Chapter 9
Expectation Values, Mean Values, and Measured Values

The probability concept is further expanded. In addition, we look at Hermitian operators in more detail. The time behavior of mean values leads to the notion of conserved quantities.

We continue the discussion started in Chap. 7 on the calculation of the mean value of measured quantities, and generalize the formalism so that it is also applicable to the continuous case. As in the algebraic approach, the formulations lead us again to Hermitian operators, which are of particular importance in quantum mechanics. Furthermore, we address *conserved quantities* and establish a connection to classical mechanics.

9.1 Mean Values and Expectation Values

9.1.1 Mean Values of Classical Measurements

In classical physics, it is assumed that there is a 'true' value of each physical quantity which can be measured. Measuring this quantity several times, e.g. the location x, one will in general obtain different values x_i, where each value occurs with the frequency of occurrence n_i. The cause of the discrepancies between different values are inadequacies in the measuring apparatus (apart from the possibly varying skill of the experimenter). For l different readings, the total number of measurements amounts to $N = \sum_{i=1}^{l} n_i$. The *mean value* $\langle x \rangle$ (average) is defined as[1]

$$\langle x \rangle = \frac{\sum_{i=1}^{l} n_i x_i}{\sum_{i=1}^{l} n_i} = \frac{\sum_{i=1}^{l} n_i x_i}{N} = \sum_{i=1}^{l} \tilde{n}_i x_i \text{ with } \sum_{i=1}^{l} \tilde{n}_i = 1, \tag{9.1}$$

[1]Instead of $\langle x \rangle$, the notation $\bar{x}$ is also common.

J. Pade, *Quantum Mechanics for Pedestrians 1*, Undergraduate Lecture Notes in Physics, https://doi.org/10.1007/978-3-030-00464-4_9

where the $\tilde{n}_i = n_i/N$ are the relative frequencies which in the limit $l \to \infty$ become the probabilities w_i (Law of Large Numbers). In this limit, the average becomes the *expected value* or 'true' value:

$$\langle x \rangle = \sum_i p_i x_i \text{ with } \sum_i p_i = 1. \tag{9.2}$$

This averaging concept is also applicable to sets of *continuous* data. We perform the familiar transition, known from school,[2] of going from a sum $\sum$ to an integral $\int$, and obtain with the probability density[3] $\rho(x)$

$$\langle x \rangle = \int \rho(x)\, x \mathrm{d}x \text{ with } \int \rho(x)\, \mathrm{d}x = 1. \tag{9.3}$$

We generalize the last equation to three dimensions:

$$\langle x \rangle = \int \rho(\mathbf{x})\ x \mathrm{d}V \text{ with } \int \rho(x)\, \mathrm{d}V = 1. \tag{9.4}$$

9.1.2 *Expectation Value of the Position in Quantum Mechanics*

We wish to transfer these ideas to quantum mechanics. $\Psi(\mathbf{r}, t)$ is the solution of the time-dependent SEq. With the probability density

$$\rho = |\Psi(\mathbf{r}, t)|^2 \tag{9.5}$$

(recall that Ψ must be normalized), we can, as described above, determine the probability w of finding the quantum object in a spatial region G as $w(G) = \int_G \rho \mathrm{d}V$. If we now ask for its mean position in x-direction, we can formulate in analogy to (9.4)

$$\langle x \rangle = \int \Psi^*(\mathbf{r}, t)\, \Psi(\mathbf{r}, t)\ x\, \mathrm{d}V. \tag{9.6}$$

For a discussion of this situation, we imagine an ensemble of N identically-prepared quantum objects, all of which we launch at time $t = 0$ from $x = 0$ (one dimensional, moving to the right). After a time T, we find the ensemble member i at the position x_i. Then the mean value of x is given by $\langle x \rangle = \sum_i x_i$, and this value agrees increasingly

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[2] See also the chapter 'Discrete and continuous' in Appendix T, Vol. 1.

[3] For the special choice $\rho(x) = \sum_i p_i \delta(x - x_i)$, we obtain the expression (9.2) from (9.3). For the delta function $\delta(x)$, see Appendix H. Vol. 1.

better with the value given by (9.6) as N increases. In the limit $N \to \infty$, (9.6) is obtained exactly.[4]

In three dimensions, it follows that

$$\langle \mathbf{r} \rangle = \int \Psi^* (\mathbf{r}, t) \, \Psi (\mathbf{r}, t) \; \mathbf{r} \, \mathrm{d}V. \tag{9.7}$$

9.1.3 Expectation Value of the Momentum in Quantum Mechanics

We now examine the momentum of the quantum object (the following calculation is one dimensional; the three-dimensional case is given below). We assume that the expectation value $\langle p \rangle$ obeys the equation

$$\frac{\mathrm{d}}{\mathrm{d}t} \langle x \rangle = \frac{1}{m} \langle p \rangle . \tag{9.8}$$

This is an *assumption* at this point,[5] which has to prove itself in the following (i.e. above all, it must lead to self-consistent results). It follows that:

$$\begin{aligned} \langle p \rangle &= m \frac{\mathrm{d}}{\mathrm{d}t} \langle x \rangle = m \frac{\mathrm{d}}{\mathrm{d}t} \int_{-\infty}^{\infty} \Psi^* \Psi x \mathrm{d}x \\ &= m \int_{-\infty}^{\infty} \left(\dot{\Psi}^* \Psi + \Psi^* \dot{\Psi} \right) x \mathrm{d}x = m \int_{-\infty}^{\infty} \dot{\Psi}^* \Psi x \mathrm{d}x + c.c. \end{aligned} \tag{9.9}$$

$c.c.$ means the complex conjugate of the preceding term. We replace the time derivatives by space derivatives by means of the SEq $i\hbar\dot{\Psi} = -\frac{\hbar^2}{2m}\Psi'' + V\Psi$. We obtain (note: $V \in \mathbb{R}$):

$$\langle p \rangle = \frac{\hbar}{2i} \int_{-\infty}^{\infty} \Psi^{*\prime\prime} \Psi x \mathrm{d}x + c.c. \tag{9.10}$$

Partial integration yields

$$\langle p \rangle = \frac{\hbar}{2i} \left[\left(\Psi^{*\prime} \Psi x \right)_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \Psi^{*\prime} \left(\Psi' x + \Psi \right) \mathrm{d}x \right] + c.c. \tag{9.11}$$

[4] In fact, we cannot measure a point-like position x_i, but instead only an interval Δx_i which contains the quantum object. However, with the idea that we can make the interval arbitrarily small, we can accept the above argument as a limiting case. More will be said on this issue in Chap. 12.

[5] $\left\langle \frac{\mathrm{d}}{\mathrm{d}t} x \right\rangle = \frac{1}{m} \langle p \rangle$ would be better.

Since the wavefunction vanishes rapidly enough at infinity,[6] the integrated part vanishes. What remains is:

$$\langle p\rangle = \left\{-\frac{\hbar}{2i}\int_{-\infty}^{\infty}\Psi^{*\prime}\Psi' x\,\mathrm{d}x - \frac{\hbar}{2i}\int_{-\infty}^{\infty}\Psi^{*\prime}\Psi\,\mathrm{d}x\right\} + c.c. \tag{9.12}$$

The first term cancels with its $c.c$. It follows that

$$\begin{aligned}\langle p\rangle &= -\frac{\hbar}{2i}\int_{-\infty}^{\infty}\Psi^{*\prime}\Psi\,\mathrm{d}x + c.c. \\ &= -\frac{\hbar}{2i}\int_{-\infty}^{\infty}\Psi^{*\prime}\Psi\,\mathrm{d}x + \frac{\hbar}{2i}\int_{-\infty}^{\infty}\Psi^{*}\Psi'\,\mathrm{d}x.\end{aligned} \tag{9.13}$$

A further integration by parts of $-\frac{\hbar}{2i}\int_{-\infty}^{\infty}\Psi^{*\prime}\Psi\mathrm{d}x$ leads to

$$\langle p\rangle = \frac{\hbar}{2i}\int_{-\infty}^{\infty}\Psi^{*}\Psi'\,\mathrm{d}x - \frac{\hbar}{2i}\left\{\Psi^{*}\Psi\big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\Psi^{*}\Psi'\,\mathrm{d}x\right\}. \tag{9.14}$$

Again, the integrated term $\Psi^{*}\Psi|_{-\infty}^{\infty}$ vanishes and we obtain the result

$$\langle p\rangle = \frac{\hbar}{i}\int_{-\infty}^{\infty}\Psi^{*}\Psi'\,\mathrm{d}x, \tag{9.15}$$

or, if the other term in (9.13) is integrated by parts:

$$\langle p\rangle = -\frac{\hbar}{i}\int_{-\infty}^{\infty}\Psi^{*\prime}\Psi\,\mathrm{d}x. \tag{9.16}$$

As one can easily see, these terms can be written by using the momentum operator. With $p = \frac{\hbar}{i}\frac{\mathrm{d}}{\mathrm{d}x}$, we obtain[7]

$$\begin{aligned}\langle p\rangle &= \int_{-\infty}^{\infty}\Psi^{*}\left(\frac{\hbar}{i}\frac{\mathrm{d}}{\mathrm{d}x}\Psi\right)\mathrm{d}x = \int_{-\infty}^{\infty}\left(\frac{\hbar}{i}\frac{\mathrm{d}}{\mathrm{d}x}\Psi\right)^{*}\Psi\,\mathrm{d}x \\ &= \int_{-\infty}^{\infty}\Psi^{*}\left(p\Psi\right)\mathrm{d}x = \int_{-\infty}^{\infty}\left(p\Psi\right)^{*}\Psi\,\mathrm{d}x.\end{aligned} \tag{9.17}$$

Two comments:

1. The equality $\int_{-\infty}^{\infty}\Psi^{*}(p\Psi)\,\mathrm{d}x = \int_{-\infty}^{\infty}(p\Psi)^{*}\Psi\mathrm{d}x$ plays an important role in quantum mechanics in a slightly different notation: it applies not only to the

[6]Recall that this behavior is necessary for the interpretation of $|\Psi|^2$ as a probability density. See Chap. 7.

[7]As usual we use the same symbol, p, for the physical quantity 'momentum' and the corresponding operator. What is meant in each case should be clear from context.

momentum, but equally to *all* measurable physical quantities. We will return to this point later.
2. The equality holds only if the wavefunction vanishes sufficiently rapidly at infinity.

In the three-dimensional case, we find accordingly[8]:

$$\begin{aligned}\langle \mathbf{p} \rangle &= \int \Psi^* \left(\frac{\hbar}{i} \nabla \Psi \right) \mathrm{d}V = \int \left(\frac{\hbar}{i} \nabla \Psi \right)^* \Psi \mathrm{d}V \\ &= \int \Psi^* (\mathbf{p}\Psi)\, \mathrm{d}V = \int (\mathbf{p}\Psi)^* \Psi \mathrm{d}V.\end{aligned} \tag{9.18}$$

Similarly, one can derive the expectation value of the energy. It follows that

$$\langle E \rangle = \langle H \rangle = \int \Psi^* H \Psi \mathrm{d}V = \int (H\Psi)^* \Psi \mathrm{d}V. \tag{9.19}$$

9.1.4 General Definition of the Expectation Value

We summarize the results obtained so far:

$$\begin{aligned}\langle \mathbf{r} \rangle &= \int \Psi^* \mathbf{r}\, \Psi\, \mathrm{d}V = \int (\mathbf{r}\, \Psi)^* \Psi\, \mathrm{d}V \\ \langle \mathbf{p} \rangle &= \int \Psi^* \mathbf{p} \Psi \mathrm{d}V = \int (\mathbf{p}\Psi)^* \Psi \mathrm{d}V \\ \langle H \rangle &= \int \Psi^* H \Psi \mathrm{d}V = \int (H\Psi)^* \Psi \mathrm{d}V.\end{aligned} \tag{9.20}$$

We generalize to an arbitrary operator A representing a measurable variable [9] and define its expectation value $\langle A \rangle$ by

$$\langle A \rangle = \int \Psi^* A \Psi \mathrm{d}V. \tag{9.21}$$

We do not require equality with $\int (A\Psi)^* \Psi \mathrm{d}V$, as we did in (9.20). Actually, this does not apply to any operator, but only to a certain class of operators (Hermitian

[8]As mentioned in Chap. 4, we use the shorthand notation of summation $\sum_n$ instead of $\sum_{n=1}^{\infty}$. Similarly, we also abbreviate integrals: $\int \Psi \mathrm{d}V$ is *not* an indefinite, but a definite integral, which is carried out over the whole domain of definition of Ψ, namely $\int \Psi \mathrm{d}V \equiv \int_{\text{domain of definition}} \Psi \mathrm{d}V$. The range of integration is explicitly specified only in exceptional cases.

[9]An example is the angular momentum, $\mathbf{l} = \mathbf{r} \times \mathbf{p}$.

operators); we come back to this point in a moment. We note that we have a tool with (9.21)[10] to connect quite generally operators of quantum mechanics with measurable quantities.[11]

We first want to recover the expressions found in Chap. 7. For this purpose we start from the eigenvalue problem

$$H\varphi_n(x) = E_n\varphi_n(x); \int \varphi_n^*(x)\,\varphi_m(x)\,\mathrm{d}x = \delta_{nm}. \tag{9.22}$$

The total state is

$$\Psi(x,t) = \sum\nolimits_n c_n\varphi_n(x)\,e^{-iE_nt/\hbar}. \tag{9.23}$$

Then it follows that

$$\begin{aligned}
\langle H\rangle = \int \Psi^* H\Psi \mathrm{d}x &= \int \sum_{n,m} c_n^*\varphi_n^*(x)\,e^{iE_nt/\hbar} H c_m\varphi_m(x)\,e^{-iE_mt/\hbar}\mathrm{d}x \\
&= \int \sum_{n,m} c_n^*\varphi_n^*(x)\,e^{iE_nt/\hbar} E_m c_m\varphi_m(x)\,e^{-iE_mt/\hbar}\mathrm{d}x \\
&= \sum_{n,m} c_n^* E_m c_m e^{i(E_n-E_m)t/\hbar} \int \varphi_n^*(x)\,\varphi_m(x)\,\mathrm{d}x \\
&= \sum_{n,m} c_n^* E_m c_m e^{i(E_n-E_m)t/\hbar}\delta_{nm} = \sum_n |c_n|^2 E_n.
\end{aligned} \tag{9.24}$$

So we have found again the familiar expression for the expectation value. As mentioned above, the definition (9.21) has the advantage that it is readily applicable to continuous variables such as the position (see exercises).

Some remarks are in order:

1. The expectation value depends on the state. If necessary, one can include this by using e.g. the notation $\langle A\rangle_\Psi = \int \Psi^* A\Psi \mathrm{d}V$.
2. In general, the expectation value is time dependent, but this is often not explicitly stated. For pure energy states (proportional to $e^{-i\omega t}$), however, the time dependence cancels out when averaging over e.g. x. In such cases, the expectation values are independent of time (see exercises).
3. A remark just to clarify our concepts: Strictly speaking, the mean value refers to a data set from the past, i.e. to a previously performed measurement, and it is formulated in terms of relative frequencies of occurrence. By contrast, the expectation value, as a conjecture about the future, is formulated with probabilities and is the theoretically-predicted mean. However, in quantum mechanics the notions

[10] Another one we have already discussed above (e.g. in Chap. 4), namely that only the eigenvalues of operators can occur as measured values.

[11] One can show that this type of averaging must follow under very general conditions (Gleason's theorem, see Appendix T, Vol. 2).

of expectation value and mean value are often used interchangeably due to a certain nonchalance of the physicists, and for a finite number of measurements, the term probability w_i is applied instead of relative frequency (as indeed 'ensemble' is used also for a finite set of identically prepared systems). A brief example in Appendix O, Vol. 1, illustrates the difference between the mean value and the expectation value.

4. As stated at the beginning of this chapter, a repeated measurement of a *classical* quantity yields a different value each time. With continued repetition, the mean value of all these measured values shows an increasingly better agreement with the true value. If the measuring instruments were *ideal*, we would obtain the same value every time.

   In contrast, in quantum mechanics, successive measurements of an identical ensemble can in general give *different* values (corresponding to different eigenvalues of the measured physical quantity) even with an ideal measurement apparatus.[12] We have already mentioned that in a single experiment we can obtain only *one eigenvalue* of the operator which corresponds to the measured physical quantity. Which one of the eigenvalues this will be cannot be predicted before the experiment (if the state is given by a superposition). In other words: Quantum-mechanical variables generally have *no* 'true' value.

   When we speak of the expectation *value* of a physical quantity A, this therefore does not imply that A *has* necessarily this value in the sense that classical quantities have 'true' values. Instead of the expectation value, it would therefore be more cautious and unbiased to speak of the *expected measured value* or the like. However, such a terminology is not often used.

9.1.5 Variance, Standard Deviation

A convenient measure of the deviation from the mean value of a classical variable A (no doubt familiar from introductory laboratory courses) is the *mean square deviation* or *variance* $(\Delta A)^2$:

$$(\Delta A)^2 = \left\langle (A - \langle A \rangle)^2 \right\rangle = \left\langle A^2 \right\rangle - \langle A \rangle^2 . \tag{9.25}$$

To obtain the same physical unit as for A, one takes the root and obtains with ΔA the *standard deviation*, also called *dispersion* or *uncertainty*. A brief motivation for the form of this expression is found in Appendix O, Vol. 1.

We adopt this concept also in quantum mechanics. Since the uncertainty ΔA depends in general on the state Ψ of the system, there is also the notation $\Delta_\Psi A$ or

[12] If we send e.g. a horizontally linearly-polarized photon through a linear analyzer, rotated by the angle φ, we obtain, as discussed in Chap. 2, different measurement results (horizontal or vertical polarization) with the probabilities $\cos^2 \varphi$ and $\sin^2 \varphi$. This is true *in principle* and is not due to shortcomings of the measurement apparatus.

the like. An example is given in the exercises, treating the uncertainty of position and momentum in the infinite potential well.

We repeat a note on the significance of the standard deviation in quantum mechanics (cf. remark 4, above): In classical physics, the standard deviation ΔA is a measure of the dispersion of the measured values which arises due to instrumental imperfections. In quantum mechanics, the meaning is quite different; ΔA is not due to instrumental errors, but is an unavoidable genuine quantum effect. Successive measurements can yield different values even for ideal measuring equipment.[13] If and only if $\Delta_\Psi A = 0$ is the quantum object in an eigenstate of the measured operator A and all members of an ensemble have the same value of the physical quantity A. An exercise illustrates that statement by considering the energy in the infinite potential well.

In this sense, the quantum-mechanical dispersion may be seen as a measure of the extent to which a system 'has' a value for A ($\Delta A = 0$) or 'has not' ($\Delta A > 0$). Thus, if in the infinite potential well (of width a), the energy eigenstate φ_n has the position uncertainty $\Delta x = \frac{a}{2}\sqrt{\frac{n^2\pi^2-6}{3n^2\pi^2}} \sim 0.3a$ (see the exercises), this does not mean that each (single) position measurement always has an error of this magnitude, but rather that the quantum object simply does not have a position in the classical sense. In other words, the concept of 'exact location' is not appropriate to this quantum-mechanical problem. More on this issue will be given in later chapters.

9.2 Hermitian Operators

An essential property of measurement results is that they are *real*. If the expectation values represent measurable quantities, they must also be real. Therefore, it must hold that

$$\langle A \rangle = \langle A \rangle^* \tag{9.26}$$

or

$$\int \Psi^* (A\Psi)\, \mathrm{d}V = \int (A\Psi)^* \, \Psi \mathrm{d}V. \tag{9.27}$$

All operators in the small table (9.20) share this property. One can furthermore show for these operators that for two arbitrary functions[14] Ψ_1 and Ψ_2, the equation

$$\int \Psi_1^* A \Psi_2 \mathrm{d}V = \int (A\Psi_1)^* \, \Psi_2 \mathrm{d}V \tag{9.28}$$

[13] In view of this, some other expression than 'standard deviation' would be more appropriate in quantum mechanics to indicate the spread of measurement results, but the mathematical simplicity of this expression has led to its widespread use.

[14] Arbitrary only insofar as the two functions have to satisfy the necessary technical requirements and the integrals have to exist. We note that the Hermiticity of operators may depend on the functions on which they act. This point is addressed explicitly in the exercises for this chapter.

holds. Generally, an operator A satisfying (9.28) is called *Hermitian*. We have already met up with Hermitian operators (and their representation as Hermitian matrices) in the algebraic approach, but these operators do not seem to have much to do with (9.28). But, contrary to that appearance, they in fact amount to the same thing, as we will see in more detail in Chap. 11 under the topic 'matrix mechanics'.

As just pointed out, the expectation values of Hermitian operators are real. This makes sense, since in quantum mechanics *all* measurable quantities are represented by Hermitian operators. In addition, Hermitian operators in general have other very practical features: they have only *real eigenvalues* (which represent the possible individual measured values), and, in the case of a nondegenerate spectrum, their *eigenfunctions* are *pairwise orthogonal* to each other (as we have already seen in the example of the infinite potential well). We now want to prove these two properties.

9.2.1 Hermitian Operators Have Real Eigenvalues

We consider the eigenvalue equation

$$Af_n = a_n f_n; \; n = 1, 2, \ldots \tag{9.29}$$

where the operator A is Hermitian:

$$\int f_m^* A f_n \mathrm{d}V = \int (Af_m)^* f_n \mathrm{d}V. \tag{9.30}$$

We want to show now that its eigenvalues are real, i.e. $a_n = a_n^*$.

To this end, we write the two equations:

$$Af_n = a_n f_n; \; (Af_n)^* = a_n^* f_n^*. \tag{9.31}$$

We multiply the left equation by f_n^* and the right one by f_n:

$$f_n^* A f_n = f_n^* a_n f_n; \; (Af_n)^* f_n = a_n^* f_n^* f_n. \tag{9.32}$$

Integration over all space yields

$$\int f_n^* A f_n \mathrm{d}V = a_n \int f_n^* f_n \mathrm{d}V; \; \int (Af_n)^* f_n \mathrm{d}V = a_n^* \int f_n^* f_n \mathrm{d}V. \tag{9.33}$$

Because of the Hermitian property of A, the two left-hand sides of these equations are the same. Therefore also the right sides have to be equal:

$$a_n \int f_n^* f_n \mathrm{d}V = a_n^* \int f_n^* f_n \mathrm{d}V \leftrightarrow \left(a_n - a_n^*\right) \int f_n^* f_n \mathrm{d}V = 0. \tag{9.34}$$

Due to $\int f_n^* f_n \mathrm{d}V = 1 \neq 0$, it follows that

$$a_n = a_n^* \leftrightarrow a_n \in \mathbb{R}. \tag{9.35}$$

We see that the eigenvalues of a Hermitian operator are real. This also holds, as said above, for the expectation values. We note again that the result of measuring a physical quantity can only be one of the eigenvalues of the corresponding operator.

9.2.2 *Eigenfunctions of Different Eigenvalues Are Orthogonal*

Given a Hermitian operator A and the eigenvalue equation

$$Af_n = a_n f_n; \tag{9.36}$$

the spectrum is assumed to be nondegenerate. Then we have

$$\int f_m^* f_n \mathrm{d}V = 0 \text{ for } n \neq m. \tag{9.37}$$

In order to show this, we begin with

$$Af_n = a_n f_n;\ (Af_m)^* = a_m f_m^*. \tag{9.38}$$

a_m is real, as we have just shown. We extend the equations

$$f_m^* Af_n = a_n f_m^* f_n;\ (Af_m)^* f_n = a_m f_m^* f_n \tag{9.39}$$

and integrate:

$$\int f_m^* Af_n \mathrm{d}V = a_n \int f_m^* f_n \mathrm{d}V;\ \int (Af_m)^* f_n \mathrm{d}V = a_m \int f_m^* f_n \mathrm{d}V. \tag{9.40}$$

Since A is Hermitian, the left sides are equal. It follows that:

$$(a_n - a_m) \int f_m^* f_n \mathrm{d}V = 0. \tag{9.41}$$

Since $n \neq m$ (and because there is no degeneracy), we have $a_n \neq a_m$. Then we conclude:

$$\int f_m^* f_n \mathrm{d}V = 0 \text{ for } n \neq m. \tag{9.42}$$

We can generalize this equation by including the case $m = n$. Since we always normalize the eigenfunctions, the result reads:

$$\int f_m^* f_n \mathrm{d}V = \delta_{nm}. \tag{9.43}$$

In other words, Hermitian operators always have real eigenvalues and their eigenfunctions constitute an ON system.

9.3 Time Behavior, Conserved Quantities

Examination of the time behavior of expectation values leads to the concept of *conserved quantities*. In addition, we can establish a connection to classical mechanics.

9.3.1 Time Behavior of Expectation Values

Since the wavefunction depends upon time, the expectation value of a physical quantity

$$\langle A \rangle = \int \Psi\left(\mathbf{r}, t\right)^* A \Psi(\mathbf{r}, t) \mathrm{d}V \tag{9.44}$$

will in general also be time dependent.

We consider the first time derivative of $\langle A \rangle$ and express the derivatives of the wavefunction using the SEq $i\hbar\dot{\Psi} = H\Psi$, while assuming that the potential V in $H = -\frac{\hbar^2}{2m}\nabla^2 + V$ is real. It follows that:

$$\begin{aligned} i\hbar \frac{\mathrm{d}}{\mathrm{d}t} \langle A \rangle &= i\hbar \int \dot{\Psi}^* A \Psi \mathrm{d}V + i\hbar \int \Psi^* \dot{A} \Psi \mathrm{d}V + i\hbar \int \Psi^* A \dot{\Psi} \mathrm{d}V \\ &= -\int \left(H\Psi\right)^* A\Psi \mathrm{d}V + i\hbar \int \Psi^* \dot{A} \Psi \mathrm{d}V + \int \Psi^* A H \Psi \mathrm{d}V \\ &\underset{H \text{ Hermitian}}{=} -\int \Psi^* H A \Psi \mathrm{d}V + i\hbar \int \Psi^* \dot{A} \Psi \mathrm{d}V + \int \Psi^* A H \Psi \mathrm{d}V \\ &= \int \Psi^* \left(AH - HA\right) \Psi \mathrm{d}V + i\hbar \left\langle \frac{\partial}{\partial t} A \right\rangle. \end{aligned} \tag{9.45}$$

Here, we have used the Hermiticity of the Hamiltonian:

$$\begin{aligned} \textstyle\int \Psi_1^* H \Psi_2 \mathrm{d}V &= \textstyle\int \left(H\Psi_1\right)^* \Psi_2 \mathrm{d}V \ \text{ or} \\ \textstyle\int \Psi^* H A \Psi \mathrm{d}V &= \textstyle\int \left(H\Psi\right)^* A\Psi \mathrm{d}V. \end{aligned} \tag{9.46}$$

$(AH - HA)$ is evidently the commutator of A and H. Then

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} \langle A \rangle = \int \Psi^* [A, H] \Psi \mathrm{d}V + i\hbar \left\langle \frac{\partial}{\partial t} A \right\rangle, \tag{9.47}$$

or in compact form,

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} \langle A \rangle = \langle [A, H] \rangle + i\hbar \left\langle \frac{\partial}{\partial t} A \right\rangle. \tag{9.48}$$

Practically all of the operators which we consider below do not depend explicitly on time.[15] In that case, $\frac{\partial}{\partial t} A$ is zero, and it thus follows that:

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} \langle A \rangle = \langle [A, H] \rangle, \text{ if } A \text{ is not explicitly time dependent.} \tag{9.49}$$

Although we will deal hereafter only with time-independent Hamiltonians, we nevertheless remark that the reasoning leading to (9.48) and (9.49) applies to both time-dependent and time-independent Hamiltonians. The key feature is the Hermiticity of H.

9.3.2 Conserved Quantities

Let us assume that we have an operator A which (i) is not explicitly time-dependent, i.e. $\frac{\partial A}{\partial t} = 0$, and which (ii) commutes with H, i.e. $[A, H] = 0$. Then it follows from (9.49) that:

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} \langle A \rangle = 0 \text{ , if } \frac{\partial}{\partial t} A = 0 \text{ and } [A, H] = 0. \tag{9.50}$$

In other words, the expectation value $\langle A \rangle$ (and the associated physical quantity) remains constant over time, in which case one speaks of a *conserved quantity* or a *constant of the motion*.[16] As is well known, conserved quantities play a special role in physics: They (or the underlying symmetries) allow for a simpler description of a system.[17] For time-independent operators, the statements 'A commutes with H' and 'A is a conserved quantity' are equivalent. Thus, we have an effective instrument at our disposal for determining whether or not a given operator represents a conserved quantity.

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[15] Examples are the momentum operator $\mathbf{p} = \frac{\hbar}{i} \nabla$ or the Hamiltonian, if the potential is time-independent.

[16] Or also of a 'good quantum number', if required.

[17] We will take a closer look at this question in Chap. 21, Vol. 2, 'Symmetries'.

9.3.3 *Ehrenfest's Theorem*

The question of whether position and momentum are conserved quantities leads to a connection with classical mechanics. It also provides a retrospective confirmation (in the sense of a self-consistent approach) of (9.8).

The physical problem is three-dimensional. We begin with the x component of the momentum. With $H = H_0 + V = \frac{p^2}{2m} + V$, we have

$$\begin{aligned}[p_x, H] &= p_x H - H p_x = p_x H_0 + p_x V - H_0 p_x - V p_x \\ &= \frac{\hbar}{i}\frac{\partial}{\partial x}V - V\frac{\hbar}{i}\frac{\partial}{\partial x} = \frac{\hbar}{i}\frac{\partial V}{\partial x} + \frac{\hbar}{i}V\frac{\partial}{\partial x} - \frac{\hbar}{i}V\frac{\partial}{\partial x} = \frac{\hbar}{i}\frac{\partial V}{\partial x}.\end{aligned} \tag{9.51}$$

For the time behavior of p_x, it follows that:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle p_x\rangle = -\left\langle\frac{\partial V}{\partial x}\right\rangle \text{ or } \frac{\mathrm{d}}{\mathrm{d}t}\langle \mathbf{p}\rangle = -\langle \nabla V\rangle\,. \tag{9.52}$$

Next, we consider the position x. We have:

$$\begin{aligned}[x, H] &= xH - Hx = xH_0 + xV - H_0 x - Vx \\ &= x\frac{p^2}{2m} - \frac{p^2}{2m}x = x\frac{p_x^2}{2m} - \frac{p_x^2}{2m}x = -\frac{\hbar^2}{2m}\left(x\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial x^2}x\right)\end{aligned} \tag{9.53}$$

and it follows that

$$[x, H] = \frac{\hbar^2}{m}\frac{\partial}{\partial x} \text{ or } [\mathbf{r}, H] = \frac{\hbar^2}{m}\nabla. \tag{9.54}$$

With $\mathbf{p} = \frac{\hbar}{i}\nabla$, this yields for the time behavior:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \mathbf{r}\rangle = \frac{1}{m}\langle \mathbf{p}\rangle\,. \tag{9.55}$$

Hence, we have recovered our starting point, (9.8), which means that we have obtained a confirmation of our *ansatz* in the sense of a self-consistent description.

We summarize the results of this section. For the expectation values of position and momentum, we have[18]:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \mathbf{r}\rangle = \frac{1}{m}\langle \mathbf{p}\rangle \text{ and } \frac{\mathrm{d}}{\mathrm{d}t}\langle \mathbf{p}\rangle = -\langle \nabla V\rangle\,. \tag{9.56}$$

The form of the equations is reminiscent of the classical Hamilton equations for a particle,

[18]So we find $m\frac{d^2}{\mathrm{d}t^2}\langle \mathbf{r}\rangle = -\langle \nabla V\rangle = \langle \mathbf{F}(\mathbf{r})\rangle$. In principle, one must still show that $\langle \mathbf{F}(\mathbf{r})\rangle = \mathbf{F}(\langle \mathbf{r}\rangle)$ (or one defines the force accordingly).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{r} = \frac{1}{m}\mathbf{p} \text{ and } \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{p} = -\nabla V, \tag{9.57}$$

which can be written in this simple case as a Newtonian equation of motion:

$$\frac{d\mathbf{p}}{\mathrm{d}t} = m\frac{d^2\mathbf{r}}{\mathrm{d}t^2} = -\nabla V = \mathbf{F}. \tag{9.58}$$

In short: The quantum-mechanical expectation values obey the corresponding classical equations. This (and therefore also the (9.56)) is called Ehrenfest's theorem.[19]

9.4 Exercises

1. Given a Hermitian operator A and the eigenvalue problem $A\varphi_n = a_n\varphi_n$, $n = 1, 2, \ldots$, show that:
   (a) The eigenvalues are real.
   (b) The eigenfunctions are pairwise orthogonal. Here, it is assumed that the eigenvalues are nondegenerate.
2. Show that the expectation value of a Hermitian operator is real.
3. Show that
$$\int \Psi_1^* A \Psi_2 \mathrm{d}V = \int (A\Psi_1)^* \Psi_2 \mathrm{d}V \tag{9.59}$$
   holds for the operators **r, p**, H. Restrict the discussion to the one-dimensional case. What conditions must the wavefunctions satisfy?
4. Show that for the infinite potential well (between 0 and a), $\langle x \rangle = \frac{a}{2}$.
5. Given the infinite potential well with walls at $x = 0$ and $x = a$; we consider the state
$$\Psi(x, t) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) e^{-i\omega_n t}. \tag{9.60}$$
   (a) Determine the position uncertainty Δx.
   (b) Determine the momentum uncertainty Δp.
6. In the infinite potential well, a normalized state is given by
$$\Psi(x, t) = c_n\varphi_n(x)e^{-i\omega_n t} + c_m\varphi_m(x)e^{-i\omega_m t}; \quad c_n, c_m \in \mathbb{C}; \quad n \neq m. \tag{9.61}$$
   Calculate $\langle x \rangle$.

[19] We note that also the general law (9.48) for the time dependence of mean values is sometimes called Ehrenfest's theorem.

7. Consider an infinite square well with potential limits at $x = 0$ and $x = a$. The initial value of the wavefunction is $\Psi(x, 0) = \Phi \in \mathbb{R}$ for $b - \varepsilon \leq x \leq b + \varepsilon$ and $\Psi(x, 0) = 0$ otherwise (of course, $0 \leq b - \varepsilon$ and $b + \varepsilon \leq a$). Remember that the eigenfunctions $\varphi_n(x) = \sqrt{\frac{2}{a}} \sin k_n x$ with $k_n = \frac{n\pi}{a}$ form a CONS.
   (a) Normalize the initial state.
   (b) Calculate $\Psi(x, t)$.
   (c) Find the probability of measuring the system in the state n.
8. Show that for the expectation value of a physical quantity A,

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} \langle A \rangle = \langle [A, H] \rangle + i\hbar \left\langle \frac{\partial}{\partial t} A \right\rangle \tag{9.62}$$

   holds. Show that for time-independent operators, the expectation value of the corresponding physical quantity is conserved, if A commutes with H.
9. Show that

$$\frac{\mathrm{d}}{\mathrm{d}t} \langle \mathbf{r} \rangle = \frac{1}{m} \langle \mathbf{p} \rangle \ \text{ and } \frac{\mathrm{d}}{\mathrm{d}t} \langle \mathbf{p} \rangle = -\langle \boldsymbol{\nabla} V \rangle. \tag{9.63}$$

10. Under which conditions is the orbital angular momentum $\mathbf{l} = \mathbf{r} \times \mathbf{p}$ a conserved quantity?
11. Given the Hamiltonian H with a discrete and nondegenerate spectrum E_n and eigenstates $\varphi_n(\mathbf{r})$, show that the energy uncertainty ΔH vanishes, iff the quantum object is in an eigenstate of the energy.