the following expression,

$$\hat{L}_z \equiv \hat{x}p_y - \hat{y}p_x = x\left(-i\hbar \frac{\partial}{\partial y}\right) - y\left(-i\hbar \frac{\partial}{\partial x}\right) = -i\hbar \frac{\partial}{\partial \phi}. \tag{5.181}$$

Writing the standard eigenproblem for the operator in this representation, $\hat{L}_z \psi_m = L_z \psi_m$, we see that it is satisfied by eigenfunctions (175), with eigenvalues $L_z = \hbar m$ - at was already conjectured in Sec. 3.5.) More specifically, let us consider a set of eigenstates $\{l, m\}$ corresponding to a certain degenerate eigenvalue of operator $\hat{L}_z$ but all possible eigenvalues of operator $\hat{L}_z$, i.e. all possible quantum numbers $m$. (At this point, $l$ is just some parameter that determines the eigenvalue of $\hat{L}_z$; it will be defined more explicitly in a minute.) In order to analyze this set, it is instrumental to introduce the so-called ladder (also called, respectively, “raising” and “lowering”) operators

$$\hat{L}_z \equiv \hat{L}_z \pm i\hat{L}_y \tag{5.182}$$

- note a substantial similarity between this definition and Eqs. (98). It is straightforward to use this definition and the last of Eqs. (178) to calculate the following commutators:

$$[\hat{L}_z, \hat{L}_z] = 2\hbar \hat{L}_z, \quad [\hat{L}_z, \hat{L}_z] = \pm \hbar \hat{L}_z, \tag{5.183}$$

and use Eq. (179) to prove another important relation:

$$\hat{L}^2 = \hbar \hat{L}_z + \hat{L}_z^2 + \hat{L}_z \hat{L}_z. \tag{5.184}$$

Now let us rewrite the last of Eqs. (183) as

$$\hat{L}_z \hat{L}_z = \hat{L}_z \hat{L}_z \pm \hbar \hat{L}_z, \tag{5.185}$$

and act by its both parts on the ket-vector $|l, m\rangle$ of the set specified above:

$$\hat{L}_z \hat{L}_z |l, m\rangle = \hat{L}_z \hat{L}_z |l, m\rangle \pm \hbar \hat{L}_z |l, m\rangle. \tag{5.186}$$

Since eigenvalues of operator $\hat{L}_z$ are equal to $\hbar m$, in the first term of the right-hand part we may write

$$\hat{L}_z |l, m\rangle = \hbar m |l, m\rangle. \tag{5.187}$$

With that, Eq. (186) may be recast as

$$\hat{L}_z (\hat{L}_z |l, m\rangle) = \hbar (m \pm 1)(\hat{L}_z |l, m\rangle) \tag{5.188}$$

In a spectacular similarity with Eqs. (111)-(112) for the harmonic oscillator, Eq. (188) means that states $\hat{L}_z |l, m\rangle$ are also the eigenstates of operator $\hat{L}_z$, corresponding to eigenvalues $(m \pm 1)$. Thus the ladder operators act exactly as the creation and annihilation operators in the oscillator, moving the system up or down a ladder of eigenstates (Fig. 9). The most significant difference is that now the state
ladder must end in both directions, because an infinite increase of \(|m|\), with whatever sign, would cause the expectation values of operator

\[
\hat{L}_x^2 + \hat{L}_y^2 = \hat{L}^2 - \hat{L}_z^2,
\]

which corresponds to a non-negative observable, to become negative. Hence there should be two states on both ends of the ladder, \(|l, m_{\text{max}}\rangle\) and \(|l, m_{\text{min}}\rangle\), for whom

\[
\hat{L}_+ |l, m_{\text{max}}\rangle = 0, \quad \hat{L}_- |l, m_{\text{min}}\rangle = 0.
\]

Due to the symmetry of the whole problem with respect to the replacement \(m \rightarrow -m\), we should have \(m_{\text{min}} = -m_{\text{max}}\). This \(m_{\text{max}}\) is exactly the quantum number that is traditionally called \(\ell\), so that

\[
-l \leq m \leq +l.
\]

Due to the symmetry of the whole problem with respect to the replacement \(m \rightarrow -m\), we should have \(m_{\text{min}} = -m_{\text{max}}\). This \(m_{\text{max}}\) is exactly the quantum number that is traditionally called \(\ell\), so that

\[
-l \leq m \leq +l.
\]

Evidently, this relation of quantum numbers \(m\) and \(\ell\) is compatible with the almost-classical image of various orientations of the angular momentum vector of the same length in various directions, with its \(z\)-component taking several \((2\ell + 1)\) possible values \(\hbar m\). In this simple picture, however, \(L^2\) would be equal to square of \((L_z)_{\text{max}}\), i.e. to \((\hbar)^2\); however, this is not so. Indeed, applying the operator equality (184) to the top state \(|l, m_{\text{max}}\rangle \equiv |l, \ell\rangle\), we get

\[
\hat{L}^2 |l, \ell\rangle = \hbar \hat{L}_x |l, \ell\rangle + \hat{L}_y^2 |l, \ell\rangle + \hat{L}_z |l, \ell\rangle = \hbar^2 |l, \ell\rangle + \hbar^2 l^2 |l, \ell\rangle + 0
\]

Since by our initial assumption, all eigenvectors \(|l, m\rangle\) correspond to the same eigenvalue of operator \(\hat{L}^2\), this result means that all these eigenvalues are equal to \(\hbar^2 (l + 1)\). Just as in case of the spin-\(1/2\) vector operators, the deviation of this result from \(\hbar^2 l^2\) may be interpreted as the result of unavoidable uncertainties (“fluctuations”) of the \(x\)- and \(y\)-components of the angular momentum, that give a finite positive contribution to \(L^2\) even if the angular momentum vector is aligned in the best possible way with the \(z\)-axis.
Now let us compare our results with those of Sec. 3.6. Using the expression of Cartesian coordinates via the spherical ones exactly as was done in Eq. (181), we get the following expressions for the ladder operators (182) in the coordinate representation:

\[
\hat{L}_z = 
\frac{\hbar e^{\pm i\varphi}}{\sqrt{2}} \left( \pm \frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \varphi} \right).
\]  

(5.193)

Now plugging this equation, together with Eq. (181), into Eq. (184), we get

\[
\hat{L}^2 = -\hbar^2 \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right].
\]

(5.194)

But this is exactly the operator (besides its division by constant parameter \(2mR^2\)) that stands in the left-hand part of Eq. (3.156). Hence that equation, which was explored by the “brute-force” (wave-mechanical) approach in Sec. 3.6, may be understood as the eigenproblem for operator \(\hat{L}^2\) in the coordinate representation, with eigenfunctions \(Y_l^m(\theta, \varphi)\) corresponding to eigenkets \(\{l, m\}\), and eigenvalues \(L_l^2 = 2mR^2E_l\). As a reminder, the main result of that, rather involved analysis was expressed by Eq. (3.163), which now may be rewritten as

\[
L_l^2 = 2mR^2E_l = \hbar^2 l(l+1),
\]

(5.195)
in a full agreement with what was obtained in this section by much more efficient means based on the bra-ket formalism. In particular, it is fascinating to see how easy are now many operations with eigenvectors \(|l, m\rangle\), albeit wavefunctions of these states, spherical harmonics \(Y_l^m(\theta, \varphi)\), have rather complex spatial behavior – please have one more look at Eq. (3.171) and Fig. 3.19.50

5.7. Spin and its addition to orbital angular momentum

Surprisingly, the theory described in the last section is useful for much more than orbital motion analysis. In particular, it helps to generalize the spin-½ results discussed in Chapter 4 to other values of spin \(s\) – the parameter still has to be defined. For that, let us notice that the commutation relations that were derived, for \(s = ½\), from the Pauli matrix properties, may be rewritten in exactly the same form as Eqs. (178) and (180) for the orbital momentum:

\[
[\hat{S}_j, \hat{S}_j' = i\hbar \delta_{jj'} \epsilon_{jj'}, \quad [\hat{S}_j^2, \hat{S}_j] = 0.
\]

(5.196)

It has been postulated (and confirmed by numerous experiments) that these relations hold true for any quantum particle. Now note that all the calculations of the last section have been based \textit{almost} exclusively on such relations – the exception will be discussed imminently. Hence, we may repeat them for spin operators, and get the relations similar to Eq. (187) and (192):

---

50 The reader is challenged to use the commutation relations discussed above to prove one more important property of the common eigenstates of operators \(\hat{L}_x\) and \(\hat{L}^2\):

\[
\langle l, m | \hat{S}_j | l', m' \rangle = 0, \quad \text{if either } l' \neq l \pm 1, \text{ or } m \neq m', \text{ or both.}
\]

This property is the basis of the \textit{selection rules} for dipole quantum transitions, to be discussed later in the course, especially in Sec. 9.3.
where \( m_s \) is a quantum number similar to the orbital number \( m \), and the non-negative constant \( s \) is defined as the maximum value of \( |m_s| \). This parameter is exactly what is called *particle’s spin* - in the narrow sense of the word.

Now let us return to the only part of our orbital moment calculations that has *not* been derived from the commutation relations. This was the fact, based on solution (175) of the orbital motion problems, that quantum numbers \( m \) (the analog of \( m_s \)) are integer. For spin, we do not have such a solution, so that the spectrum of numbers \( m_s \) (and hence its limits \( \pm s \)) should be found from the more loose requirement that the eigenstate ladder, extending from \(-s\) to \(+s\), has an integer number of steps. Hence, \( 2s \) has to be integer, i.e. spin \( s \) of a quantum particle may be either integer (as it is, for example, for photons and gluons), or half-integer (e.g., for all quarks and leptons including electrons).  

For \( s = \frac{1}{2} \), this picture yields all spin properties of electron that were derived in Chapter 4 from postulate (4.117). In particular, operators \( \hat{S}_x \) and \( \hat{S}_z \) have only 2 common eigenstates, with \( S_z = \hbar m_s = \pm \hbar/2 \), and both with \( S_x = s(s + 1)\hbar^2 = (3/4)\hbar^2 \). Note that this analogy with the angular momentum sheds a new light on the symmetry properties of electrons. Indeed, the fact that \( m \) in Eq. (175) is integer was derived in Sec. 3.5 from the requirement that making a full circle around axis \( z \), we should find a similar value of wavefunction \( \psi_m \), which differs from the initial one by an inconsequential factor \( \exp{2\pi im} \). With the replacement \( m \to m_s = \pm \frac{1}{2} \), such operation would multiply the wavefunction by \( \exp{\pm \pi i} \), i.e. reverse its sign. On course, spin cannot be described by a usual wavefunction, but this odd parity of electrons (and all other spin-\( \frac{1}{2} \) particles) is clearly revealed in multiparticle systems – see Chapter 8.

Now we are sufficiently equipped to analyze particles that have both the orbital momentum and the spin. In classical mechanics, such a particle would be characterized by the *total angular momentum* vector \( \mathbf{J} = \mathbf{L} + \mathbf{S} \). Following the correspondence principle, we may make an assumption that quantum-mechanical properties of this observable may be analyzed using the similarly defined vector operator:

\[
\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}},
\]

with Cartesian components

\[
\hat{J}_x \equiv \hat{L}_x + \hat{S}_x,
\]

\[
\hat{J}_y \equiv \hat{L}_y + \hat{S}_y,
\]

\[
\hat{J}_z \equiv \hat{L}_z + \hat{S}_z,
\]

etc, and the magnitude squared equal to

\[
\hat{J}^2 \equiv \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2.
\]

Let us examine the properties of this vector operator. Since its two components describe different degrees of freedom of the particle (again, you may say “belong to different Hilbert spaces”), they may be considered as completely commuting:

\[
\left[ \hat{L}_j, \hat{S}_j \right] = 0, \quad \left[ \hat{L}_j^2, \hat{S}_j^2 \right] = 0.
\]

\[51\] As a reminder, in the Standard Model of particle physics, such hadrons as mesons and baryons (notably including protons and neutrons) are essentially composite particles, with the spin equal to the sum of its component quark spins. However, at non-relativistic energies, protons and neutrons may be considered fundamental particles with \( s = \frac{1}{2} \).
These above equalities are sufficient to derive the commutation rules of the total angular momentum, and, not surprisingly, they turn out to be absolutely similar to those of its components:

$$\left[ \hat{J}_x, \hat{J}_y \right] = i \hbar \hat{J}_z \varepsilon_{xzy}, \quad \left[ \hat{J}_z, \hat{J}_x \right] = 0. \quad (5.202)$$

Now repeating all arguments of the last section, we may derive the following expressions for the common eigenstates of operators $\hat{J}^2$ and $\hat{J}_z$:

$$J_z | j, m_j \rangle = \hbar m_j | j, m_j \rangle, \quad \hat{J}^2 | j, m_j \rangle = \hbar^2 j(j+1) | j, m_j \rangle, \quad 0 \leq j, \quad -j \leq m_j \leq +j, \quad (5.203)$$

where $j$ and $m_j$ are new quantum numbers. Repeating the arguments made for $m_s$, we may conclude that $j$ and $m_j$ may be either integer or half-integer.

Before we proceed, one remark on notation: it is very convenient to use the same letter $m$ for numbering eigenstates of all momentum components participating in Eq. (199), with corresponding indices ($j$, $l$, and $s$), in particular, to replace what we called $m$ with $m_l$. With this replacement, the main results of the last section may be summarized in the form similar to Eqs. (197) and (203):

$$\hat{L}_z | l, m_l \rangle = \hbar m_l | l, m_l \rangle, \quad \hat{L}^2 | l, m_l \rangle = \hbar^2 l(l+1) | l, m_l \rangle, \quad 0 \leq l, \quad -l \leq m_l \leq +l. \quad (5.204)$$

In order to understand which eigenstates used in Eqs. (197), (203), and (204) are compatible with each other, let us use Eqs. (198)-(202) to calculate the mutual commutators of the operators squared and their $z$-components. The result is

$$\left[ \hat{J}^2, \hat{J}^2 \right] = 0, \quad \left[ \hat{J}^2, \hat{S}^2 \right] = 0, \quad (5.205)$$

$$\left[ \hat{J}^2, \hat{L}_z \right] \neq 0, \quad \left[ \hat{J}^2, \hat{S}_z \right] \neq 0. \quad (5.206)$$

This result may be presented schematically on the following Venn diagram (Fig. 10), in which the crossed arrows indicate the only non-commuting pairs of operators.

![Venn diagram](image)  
Fig. 5.10. Venn diagram for angular momentum operators, and their mutually-commuting groups.

This means that just as for each component angular momentum ($\bf{J}$, $\bf{L}$, and $\bf{S}$) considered separately we could select a group of common eigenstates for its magnitude squared and the $z$-component, we also may find eigenstates shared by two broader groups of operators, encircled with colored lines in Fig. 10. The first group (within the red circle), consists of all operators but $\hat{J}_z$. This means that there are eigenstates shared by 5 remaining operators, and they may be characterized by certain values of the corresponding quantum numbers: $l$, $m_l$, $s$, $m_s$, and $m_j$. Actually, only 4 of these
numbers are independent, because due to Eq. (199) for these compatible operators, for each eigenstate of the group, their “magnetic” quantum numbers \( m \) have to satisfy the following relation:

\[
m_j = m_l + m_s.
\] (5.207)

Hence the common eigenstates of the operators of this group are fully defined by just 4 quantum numbers, for example, \( l, m_l, s, \) and \( m_s \). For some calculations, especially those for systems whose Hamiltonians include only operators of this group, it is convenient to use this set of eigenstates as the basis; frequently this is called the \textit{uncoupled representation}.

However, in some situations we cannot ignore interactions between the orbital and spin degrees of freedom (in the common jargon, the \textit{spin-orbit coupling}), which leads in particular to splitting (called the \textit{fine structure}) of atomic energy levels even in the absence of external magnetic field. I will discuss these effects in detail in the next chapter, and now will only note that they may be described by a separate term, proportional to product \( \hat{L} \cdot \hat{S} \), in the system’s Hamiltonian. If this term is not negligible, the uncoupled representation becomes inconvenient. Indeed, writing

\[
\hat{J}^2 = (\hat{L} + \hat{S})^2 = \hat{L}^2 + \hat{S}^2 + 2\hat{L} \cdot \hat{S},
\] (5.208)

and looking at Fig. 10 again, we see that the operator \( \hat{L} \cdot \hat{S} \), describing the spin-orbit coupling, does not commute with operators \( \hat{L}_z \) and \( \hat{S}_z \). This means that stationary states of the system with such term in the Hamiltonian do not belong to the uncoupled representation basis. On the other hand, Eq. (208) shows that operator \( \hat{L} \cdot \hat{S} \) does commute with all 4 operators of another group, encircled with the blue line in Fig. 10. According to Eqs. (201), (202), and (205), all operators of that group also commute to each other, so that they have common eigenstates that may be marked by the corresponding quantum numbers, \( l, s, j, \) and \( m_j \). This group is the basis for the \textit{coupled representation} of particle’s state.

Excluding the quantum numbers \( l \) and \( s \), common for both groups, from notation, it is convenient to denote the common ket-vectors of each group as, respectively,

\[
\begin{align*}
|j, m_j\rangle, & \quad \text{for the uncoupled representation's basis,} \\
|m_l, m_s\rangle, & \quad \text{for the coupled representation's basis.}
\end{align*}
\] (5.209)

As we will see in the next chapter, for solution of some important problems (e.g., the fine structure of atomic spectra and the Zeeman effect), we will need the relation between the kets \( |j, m_j\rangle \) and the kets \( |m_l, m_s\rangle \). This relation may be represented as the usual linear superposition,

\[
|j, m_j\rangle = \sum_{m_l, m_s} \langle m_l, m_s | j, m_j \rangle |m_l, m_s\rangle,
\] (5.210)

whose bra-kets (\( c \)-numbers), essentially the elements of the unitary matrix of the transformation between two eigenstate bases (209), are called the \textit{Clebsch-Gordan coefficients}.

The best (though imperfect) classical interpretation of Eq. (210) I can offer is as follows. If the lengths of vectors \( \mathbf{L} \) and \( \mathbf{S} \) (in quantum mechanics associated with numbers \( l \) and \( s \), respectively), and also their scalar product \( \mathbf{L} \cdot \mathbf{S} \), are all fixed, then so is the length of vector \( \mathbf{J} = \mathbf{L} + \mathbf{S} \) (whose length in quantum mechanics is described by quantum number \( j \)). Hence, the classical image of a specific eigenket \( |j, m_j\rangle \), in which \( l, s, j, \) and \( m_j \) are all fixed, is a state in which \( L^2, S^2, J^2, \) and \( J_z \) are fixed.
However, this fixation still allows for an arbitrary rotation of the pair of vectors $\mathbf{L}$ and $\mathbf{S}$ (with a fixed angle between them, and hence fixed $\mathbf{L} \cdot \mathbf{S}$ and $\hat{J}^2$) about the direction of vector $\mathbf{J}$ - see Fig. 11.

However, this fixation still allows for an arbitrary rotation of the pair of vectors $\mathbf{L}$ and $\mathbf{S}$ (with a fixed angle between them, and hence fixed $\mathbf{L} \cdot \mathbf{S}$ and $\hat{J}^2$) about the direction of vector $\mathbf{J}$ - see Fig. 11.

Hence the components $L_z$ and $S_z$ in these conditions are not fixed, and in classical mechanics may take a continuum of values, two of which (with the largest and smallest possible values of $S_z$) are shown in Fig. 11. In quantum mechanics, these components are quantized, with their states represented by eigenkets $|m_l, m_s\rangle$, so that a linear combination of such kets is necessary to represent ket $|j, m_j\rangle$. This is exactly what Eq. (210) does.

Some of properties of the Clebsch-Gordan coefficients $\langle m_l, m_s|j, m_j\rangle$ may be readily established. For example, the coefficients do not vanish only if the involved magnetic quantum numbers satisfy Eq. (207); let us prove this fact.\footnote{One may think that Eq. (207) is a trivial corollary of Eq. (199). However, now we should be a bit more careful, because in the Clebsch-Gordan coefficients, these quantum numbers characterize different groups of eigenstates.} All matrix elements of the null-operator

$$\hat{J}_z - (\hat{L}_z + \hat{S}_z) = 0$$

(5.211)

should equal zero in any basis; in particular

$$\langle j, m_j|(\hat{J}_z - (\hat{L}_z + \hat{S}_z))|m_l, m_s\rangle = 0.$$  

(5.212)

Acting by operator $\hat{J}_z$ on the bra-vector, and by the sum $(\hat{L}_z + \hat{S}_z)$ on the ket-vector, we get

$$[m_j - (m_l + m_s)]\langle j, m_j|m_l, m_s\rangle = 0,$$

(5.213)

thus proving that $\langle m_l, m_s| j, m_j\rangle \equiv \langle j, m_j|m_l, m_s\rangle^* = 0$, if $m_j - (m_l + m_s) \neq 0$.

For the most important case of spin-$\frac{1}{2}$ particles ($s = \frac{1}{2}$, and hence $m_s = \pm \frac{1}{2}$), whose uncoupled representation basis includes $2 \times (2l + 1)$ states, restriction (207) enables the representation of all nonvanishing Clebsch-Gordan coefficients on the simple diagram shown in Fig. 12. Indeed, each coupled-representation eigenket $|j, m_j\rangle$, with $m_l = m_l + m_s = m_l \pm \frac{1}{2}$, may be related with non-zero Clebsch-Gordan coefficients to at most two uncoupled-representation eigenstates $|m_l, m_s\rangle$. Since $m_l$ may only take integer values from $-l$ to $+l$, $m_l$ may only take semi-integer values on the interval $[-l - \frac{1}{2}, l + \frac{1}{2}]$. Hence, by the definition of $j$ as $(m_l)_{\text{max}}$, its maximum value has to be $l + \frac{1}{2}$, and for $m_j = l + \frac{1}{2}$, this is the only possible value. This means that the uncoupled state with $m_l = l$ and $m_s = \frac{1}{2}$ should be identical to the coupled-representation state with $j = l + \frac{1}{2}$ and $m_j = l + \frac{1}{2}$:

$$|j = l + \frac{1}{2}, m_j = l + \frac{1}{2}\rangle = |m_l = m_l - \frac{1}{2}, m_s = \frac{1}{2}\rangle.$$  

(5.214)
However, already for the next value, \( m_j = l - \frac{1}{2} \), we need to have two values of \( j \), so that two \(|m_l, m_s\rangle\) kets is to be related to two \(|j, m_j\rangle\) kets by two Clebsch-Gordan coefficients. Since \( l \) changes in unit steps, these values of \( j \) have to be \( l \pm \frac{1}{2} \). This choice,

\[
j = l \pm \frac{1}{2},
\]

(5.215)
evidently satisfies all lower values of \( m_j \) (again, with only one value, \( j = l + \frac{1}{2} \), necessary for the lowest \( m_j = l - \frac{1}{2} \)) \text{ – see Fig. 12.} Note that the total number of the coupled-representation states is \( 1 + 2 \times 2l + 1 = 2(2l + 1) \), i.e. the same as in the uncoupled representation. So, each sum (210), for fixed \( j, m_j \) (and fixed common parameter \( l \)), has at most 2 terms, i.e. involves at most 2 Clebsch-Gordan coefficients.

These coefficients may be calculated in a few steps, all but the last one rather simple even for arbitrary spin \( s \). First, the matrix elements of ladder operators \( \hat{L}_z \) in the standard \( z \)-basis (i.e. in the basis of kets \(|m_l\rangle\)) may be calculated from Eq. (184). Next, the similarity of vector operators \( \hat{J}_z \) and \( \hat{S}_z \) to operators \( \hat{L}_z \), expressed by Eqs. (197), (203), and (204), may be used to argue that the matrix elements of operators \( \hat{J}_z \) and \( \hat{S}_z \), defined absolutely similarly to \( \hat{L}_z \), have similar matrix elements in the bases of kets \(|m_j\rangle\) and \(|m_i\rangle\), respectively. After that, acting by operator \( \hat{J}_z = \hat{L}_z + \hat{S}_z \) upon both parts of Eq. (210), and then inner-multiplying the result by the bra vector \( \langle m_i, m_s | \) and using the above matrix elements, we get recurrence relations for the Clebsch-Gordan coefficients. Finally, these relations may be recurrently applied to the adjacent states in both representations, starting from any of the two states common for them – for example, from state with ket-vectors (214), corresponding to the top right point in Fig. 12. Let me leave these straightforward but a bit tedious calculations for reader’s exercise and just cite the final result of this procedure for \( s = \frac{1}{2} \):\(^{53}\)

\[
\begin{align*}
\langle m_i = m_j - \frac{1}{2}, m_s = +\frac{1}{2} | j = l \pm \frac{1}{2}, m_j \rangle &= \pm \left( \frac{l \pm m_j + 1/2}{2l + 1} \right)^{1/2}, \\
\langle m_i = m_j + \frac{1}{2}, m_s = -\frac{1}{2} | j = l \pm \frac{1}{2}, m_j \rangle &= \pm \left( \frac{l \mp m_j + 1/2}{2l + 1} \right)^{1/2}.
\end{align*}
\]

(5.216a)

\(^{53}\) For arbitrary spin \( s \), the calculations and even the final expressions for the Clebsch-Gordan coefficients are rather bulky. They may be found, typically in a table form, mostly in special monographs – see, e.g., A. R. Edmonds, *Angular Momentum in Quantum Mechanics*, Princeton U. Press, 1957.
For applications, it may be more convenient to use this result in the following equivalent form:

\[
\begin{array}{l}
\left| j = l \pm \frac{1}{2}, m_j \right> \\
= \pm \left( \frac{l \pm m_j + 1/2}{2l + 1} \right)^{1/2} \left| m_i = m_j - \frac{1}{2}, m_s = \pm \frac{1}{2} \right> + \left( \frac{l \mp m_j + 1/2}{2l + 1} \right)^{1/2} \left| m_i = m_j + \frac{1}{2}, m_s = -\frac{1}{2} \right>
\end{array}
\]

(5.216b)

We will use this relation in Sec. 6.4 for an analysis of the anomalous Zeeman effect, based on the perturbation theory. Moreover, most of the angular momentum addition theory described above is immediately applicable to the addition of angular momenta in multiparticle systems, so we will revisit it in Chapter 8.

To conclude this section, I have to note that the Clebsch-Gordan coefficients (for arbitrary \( s \)) participate also in the so-called Wigner-Eckart theorem that expresses matrix elements of certain spherical tensors, in the coupled-representation basis \( | j, m_j \rangle \), via a reduced set of matrix elements. Unfortunately, a discussion of this theorem and its applications would require a higher mathematical background than I can expect from my readers, and more time/space than I can afford.\(^{54}\)

5.8. Exercise problems

5.1. Use the discussion of Sec. 1 to find an alternative solution of Problem 4.17.

5.2. A two-level system is in a quantum state \( \alpha \), described by ket-vector \( | \alpha \rangle = \alpha_\uparrow | \uparrow \rangle + \alpha_\downarrow | \downarrow \rangle \), with given (generally, complex) \( c \)-number coefficients \( \alpha_\uparrow, \alpha_\downarrow \). Prove that we can always select a 3-component vector \( \mathbf{a} = \{ a_x, a_y, a_z \} \) of real \( c \)-numbers, such that \( \alpha \) is an eigenstate of operator \( \mathbf{a} \cdot \mathbf{\hat{\sigma}} \), where \( \mathbf{\hat{\sigma}} \) is the operator described, in \( z \)-basis, by the Pauli matrix vector. Find all possible values of \( \mathbf{a} \) satisfying this condition, and the second eigenstate of operator \( \mathbf{a} \cdot \mathbf{\hat{\sigma}} \), orthogonal to the given \( \alpha \). Give a Bloch-sphere interpretation of your result.

5.3. A spin-\( \frac{1}{2} \) particle is in a constant vertical field, so that its Hamiltonian

\[
\hat{H} = \frac{\hbar \Omega}{2} \hat{\sigma}_z,
\]

but its spin’s initial state is an eigenstate of a different Hamiltonian:\(^{55}\)

\[
\hat{H}_{\text{ini}} = \mathbf{a} \cdot \mathbf{\hat{\sigma}} \equiv a_x \hat{\sigma}_x + a_y \hat{\sigma}_y + a_z \hat{\sigma}_z.
\]

Use any approach you like to calculate the time evolution of the expectation values of the spin components. Interpret the results.

5.4. For any periodic motion of a single particle in a confining potential \( U(r) \), the virial theorem of non-relativistic classical mechanics\(^{56}\) is reduced to the following equality:

---


\(^{55}\) Cf. Problems 4.22, 4.23, 5.2.

\(^{56}\) See, e.g., CM Problem 1.12.
\[ \overline{T} = \frac{1}{2} \mathbf{r} \cdot \nabla U, \]

where \( T \) is particle’s kinetic energy, and the top bar means averaging over the period of motion. Prove the quantum-mechanical version of the theorem for an arbitrary stationary quantum state, in the absence of spin effects:

\[ \langle T \rangle = \frac{1}{2} \langle \mathbf{r} \cdot \nabla U \rangle, \]

where the angular brackets mean, as everywhere in these notes, the expectation value of the variable inside them.

*Hint:* Mimicking the proof of the classical virial theorem, consider the time evolution of operator

\[ \hat{G} \equiv \hat{\mathbf{r}} \cdot \hat{\mathbf{p}}. \]

5.5. A constant force \( F \) is applied to an (otherwise free) 1D particle of mass \( m \). Calculate the eigenfunctions of the problem, using

(i) the coordinate representation, and
(ii) the momentum representation.

Discuss the relation between the results.

5.6. The momentum representation of an operator, defined in the Hilbert space of 1D orbital states of a particle, equals \( p^{-1} \). Find its coordinate representation.

5.7*. For a particle moving in a 3D periodic potential, develop the bra-ket formalism for the \( \mathbf{q} \)-representation, in which a complex amplitude similar to \( a_q \) in Eq. (2.234) (but generalized to 3D and all energy bands) plays the role of the wavefunction. In particular, calculate operators \( \mathbf{r} \) and \( \mathbf{v} \) in this representation, and use the result to prove Eq. (2.237) for 1D motion in the low-field limit.

*Hint:* Try to generalize the analysis of the momentum representation in Sec. 5.2.

5.8. In the Heisenberg picture of quantum dynamics, find the operator of velocity and acceleration,

\[ \hat{\mathbf{v}} \equiv \frac{d\hat{\mathbf{r}}}{dt} \quad \text{and} \quad \hat{\mathbf{a}} \equiv \frac{d\hat{\mathbf{v}}}{dt}, \]

of an electron moving in an arbitrary electromagnetic field. Compare the results with the corresponding classical expressions.

5.9. Calculate, in the WKB approximation, the transmission coefficient \( T \) for tunneling of a 2D particle with energy \( E < U_0 \) through a saddle-shaped potential “pass”

\[ U(x, y) = U_0 \left( 1 + \frac{xy}{a^2} \right), \]

where \( U_0 \) and \( a \) are real constants.
5.10. Calculate the so-called Gamow factor\(^{57}\) for the alpha decay of atomic nuclei, i.e. the exponential factor in the transparency of the tunnel barrier, resulting from the following simple model of the particle’s potential energy as a function of its distance from the nuclear center:

\[
U(r) = \begin{cases} 
U_0 < 0, & \text{for } r < R, \\
\frac{ZZ'e^2}{4\pi\varepsilon_0 r}, & \text{for } R < r,
\end{cases}
\]

(where \(Z'e = 2e > 0\) is the charge of the alpha-particle, \(Z'e > 0\) is that of the nucleus after the decay, and \(R\) is the nucleus’ radius), in the WKB approximation.

5.11. For a 1D harmonic oscillator with mass \(m\) and frequency \(\omega_0\), calculate:

(i) all matrix elements \(\langle n | \hat{x}^3 | n' \rangle\), and

(ii) diagonal matrix elements \(\langle n | \hat{x}^4 | n \rangle\),

where \(n\) are the Fock states.

5.12. Calculate the sum (over all \(n > 0\)) of the so-called oscillator strengths,

\[
f_n = \frac{2m}{\hbar^2} (E_n - E_0) \langle n | \hat{x} | 0 \rangle^2,
\]

of quantum transitions between the \(n^{th}\) energy level and the ground state, for

(i) a 1D harmonic oscillator, and

(ii) a 1D particle confined in an arbitrary stationary potential.

5.13.* Prove the so-called the Bethe sum rule,

\[
\sum_{n'} (E_{n'} - E_n) \langle n | e^{ikx} | n' \rangle^2 = \frac{\hbar^2 k^2}{2m}
\]

(where \(k\) is a \(c\)-number), valid for a 1D particle moving in an arbitrary time-independent potential \(U(x)\), and discuss its relation with the Thomas-Reiche-Kuhn sum rule, whose derivation was the subject of the previous problem.

*Hint: Calculate the expectation value, in a stationary state \(n\), of the following double commutator,

\[
\hat{D} \equiv [\hat{H}, e^{ikx}] e^{-ikx},
\]

in two ways – first, just spelling out both commutators, and, second, using the commutation relations between operators \(\hat{p}\) and \(e^{\pm ikx}\), and compare the results.

5.14. Simplify the following operators:

(i) \(\exp\{i a \hat{x}\} \hat{p} \exp\{-i a \hat{x}\}\), and

---

\(^{57}\) Named after G. Gamow, who made this calculation as early as in 1928.
(ii) \( \exp\{+ia\hat{p}_x\}\hat{x}\exp\{-ia\hat{p}_x\}, \)
where \( a \) is a \( c \)-number.

5.15. Use the Heisenberg equation of motion for a direct derivation of time evolution law (5.171) of the creation and annihilation operators of a harmonic oscillator.

5.16. Calculate:
(i) the expectation value of energy, and
(ii) the laws of time evolution of expectation values of the coordinate and momentum
for a 1D harmonic oscillator, provided that in the initial moment \( (t=0) \) it was in state
\[ |\alpha\rangle = \frac{1}{\sqrt{2}} (|15\rangle + |16\rangle), \]
where \( |n\rangle \) are ket-vectors of the stationary (Fock) states of the oscillator.

5.17. Re-derive the London dispersion force potential between two 3D harmonic oscillators (already calculated in Problem 3.19), using the language of mutually-induced polarization.

5.18. The discussion of the Glauber state properties in Sec. 5 has used the following general statement: if
\[ \hat{A}, \hat{B} = \mu \hat{d}, \]
where \( \hat{A} \) and \( \hat{B} \) are arbitrary operators, and \( \mu \) is an arbitrary \( c \)-number, then
\[ \exp\{+\hat{A}\hat{B}\exp\{-\hat{A}\} = \hat{B} + \mu \hat{d}. \]
Prove the statement.

\textit{Hint:} One (of several) ways to prove the statement is to expand operator
\( \hat{f}(\lambda) = \exp\{\lambda\hat{A}\hat{B}\exp\{-\lambda\hat{A}\} \) into the Taylor series in \( c \)-number \( \lambda \), and then evaluate it at \( \lambda = 1. \)

5.19. An external force pulse \( F(t) \), of a finite time duration \( \tau \), is exerted on a 1D harmonic oscillator, initially in its ground state. Use the Heisenberg-picture equations of motion to calculate the expectation value of oscillator’s energy at the end of the pulse.

5.20. Calculate the energy of the squeezed ground state \( s \) of a harmonic oscillator, defined by Eq. (172).

5.21. Use Eqs. (5.178) of the lecture notes to prove that operators \( \hat{L}_j \) and \( \hat{L}^2 \) commute with the Hamiltonian of a spinless particle placed in any central potential field.

5.22. Prove the following relations for the operators of the angular momentum:
\[ \hat{L}^2 = \hat{L}_z^2 + \hat{L}_+ \hat{L}_- - \hbar \hat{L}_z = \hat{L}_z^2 + \hat{L}_- \hat{L}_+ + \hbar \hat{L}_z. \]
5.23. According to Eqs. (188) and their discussion, action of the ladder operators on the common eigenkets $|l, m\rangle$ of operators $\hat{L}^z$ and $\hat{L}_z$ may be described as

$$\hat{L}_z |l, m\rangle = L_z^{(m)} |l, m \pm 1\rangle.$$ 

Calculate coefficients $L_z^{(m)}$, assuming that the eigenstates are normalized: $\langle l, m| l, m \rangle = 1$.

5.24. In the basis of common eigenstates of operators $\hat{L}_z$ and $\hat{L}^z$, described by eigenkets $|l, m\rangle$:

(i) calculate matrix elements $\langle l, m| \hat{L}_z |l, m_1\rangle$ and $\langle l, m_1| \hat{L}^z |l, m_2\rangle$;

(ii) spell out your results for diagonal matrix elements (with $m_1 = m_2$) and their $y$-axis counterparts; and

(iii) calculate diagonal matrix elements $\langle l, m| \hat{L}_z \hat{L}_z |l, m\rangle$ and $\langle l, m| \hat{L}_z \hat{L}_z |l, m\rangle$.

5.25. For the state described by the common eigenket $|l, m\rangle$ of operators $\hat{L}_z$ and $\hat{L}^z$ in a reference frame $\{x, y, z\}$, calculate the expectation values $\langle L_z \rangle$ and $\langle L_z^2 \rangle$ in the reference frame whose axis $z'$ forms angle $\theta$ with axis $z$.

5.26. Write down the matrices of the following angular momentum operators:

$\hat{L}_z, \hat{L}_y, \hat{L}_z$, and $\hat{L}_z$ in the $z$-basis of states with $l = 1$.

5.27. Find the angular part of the orbital wavefunction of a particle with a definite value of $L^2$, equal to $6\hbar^2$, and the largest possible value of $L_x$. What is this value?

5.28.* A charged 2D particle is trapped in a soft in-plane potential well $U(x, y) = m\omega_0^2(x^2 + y^2)/2$. Calculate its energy spectrum in the presence of an additional uniform magnetic field $\mathcal{B}$, normal to the plane.

5.29. Calculate the spectrum of rotational energies of an axially-symmetric, rigid molecule.

5.30. For the state with wavefunction $\psi = Cxye^{-\lambda r}$, with a real, positive $\lambda$, calculate:

(i) the expectation values of observables $L_x, L_y, L_z$ and $L^2$, and

(ii) the normalization constant $C$.

5.31. An angular state of a spinless particle is described by the following ket-vector:

$$|\alpha\rangle = \frac{1}{\sqrt{2}} (|l = 3, m = 0\rangle + |l = 3, m = 1\rangle).$$

Find the expectation values of the $x$- and $y$-components of its angular momentum. Is it sensitive to a possible phase shift between two component eigenkets?
5.32. Simplify the following double commutator: \[ [\hat{A}_j, [\hat{J}_j, \hat{L}^2, \hat{L}_j]]. \]

5.33. Express the commutators listed in Eq. (206), \([\hat{J}^2, \hat{L}_z]\) and \([\hat{J}^2, \hat{S}_z]\), via \(\hat{L}_j\) and \(\hat{S}_j\).

5.34. Find the operator \(\hat{T}_\phi\) describing the state rotation by angle \(\phi\) about a certain axis, using the similarity of this operation with the shift of a Cartesian coordinate, discussed in Sec. 5. Then use it to calculate the probabilities of measurements of a beam of particles with \(z\)-polarized spin-\(\frac{1}{2}\), by a Stern-Gerlach instrument turned by angle \(\theta\) within the \([z, x]\) plane (where \(y\) is the axis of particle propagation – see Fig. 4.1).\(^{58}\)

5.35. The rotation ("angle translation") operators \(\hat{T}_\alpha\), analyzed in the previous problem, and the coordinate translation operator \(\hat{T}_x\), discussed in Sec. 5.5 of the lecture notes, have a similar structure:
\[
\hat{T}_\lambda = \exp \left\{ -i \frac{\hat{C} \lambda}{\hbar} \right\},
\]

where \(\lambda\) is a real \(c\)-number, characterizing shift’s magnitude, and \(\hat{C}\) is a Hermitian operator that does not explicitly depend on time.

(i) Prove that all such operators \(\hat{T}_\lambda\) are unitary.

(ii) Prove that if the shift by \(\lambda\), induced by operator \(\hat{T}_\lambda\), leaves the Hamiltonian of some system unchanged for any \(\lambda\), then the variable \(C\), corresponding to the operator \(\hat{C}\), is a constant of motion.

(iii) Discuss what does the last conclusion give for the particular operators \(\hat{T}_x\) and \(\hat{T}_\phi\).

5.36. A particle is in a state \(\alpha\) with the orbital wavefunction proportional to the spherical harmonic \(Y^l_m(\theta, \phi)\). Find the angular dependence of the wavefunctions corresponding to the following ket-vectors:

(i) \(\hat{L}_x |\alpha\rangle\), (ii) \(\hat{L}_y |\alpha\rangle\), (iii) \(\hat{L}_z |\alpha\rangle\), (iv) \(\hat{L}_x \hat{L}_x |\alpha\rangle\), and (v) \(\hat{L}_z^2 |\alpha\rangle\).

5.37. For a state with definite quantum numbers \(l\) and \(j\), prove that observable \(\mathbf{L} \cdot \mathbf{S}\) also has a definite value, and calculate this value.

5.38. Derive the general recurrence relations for the Clebsh-Gordan coefficients.

*Hint*: Using the similarity of commutation relations, discussed in Sec. 7, generalize the solution of Problem 19 to all angular momentum operators, and apply them to Eq. (198).

5.39. The byproduct of the solution of the previous problem is the general relation for the spin operators (valid for any spin \(s\)), which may be rewritten as

\(^{58}\) Note that the last task is just a particular case of Problem 4.17 (see also Problem 1).
\[ \langle m_s \pm 1 | \hat{S}_z | m_s \rangle = \hbar [s \pm m_s + 1][s \mp m_s]^{1/2}, \]

provided that all other quantum numbers are fixed. Use this result to spell out the matrices \( S_x, S_y, S_z, \) and \( S^2 \) of a particle with \( s = 1 \), in the \( z \)-basis - defined as the basis in which the matrix \( S_z \) is diagonal.

5.40. For a particle with spin \( s \), moving in a spherically-symmetric field, find the ranges of possible values of quantum numbers \( m_l \) and \( j \), necessary to describe, in the coupled representation basis:

(i) all states with a definite quantum number \( l \), and
(ii) a state with definite value of not only \( l \), but also \( m_l \) and \( m_s \).

Give an interpretation of your results in terms of the classical geometric vector diagram (see Fig. 11).

5.41. A spin-\( \frac{1}{2} \) particle moves in a centrally-symmetric potential \( U(r) \). Using Eqs. (216) for the Clebsch-Gordan coefficients,

(i) write explicit expressions for the ket vectors for states that would be simultaneously the eigenstates of operators \( \hat{L}_z \), \( \hat{J}_z \), and \( \hat{J}_z \), via spin eigenkets \( |\uparrow\rangle \) and \( |\downarrow\rangle \);

(ii) for each such state, find all the possible values of observables \( L_z, L_2, S_2, \) and \( S_z \), the probability of each listed value, and the expectation value for each of the observables.

5.42. Taking into account electron’s spin, find the energy spectrum of an electron, free to move within a plane, besides being placed into a uniform magnetic field \( \mathbf{B} \), normal to the plane. Compare the result with the Landau level picture discussed in Sec. 3.2.