4.5: Observables- Expectation Values and Uncertainties

After this particular (and hopefully inspiring) example, let us discuss the general relation between the Dirac formalism and experiment in more detail. The expectation value of an observable over any statistical ensemble (not necessarily coherent) may be always calculated using the general statistical rule (1.37). For the particular case of a coherent superposition (118), we can combine that rule with Eq. (120) and the second of Eqs. (118):

$$\langle A\rangle=\sum_j A_j W_j=\sum_j \alpha_j^* A_j \alpha_j=\sum_j \langle\alpha \mid a_j\rangle A_j \langle a_j \mid \alpha\rangle \equiv\left\langle\alpha\left|\left(\sum_j |a_j\rangle A_j \langle a_j|\right)\right| \alpha\right\rangle . \tag{4.5.1}$$

Now using Eq. (59) for the particular case of the eigenstate basis $\{a\}$, for which Eq. (98) is valid, we arrive at a very simple and important formula [26]

$$\langle A\rangle=\langle\alpha|\hat{A}|\alpha\rangle . \tag{4.5.2}$$

This is a clear analog of the wave-mechanics formula (1.23) - and as we will see soon, may be used to derive it. A big advantage of Eq. (125) is that it does not explicitly involve the eigenvector set of the corresponding operator, and allows the calculation to be performed in any convenient basis. [27]

For example, let us consider an arbitrary coherent state α of spin- $1/2, 28$ and calculate the expectation values of its components. The calculations are easiest in the z-basis because we know the matrix elements of the spin operator components in that basis. Representing the ket- and bra-vectors of the given state as linear superpositions of the corresponding vectors of the basis states $\uparrow$ and $\downarrow$,

$$|\alpha\rangle=\alpha_{\uparrow}|\uparrow\rangle+\alpha_{\downarrow}|\downarrow\rangle, \quad\langle\alpha|=\langle\uparrow| \alpha_{\uparrow}^*+\langle\downarrow| \alpha_{\downarrow}^* . \tag{4.5.3}$$

and plugging these expressions to Eq. (125) written for the observable S_z, we get

$$\begin{aligned}
\langle S_z\rangle & =\left(\left\langle\uparrow\left|\alpha_{\uparrow}^*+\langle\downarrow\right| \alpha_{\downarrow}^*\right) \hat{S}_z\left(\alpha_{\uparrow}|\uparrow\rangle+\alpha_{\downarrow}|\downarrow\rangle\right)\right. \\
& =\alpha_{\uparrow} \alpha_{\uparrow}^*\left\langle\uparrow\left|\hat{S}_z\right| \uparrow\right\rangle+\alpha_{\downarrow} \alpha_{\downarrow}^*\left\langle\downarrow\left|\hat{S}_z\right| \downarrow\right\rangle+\alpha_{\uparrow} \alpha_{\downarrow}^*\left\langle\downarrow\left|\hat{S}_z\right| \uparrow\right\rangle+\alpha_{\downarrow} \alpha_{\uparrow}^*\left\langle\uparrow\left|\hat{S}_z\right| \downarrow\right\rangle
\end{aligned}$$

Now there are two equivalent ways (both very simple) to calculate the long brackets in this expression. The first one is to represent each of them in the matrix form in the z-basis, in which the braand ket-vectors of states $\uparrow$ and $\downarrow$ are the matrix-rows $(1,0)$ and $(0,1)$, or similar matrix-columns - the exercise highly recommended to the reader. Another (perhaps more elegant) way is to use the general Eq. (59), in the z-basis, together with the spin-1/2-specific Eqs. (116a) and (105) to write

$$\hat{S}_x=\frac{\hbar}{2}(|\uparrow\rangle\langle\downarrow|+|\downarrow\rangle\langle\uparrow|), \quad \hat{S}_y=-i \frac{\hbar}{2}(|\uparrow\rangle\langle\downarrow|-|\downarrow\rangle\langle\uparrow|), \quad \hat{S}_z=\frac{\hbar}{2}(|\uparrow\rangle\langle\uparrow|-|\downarrow\rangle\langle\downarrow|) \tag{4.5.4}$$

For our particular calculation, we may plug the last of these expressions into Eq. (127), and use the orthonormality conditions (38):

$$\langle\uparrow | \uparrow\rangle=\langle\downarrow | \downarrow\rangle=1, \quad\langle\uparrow | \downarrow\rangle=\langle\downarrow | \uparrow\rangle=0 . \tag{4.5.5}$$

Both approaches give (of course) the same result:

$$\langle S_z\rangle=\frac{\hbar}{2}\left(\alpha_{\uparrow} \alpha_{\uparrow}^*-\alpha_{\downarrow} \alpha_{\downarrow}^*\right) . \tag{4.5.6}$$

This particular result might be also obtained using Eq. (120) for the probabilities $W_{\uparrow}=\alpha \uparrow \alpha \uparrow^*$ and $W_{\downarrow}=\alpha \downarrow \alpha \downarrow^*$, namely:

$$\langle S_z\rangle=W_{\uparrow}\left(+\frac{\hbar}{2}\right)+W_{\downarrow}\left(-\frac{\hbar}{2}\right)=\alpha_{\uparrow} \alpha_{\uparrow}^*\left(+\frac{\hbar}{2}\right)+\alpha_{\downarrow} \alpha_{\downarrow}^*\left(-\frac{\hbar}{2}\right) . \tag{4.5.7}$$

The formal way (127), based on using Eq. (125), has, however, an advantage of being applicable, without any change, to finding the observables whose operators are not diagonal in the z-basis, as well. In particular, absolutely similar calculations give

$$\begin{aligned}
& \langle S_x\rangle=\alpha_{\uparrow} \alpha_{\uparrow}^*\left\langle\uparrow\left|\hat{S}_x\right| \uparrow\right\rangle+\alpha_{\downarrow} \alpha_{\downarrow}^*\left\langle\downarrow\left|\hat{S}_x\right| \downarrow\right\rangle+\alpha_{\uparrow} \alpha_{\downarrow}^*\left\langle\downarrow\left|\hat{S}_x\right| \uparrow\right\rangle+\alpha_{\downarrow} \alpha_{\uparrow}^*\left\langle\uparrow\left|\hat{S}_x\right| \downarrow\right\rangle=\frac{\hbar}{2}\left(\alpha_{\uparrow} \alpha_{\downarrow}^*+\alpha_{\downarrow} \alpha_{\uparrow}^*\right), \\
& \langle S_y\rangle=\alpha_{\uparrow} \alpha_{\uparrow}^*\left\langle\uparrow\left|\hat{S}_y\right| \uparrow\right\rangle+\alpha_{\downarrow} \alpha_{\downarrow}^*\left\langle\downarrow\left|\hat{S}_y\right| \downarrow\right\rangle+\alpha_{\uparrow} \alpha_{\downarrow}^*\left\langle\downarrow\left|\hat{S}_y\right| \uparrow\right\rangle+\alpha_{\downarrow} \alpha_{\uparrow}^*\left\langle\uparrow\left|\hat{S}_y\right| \downarrow\right\rangle=i \frac{\hbar}{2}\left(\alpha_{\uparrow} \alpha_{\downarrow}^*-\alpha_{\downarrow} \alpha_{\uparrow}^*\right),
\end{aligned}$$

Let us have a good look at a particular spin state, for example the spin-up state $\uparrow$. According to Eq. (126), in this state $\alpha \uparrow = 1$ and $\alpha_\downarrow = 0$, so that Eqs. (130)-(133) yield:

$$\langle S_z \rangle = \frac{\hbar}{2}, \quad \langle S_x \rangle = \langle S_y \rangle = 0. \tag{4.5.8}$$

Now let us use the same Eq. (125) to calculate the spin component uncertainties. According to Eqs. (105) and (116)-(117), the operator of each spin component squared is equal to $(\hbar/2)^2 \hat{I}$, so that the general Eq. (1.33) yields

$$\begin{gathered}
(\delta S_z)^2 = \langle S_z^2 \rangle - \langle S_z \rangle^2 = \left\langle \uparrow \left| \hat{S}_z^2 \right| \uparrow \right\rangle - \left(\frac{\hbar}{2}\right)^2 = \left(\frac{\hbar}{2}\right)^2 \langle \uparrow | \hat{I} | \uparrow \rangle - \left(\frac{\hbar}{2}\right)^2 = 0 \\
(\delta S_x)^2 = \langle S_x^2 \rangle - \langle S_x \rangle^2 = \left\langle \uparrow \left| \hat{S}_x^2 \right| \uparrow \right\rangle - 0 = \left(\frac{\hbar}{2}\right)^2 \langle \uparrow | \hat{I} | \uparrow \rangle = \left(\frac{\hbar}{2}\right)^2 \\
(\delta S_y)^2 = \langle S_y^2 \rangle - \langle S_y \rangle^2 = \left\langle \uparrow \left| \hat{S}_y^2 \right| \uparrow \right\rangle - 0 = \left(\frac{\hbar}{2}\right)^2 \langle \uparrow | \hat{I} | \uparrow \rangle = \left(\frac{\hbar}{2}\right)^2
\end{gathered}$$

While Eqs. (134) and (135a) are compatible with the classical notion of the angular momentum of magnitude $\hbar/2$ being directed exactly along the z-axis, this correspondence should not be overstretched, because such classical picture cannot explain Eqs. (135b) and (135c). The best (but still imprecise!) classical image I can offer is the spin vector S oriented, on average, in the z-direction, but still having its x - and y-components strongly "wobbling" (fluctuating) about their zero average values.

It is straightforward to verify that in the x-polarized and y-polarized states the situation is similar, with the corresponding change of axis indices. Thus, in neither of these states all three spin components have definite values. Let me show that this is not just an occasional fact, but reflects the perhaps most profound property of quantum mechanics, the uncertainty relations. For that, let us consider two measurable observables, A and B, of the same quantum system. There are two possibilities here. If the operators corresponding to these observables commute,

$$[\hat{A}, \hat{B}] = 0 \tag{4.5.9}$$

then all matrix elements of the commutator in any orthogonal basis (in particular, in the basis of eigenstates a_j of the operator $\hat{A}$) have to equal zero:

$$\left\langle a_j | [\hat{A}, \hat{B}] | a_{j'} \right\rangle \equiv \left\langle a_j | \hat{A}\hat{B} | a_{j'} \right\rangle - \left\langle a_j | \hat{B}\hat{A} | a_{j'} \right\rangle = 0. \tag{4.5.10}$$

In the first bracket of the middle expression, let us act by the (Hermitian!) operator $\hat{A}$ on the bra-vector, while in the second one, on the ket-vector. According to Eq. (68), such action turns the operators into the corresponding eigenvalues, which may be taken out of the long brackets, so that we get

$$A_j \left\langle a_j | \hat{B} | a_{j'} \right\rangle - A_{j'} \left\langle a_j | \hat{B} | a_{j'} \right\rangle \equiv \left(A_j - A_{j'}\right) \left\langle a_j | \hat{B} | a_{j'} \right\rangle = 0. \tag{4.5.11}$$

This means that if all eigenstates of operator $\hat{A}$ are non-degenerate (i.e. $A_j \neq A_j$, if $j \neq j$ '), the matrix of operator $\hat{B}$ has to be diagonal in the basis $\{a\}$, i.e., the eigenstate sets of the operators $\hat{A}$ and $\hat{B}$ coincide. Such pairs of observables (and their operators) that share their eigenstates, are called compatible. For example, in the wave mechanics of a particle, its momentum (1.26) and kinetic energy (1.27) are compatible, sharing their eigenfunctions (1.29). Now we see that this is not occasional, because each Cartesian component of the kinetic energy is proportional to the square of the corresponding component of the momentum, and any operator commutes with an arbitrary integer power of itself:

$$\left[\hat{A}, \hat{A}^n\right] \equiv [\hat{A}, \underbrace{\hat{A}\hat{A} \ldots \hat{A}}_{n}] = \hat{A}\underbrace{\hat{A}\hat{A} \ldots \hat{A}}_{n} - \underbrace{\hat{A}\hat{A} \ldots \hat{A}}_{n}\hat{A} = 0. \tag{4.5.12}$$

Now, what if operators $\hat{A}$ and $\hat{B}$ do not commute? Then the following general uncertainty relation is valid:

$$\delta A \delta B \geq \frac{1}{2} |\langle [\hat{A}, \hat{B}] \rangle|, \tag{4.5.13}$$

where all expectation values are for the same but arbitrary state of the system. The proof of Eq. (140) may be divided into two steps, the first one proving the so-called Schwartz inequality for any two possible states, say α and β : 29

$$\langle\alpha \mid \alpha\rangle\langle\beta \mid \beta\rangle \geq|\langle\alpha \mid \beta\rangle|^{2} \tag{4.5.14}$$

Its proof may be readily achieved by applying the postulate (16) - that the norm of any legitimate state of the system cannot be negative - to the state with the following ket-vector:

$$|\delta\rangle \equiv|\alpha\rangle-\frac{\langle\beta \mid \alpha\rangle}{\langle\beta \mid \beta\rangle}|\beta\rangle \tag{4.5.15}$$

where α and β are possible, non-null states of the system, so that the denominator in Eq. (142) is not equal to zero. For this case, Eq. (16) gives

$$\left(\left\langle\alpha\left|-\frac{\langle\alpha \mid \beta\rangle}{\langle\beta \mid \beta\rangle}\langle\beta|\right)\left(|\alpha\rangle-\frac{\langle\beta \mid \alpha\rangle}{\langle\beta \mid \beta\rangle}|\beta\rangle\right) \geq 0\right.\right. \tag{4.5.16}$$

Opening the parentheses, we get

$$\langle\alpha \mid \alpha\rangle-\frac{\langle\alpha \mid \beta\rangle}{\langle\beta \mid \beta\rangle}\langle\beta \mid \alpha\rangle-\frac{\langle\beta \mid \alpha\rangle}{\langle\beta \mid \beta\rangle}\langle\alpha \mid \beta\rangle+\frac{\langle\alpha \mid \beta\rangle\langle\beta \mid \alpha\rangle}{\langle\beta \mid \beta\rangle^{2}}\langle\beta \mid \beta\rangle \geq 0 \tag{4.5.17}$$

After the cancellation of one inner product $\langle\beta \mid \beta\rangle$ in the numerator and the denominator of the last term, it cancels with the 2^{nd} (or the 3^{rd}) term. What remains is the Schwartz inequality (141).

Now let us apply this inequality to states

$$|\alpha\rangle \equiv \hat{\tilde{A}}|\gamma\rangle \text { and }|\beta\rangle \equiv \hat{\tilde{B}}|\gamma\rangle, \tag{4.5.18}$$

where, in both relations, γ is the same (but otherwise arbitrary) possible state of the system, and the deviation operators are defined similarly to the deviations of the observables (see Sec. 1.2):

$$\hat{\tilde{A}} \equiv \hat{A}-\langle A\rangle, \quad \hat{\tilde{B}} \equiv \hat{B}-\langle B\rangle. \tag{4.5.19}$$

With this substitution, and taking into account again that the observable operators $\hat{A}$ and $\hat{B}$ are Hermitian, Eq. (141) yields

$$\left\langle\gamma\left|\hat{\tilde{A}}^{2}\right| \gamma\right\rangle\left\langle\gamma\left|\hat{\tilde{B}}^{2}\right| \gamma\right\rangle \geq|\langle\gamma| \hat{\tilde{A}} \hat{\tilde{B}}|\gamma\rangle|^{2}. \tag{4.5.20}$$

Since the state γ is arbitrary, we may use Eq. (125) to rewrite this relation as an operator inequality:

$$\delta A \delta B \geq|\langle\hat{\tilde{A}} \hat{\tilde{B}}\rangle|. \tag{4.5.21}$$

Actually, this is already an uncertainty relation, even "better" (stronger) than its standard form (140); moreover, it is more convenient in some cases. To prove Eq. (140), we need a couple of more steps. First, let us notice that the operator product participating in Eq. (148) may be recast as

$$\hat{\tilde{A}} \hat{\tilde{B}}=\frac{1}{2}\{\hat{\tilde{A}}, \hat{\tilde{B}}\}-\frac{i}{2} \hat{C}, \quad \text { where } \hat{C} \equiv i[\hat{\tilde{A}}, \hat{\tilde{B}}]. \tag{4.5.22}$$

Any anticommutator of Hermitian operators, including that in Eq. (149), is a Hermitian operator, and its eigenvalues are purely real, so that its expectation value (in any state) is also purely real. On the other hand, the commutator part of Eq. (149) is just

$$\hat{C} \equiv i[\hat{\tilde{A}}, \hat{\tilde{B}}] \equiv i(\hat{A}-\langle A\rangle)(\hat{B}-\langle B\rangle)-i(\hat{B}-\langle B\rangle)(\hat{A}-\langle A\rangle) \equiv i(\hat{A} \hat{B}-\hat{B} \hat{A}) \equiv i[\hat{A}, \hat{B}]. \tag{4.5.23}$$

Second, according to Eqs. (52) and (65), the Hermitian conjugate of any product of the Hermitian operators $\hat{A}$ and $\hat{B}$ is just the product of these operators swapped. Using the fact, we may write

$$\hat{C}^{\dagger}=(i[\hat{A}, \hat{B}])^{\dagger}=-i(\hat{A} \hat{B})^{\dagger}+i(\hat{B} \hat{A})^{\dagger}=-i \hat{B} \hat{A}+i \hat{A} \hat{B}=i[\hat{A}, \hat{B}]=\hat{C}, \tag{4.5.24}$$

so that the operator $\hat{C}$ is also Hermitian, i.e. its eigenvalues are also real, and thus its expectation value is purely real as well. As a result, the square of the expectation value of the operator product (149) may be represented as

$$\langle\hat{\tilde{A}} \hat{\tilde{B}}\rangle^{2}=\left\langle\frac{1}{2}\{\hat{\tilde{A}}, \hat{\tilde{B}}\}\right\rangle^{2}+\left\langle\frac{1}{2} \hat{C}\right\rangle^{2}. \tag{4.5.25}$$

Since the first term on the right-hand side of this equality cannot be negative, we may write

$$\langle\hat{\tilde{A}}\hat{\tilde{B}}\rangle^2 \geq \left\langle\frac{1}{2}\hat{C}\right\rangle^2 = \left\langle\frac{i}{2}[\hat{A},\hat{B}]\right\rangle^2, \tag{4.5.26}$$

and hence continue Eq. (148) as

$$\delta A\delta B \geq |\langle\hat{\tilde{A}}\hat{\tilde{B}}\rangle| \geq \frac{1}{2}|\langle[\hat{A},\hat{B}]\rangle|, \tag{4.5.27}$$

thus proving Eq. (140).

For the particular case of operators $\hat{x}$ and $\hat{p}_x$ (or a similar pair of operators for another Cartesian coordinate), we may readily combine Eq. (140) with Eq. (2.14b) and to prove the original Heisenberg's uncertainty relation (2.13). For the spin-1/2 operators defined by Eq. (116)-(117), it is very simple (and highly recommended to the reader) to show that

$$\left[\hat{\sigma}_j,\hat{\sigma}_{j'}\right] = 2i\varepsilon_{jj'j''}\hat{\sigma}_{j''}, \quad \text{i.e. } \left[\hat{S}_j,\hat{S}_{j'}\right] = i\varepsilon_{jj'j'}\hbar\hat{S}_{j''}, \tag{4.5.28}$$

where ε_{ijj} " is the Levi-Civita permutation symbol - see, e.g., MA Eq. (13.2). As a result, the uncertainty relations (140) for all Cartesian components of spin- $-\frac{1}{2}$ systems are similar, for example

$$\delta S_x\delta S_y \geq \frac{\hbar}{2}|\langle S_z\rangle|, \text{ etc.} \tag{4.5.29}$$

In particular, as we already know, in the $\uparrow$ state the right-hand side of this relation equals $(\hbar/2)^2 > 0$, so that neither of the uncertainties $\delta S_x, \delta S_y$ can equal zero. As a reminder, our direct calculation earlier in this section has shown that each of these uncertainties is equal to $\hbar/2$, i.e. their product is equal to the lowest value allowed by the uncertainty relation (156) - just as the Gaussian wave packets (2.16) provide the lowest possible value of the product $\delta x\delta p_x$, allowed by the Heisenberg relation (2.13).

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[26] This equality reveals the full beauty of Dirac's notation. Indeed, initially in this chapter the quantummechanical brackets just reminded the angular brackets used for the statistical averaging. Now we see that in this particular (but most important) case, the angular brackets of these two types may be indeed equal to each other!

[27] Note also that Eq. (120) may be rewritten in a form similar to Eq. (125): $W_j = \left\langle\alpha\left|\hat{\Lambda}_j\right|\alpha\right\rangle$, where $\hat{\Lambda}_j$ is the operator (42) of the state's projection upon the j^{th} eigenstate a_j.

[28] For clarity, the noun "spin- $1/2$ " is used, here and below, to denote the spin degree of freedom of a spin- $1/2$ particle, independent of its orbital motion.

[29] This inequality is the quantum-mechanical analog of the usual vector algebra's result $\alpha^2\beta^2 \geq |\boldsymbol{\alpha}\cdot\boldsymbol{\beta}|^2$.
