Chapter 11
Abstract Notation

We are now starting to bring together the analytical and the algebraic approaches to quantum mechanics. In this chapter, we first consider the vector space of solutions of the SEq in more detail. After a brief excursion into matrix mechanics, we treat the abstract representation of quantum mechanics, which is formulated in terms of the familiar bras and kets.

In Chap. 10, we saw that the analytic and the algebraic approaches lead to very similar formulations. We deepen this parallelism in the following sections by showing that the expression $\int \Phi^* \Psi \mathrm{d}V$ is a scalar product. With some additional assumptions, it follows that the vector spaces of both the algebraic and analytic approaches are Hilbert spaces. With this background, we can then formulate a representation-independent, i.e. an *abstract* notation.

All the spectra which we consider in this chapter are discrete and non-degenerate.

11.1 Hilbert Space

11.1.1 Wavefunctions and Coordinate Vectors

In Chap. 10, we ventured the guess that $\int \Phi^* \Psi \mathrm{d}V$ is a scalar product. We now want to provide some additional motivation for this assumption.

We start with a Hamiltonian H (with a discrete and non-degenerated energy spectrum). Its eigenfunctions $\varphi_n(\mathbf{r})$, i.e. the solutions of the stationary SEq

$$H\varphi_n(\mathbf{r}) = E_n \varphi_n(\mathbf{r}); \; n = 1, 2, \ldots \tag{11.1}$$

are known and form a CONS. Because of the completeness of $\varphi_n(\mathbf{r})$, we can write any solution $\psi(\mathbf{r}, t)$ of the time-dependent SEq as

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$$\psi(\mathbf{r}, t) = \sum\nolimits_n c_n \varphi_n(\mathbf{r})\, e^{-i\frac{E_n t}{\hbar}};\ c_n \in \mathbb{C}. \tag{11.2}$$

To save writing, we restrict the following considerations to the initial state (i.e. we freeze time at $t = 0$):

$$\psi(\mathbf{r}, 0) = \sum\nolimits_n c_n \varphi_n(\mathbf{r}). \tag{11.3}$$

The total time evolution can be determined easily from (11.2). Due to the orthonormality of the eigenfunctions, the coefficients c_n are specified uniquely by the initial condition $\psi(\mathbf{r}, 0)$:

$$c_n = \int \varphi_n^*(\mathbf{r})\, \psi(\mathbf{r}, 0)\, \mathrm{d}V. \tag{11.4}$$

We can understand this situation a little differently. To this end, we take into account the fact that the eigenfunctions $\{\varphi_n(\mathbf{r})\}$ represent an orthonormal basis of the vector space $\mathcal{V}$ of solutions of the SEq—analogous to the three unit vectors $\mathbf{e}_x$, $\mathbf{e}_y$ and $\mathbf{e}_z$ in the visual space or $\mathbb{R}^3$. In the latter space, we can represent a general vector $\mathbf{v}$ as $\mathbf{v} = v_x\mathbf{e}_x + v_y\mathbf{e}_y + v_z\mathbf{e}_z$, where the components or expansion coefficients v_x, v_y, v_z are usually called the *coordinates* of $\mathbf{v}$. It makes no difference whether we specify $\mathbf{v}$ or v_x, v_y, v_z—we can calculate $\mathbf{v}$ uniquely from v_x, v_y, v_z and *vice versa*, if the unit vectors are known.

The situation described in (11.3) and (11.4) is quite analogous - only we are dealing with the function $\psi(\mathbf{r}, 0)$ instead of the vector $\mathbf{v}$, the eigenfunctions φ_n instead of the unit vectors $\mathbf{e}_i$, and the constants c_n instead of the coordinates v_x. For example, the c_n can be determined uniquely (for known φ_n), if $\psi(\mathbf{r}, 0)$ is given, and *vice versa*. We can thus denote the expansion coefficients c_n as coordinates and have the same information (always assuming that φ_n is known), whether we are given $\psi(\mathbf{r}, 0)$ or the coordinate vector

$$\mathbf{c} = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \end{pmatrix} \tag{11.5}$$

We now consider two wavefunctions $\psi = \sum_i c_i\varphi_i$ and $\chi = \sum_j d_j\varphi_j$. Because of the orthonormality of the eigenfunctions, we have

$$\int \psi^*\chi \mathrm{d}V = \sum_{ij} c_i^* d_j \int \varphi_i^*\varphi_j \mathrm{d}V = \sum_{ij} c_i^* d_j \delta_{ij} = \sum_i c_i^* d_i. \tag{11.6}$$

We find exactly the same result when we take the dot product of the two coordinate vectors $\mathbf{c}$ and $\mathbf{d}$; it is

$$\mathbf{c}^{\dagger}\mathbf{d} = \left(c_1^* \; c_2^* \; \ldots\right) \cdot \begin{pmatrix} d_1 \\ d_2 \\ \vdots \end{pmatrix} = \sum_i c_i^* d_i \tag{11.7}$$

Comparing (11.6) and (11.7), we see that the expression $\int \psi^* \chi \mathrm{d}V$ is clearly a scalar product.[1]

11.1.2 The Scalar Product

The formal confirmation that $\int \psi^* \chi \mathrm{d}V$ is a scalar product is found in mathematics. There, the scalar product is generally defined as a rule which assigns to two elements x and y of a vector space a scalar (x, y), where the following properties must apply: (x, y) is (i) positive definite: $(x, x) \geq 0$ and $(x, x) = 0 \leftrightarrow x = 0$; (ii) linear: $(x, \alpha y + \beta z) = \alpha (x, y) + \beta (x, z)$; (iii) Hermitian or conjugate symmetric: $(x, y) = (y, x)^*$ (see also Appendix F, Vol. 1). *Any* rule that meets these requirements is a scalar product (also called *Hermitian form*).

In order to test $\int f^* g \mathrm{d}V$ for these properties, we do not choose the notation (f, g), but refer instead to the algebraic approach $\langle f \mid g \rangle$, i.e.

$$\langle f \mid g \rangle := \int f^* g \mathrm{d}V. \tag{11.8}$$

At this point is not clear how a ket $|g\rangle$ and a bra $\langle f|$ are specifically defined; we address this question in Chap. 12. But notwithstanding this, we can easily show that $\int f^* g \mathrm{d}V$ is a scalar product - even though the expression may not have looked like one when we wrote it down for the first time in Chap. 5. For it is immediately apparent that $\int f^* g \mathrm{d}V$ assigns a number to two elements.[2] Furthermore, $\int f^* g \mathrm{d}V$ is

1. positive definite: $\langle f \mid f \rangle = \int f^* f \mathrm{d}V \geq 0, \in \mathbb{R}$ where $\langle f \mid f \rangle = 0 \Leftrightarrow f \equiv 0$.
2. linear[3]: $\langle f \mid \alpha g + \beta h \rangle = \int f^* (\alpha g + \beta h) \, \mathrm{d}V = \alpha \int f^* g \mathrm{d}V + \beta \int f^* h \mathrm{d}V = \alpha \langle f \mid g \rangle + \beta \langle f \mid h \rangle$.
3. Hermitian or conjugate symmetric: $\langle f \mid g \rangle = \int f^* g \mathrm{d}V = \left(\int f g^* \mathrm{d}V\right)^* = \langle g \mid f \rangle^*$.

[1] We see, by the way, that the scalar product is independent of the representation. The left-hand sides of (11.6) and (11.7) are two different representations of the same expression.

[2] We remark again that in general, we do not specify the integration limits for integrals as in (11.8). It is tacitly assumed that one integrates over the entire domain of definition of the integrand. Contrary to the initial impression, these integrals are *definite* integrals - in other words, scalars (which may be time dependent).

[3] More precisely, semi-linear in the first and linear in the second component (also denoted as anti-linear or conjugate linear in the first argument and linear in the second argument). Therefore, the form is not called bilinear, but sesquilinear. In mathematics, the form is usually defined the other way around, as antilinear in the second argument.

By means of the scalar product $\int f^* g \mathrm{d}V$, we can therefore not only define as usual the length or norm of wavefunctions by $||\varphi|| = \sqrt{\langle\varphi|\,\varphi\rangle} = \sqrt{\int \varphi^* \varphi \mathrm{d}V}$ and the orthogonality of two wave functions (as elements of the vector space) by $\langle\varphi|\,\psi\rangle = \int \varphi^* \psi \mathrm{d}V = 0$, but also we can use general statements about scalar products (e.g. the Schwarz and the triangle inequalities) without further ado.

Thus, the solutions of the SEq span a complex vector space in which a scalar product is defined. Such spaces are called *unitary spaces*, as we know already from the algebraic approach (Chap. 4). At this point it is perhaps possible to understand somewhat better why the eigenfunctions φ_m, φ_n, obeying $\int \varphi_m^* \varphi_n \mathrm{d}V = \delta_{nm}$, are called orthonormal. On the one hand, one can call an element of a vector space a 'vector'—an eigenfunction as an element of a vector space is an eigenvector. On the other hand, $\int \varphi_m^* \varphi_n \mathrm{d}V = 0$ for $n \neq m$ means in the sense of a scalar product that the eigenfunctions (as eigenvectors) are pairwise orthogonal,[4] and $\int \varphi_n^* \varphi_n \mathrm{d}V = 1$ means that they have length 1 or are normalized.

11.1.3 Hilbert Space

The way we constructed it, our unitary space is *separable*.[5] This means, essentially, that there is a CONS of at most *countably infinite dimension*. Any vector ψ can be expanded in terms of this CONS (*expansion theorem*):

$$\psi(\mathbf{r}, t) = \sum\nolimits_n d_n(t) \varphi_n(\mathbf{r}) \text{ with } d_n(t) = \int \varphi_n^*(\mathbf{r}) \psi(\mathbf{r}, t) \,\mathrm{d}V. \tag{11.9}$$

This sum and others like $|\psi(\mathbf{r}, t)|^2 = \sum\limits_n |d_n(t)|^2$ must of course be meaningful, i.e. they must converge to an element which itself belongs to the vector space. We therefore require that the vector space be *complete*, which means that sequences[6] have limits which are themselves elements of the vector space.[7] A space with all these ingredients is called a (separable)[8] *Hilbert space* $\mathcal{H}$. A quantum-mechanical state is an element of $\mathcal{H}$ and thus may be denoted, as stated above, as a vector, even if it is in fact a function in the concrete representation.

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[4] As said above, this does not mean that the graphs of the functions are orthogonal to each other or something similar. The statement refers only to the (abstract) angle between two vectors in the vector space.

[5] The term 'separable' which occurs here has nothing to do with the requirement of 'separability,' which means that a system (function) is separable into functions of space and of time.

[6] The technical term is Cauchy sequences, see Appendix G, Vol. 1.

[7] The requirement of completeness has no straightforward physical meaning, but it occurs in many proofs of laws concerning Hilbert spaces.

[8] There are also non-separable Hilbert spaces (for example, in the quantization of fields). But in 'our' quantum mechanics, they play no role, so here 'Hilbert space' means in general 'separable Hilbert space.'

We see in retrospect that the unitary spaces which we considered in the algebraic approach are also separable Hilbert spaces. Now, the punchline of this story is that *all* Hilbert spaces of the same dimension are *isomorphic*, i.e. there are reversible unique (one-to-one, bijective) mappings between them. That is why we also often speak of *the* Hilbert space $\mathcal{H}$ of dimension N, for which there are various realizations or representations. In particular, the space of solutions (11.2) of the SEq, as spanned by $\{\varphi_n(\mathbf{r})\}$, and the space of the coordinate vectors $\mathbf{c}$ are isomorphic; that is they are just different representations of the same systems. Of course, the question arises as to whether there is a *representation-independent*, i.e. *abstract* formulation of these systems. We take up this issue below.

If we disregard the technical issues (which we do not consider to a greater extent in the following), then $\mathcal{H}$ is basically a very intuitive structure. As we have already indicated above, we can in principle imagine everything as in $\mathbb{R}^3$, despite the possibly much higher dimensionality of the Hilbert space and its use of complex numbers. In both spaces, mutually orthogonal and normalized vectors, i.e. unit vectors, constitute a basis and span the entire space; any vector can therefore be represented as a linear combination of basis vectors. In addition, we also have an inner product in both spaces, which automatically defines a norm. We can imagine an intuitive analog to the time-dependent (normalized) state vector $\psi(\mathbf{r}, t) \in \mathcal{H}$ of (11.9): In $\mathbb{R}^3$ this would be a vector of length 1, which moves in the course of time. A state with a sharp energy $\in \mathcal{H}$ corresponds to a circular motion in $\mathbb{R}^3$, because the time dependence in $\mathcal{H}$ is given by $\exp(-i\omega t)$.[9]

11.2 Matrix Mechanics

We have seen that we obtain the same information if we specify the vector $\mathbf{c}$ instead of the wavefunction $\psi(\mathbf{r}, 0)$. We will now apply this 'algebraization' to eigenvalue problems, also.

In fact, in the early days of quantum mechanics there were two competing formulations: *Matrix mechanics* (associated with the name W. Heisenberg, corresponding essentially to our algebraic approach), and *wave mechanics* (linked to the name Schrödinger, corresponding essentially to our analytic approach). Quite soon it became clear that these formulations, for the same initial physical situation, were just two different descriptions of the same facts, which hence could be converted one-to-one into each other. This can be shown rather simply in a way similar to the above provisional representation using coordinates.

We start from the formulation of an eigenvalue problem of wave mechanics, considering a wavefunction $\Psi(x)$ and an operator A with a discrete and non-degenerate spectrum:

[9] We note that approaching quantum mechanics by means of the Hilbert space is not the only possible option. As a starting point, one could for example consider a C^*-algebra (see Appendix G, Vol. 1), or the aforementioned replacement process $\{,\}_{\text{Poisson}} \rightarrow \frac{1}{i\hbar}[,]_{\text{commutator}}$. This method is called canonical quantization, see Appendix W, Vol. 2.

$$A\Psi(x) = a\Psi(x). \tag{11.10}$$

This problem can be written as a *matrix equation* (that is, among other things: with no spatial dependence). To demonstrate this, in a first step we expand the wavefunction in terms of the eigenfunctions $\{\varphi_i\}$ of the Hamiltonian (or any other basis system in $\mathcal{H}$) as $\Psi = \sum_n c_n \varphi_n(x)$, and obtain

$$A\sum\nolimits_n c_n \varphi_n(x) = a\sum\nolimits_n c_n \varphi_n(x). \tag{11.11}$$

Then we multiply by φ_m^* and take the scalar product:

$$\sum\nolimits_n c_n \int \varphi_m^* A \varphi_n \mathrm{d}V = \sum\nolimits_n c_n \int \varphi_m^* \varphi_n \mathrm{d}V = a c_m \tag{11.12}$$

The integral $\int \varphi_m^* A \varphi_n \mathrm{d}V$ is a *number* that depends on n and m. We call this number A_{mn}:

$$\sum\nolimits_n c_n A_{mn} = a c_m. \tag{11.13}$$

The expression on the left side is simply the product of the matrix $\{A_{mn}\} \equiv \mathbb{A}$ with the column vector $\mathbf{c}$:

$$\mathbb{A}\mathbf{c} = a\mathbf{c}. \tag{11.14}$$

The column vector $\mathbf{c}$ is of course just the coordinate vector introduced above. In this way, we can formulate quantum mechanics as matrix mechanics, representing operators as matrices and states as column vectors. In practice, this is not done in general, but only in cases where this approach is particularly well-suited (e.g. in lower-dimensional systems).

11.3 Abstract Formulation

Thus far, we have met up with various formulations of states, which at first glance seem to have little in common. In the analytical approach, we started from the wavefunction $\psi(\mathbf{r})$, but instead we could have chosen the coordinate vector $\mathbf{c}$. Moreover, there are other possibilities, e.g. the Fourier transform of $\varphi(\mathbf{k}) = \int \psi(\mathbf{r}) e^{i\mathbf{kr}} d^3r$, which provides the same information as the wavefunction itself. In the algebraic approach, we worked with kets, for which the various representations in the form of a column vector are possible. An analogous consideration applies to different formulations of operators: We have just seen that we can likewise write the operators of the analytical approach as matrices. In the algebraic approach, we defined operators as dyadic products, or represented them as matrices. All together, we have quite different but equivalent ways at hand to describe the same facts.

The circumstance that Hilbert spaces of the same dimension are isomorphic is beyond the parallelism of the two approaches established in Chap. 10, and it shows that the analytical and the algebraic approaches are actually just different manifestations of the same facts. For whether we work in a Hilbert space of one or the other approach (and in which one) is irrelevant, insofar as there are one-to-one transformations between all Hilbert spaces of the same dimension. But if we have very different representations for the same facts, there *must* exist a representation-independent, i.e. abstract core.[10]

The fact that we can represent one and the same (physical) situation in many different ways is known to us in a similar form e.g. from $\mathbb{R}^3$. There, a vector also has different representations (components), depending on how we define our coordinate system in space. We can specify this vector abstractly, i.e. in a coordinate-free manner, by writing it not just as a column vector with several components, but instead by denoting it as $\mathbf{a}$ or $\vec{a}$ or something similar. That will not only suffice for many formulations (e.g. $\mathbf{l} = \mathbf{r} \times \mathbf{p}$), but it also facilitates them or renders them expressible in a compact form; think of e.g. the Maxwell equations. For concrete calculations, however, one often has to specify the vectors in some particular representation.[11]

Here, we are in a similar situation, seeking an abstract designation for the elements of the Hilbert space. The notations $\mathbf{a}$ or $\vec{a}$ are 'used up' and also too strongly suggest a column vector. Instead, the convention of writing an abstract vector of the Hilbert space as a ket, $|\Psi\rangle$ has been adopted. It is for this reason that we denoted states as kets from the start in the algebraic approach[12] (a justification in retrospect, so to speak).

In this way, we can write for example an eigenvalue equation like

$$A_{\text{spatial}}\Psi(x) = a\Psi(x)\,;\; A_{\text{matrix}}\mathbf{c} = a\mathbf{c} \tag{11.15}$$

in the abstract formulation as

$$A_{\text{abstract}}\,|\Psi\rangle = a\,|\Psi\rangle\,. \tag{11.16}$$

Some remarks are in order:

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[10] Only the dimension of the state space matters here. The physical system can take a variety of forms. The electronic spin with its two orientations, the polarization of a photon, e.g. with horizontally and vertically linearly-polarized states, the MZI with the basis states $|H\rangle$ and $|V\rangle$, in a certain sense the ammonia molecule (NH_3, where the N atom can tunnel through the H_3 plane and occupy two states with respect to it) are some examples of physically different systems which all 'live' in a two-dimensional Hilbert space.

[11] In fact, the notation $\mathbf{a}$ is very abstract—it does not reveal anything about the dimension nor the individual components. We know nothing more than simply that it is a vector. Nevertheless, this notation is often not perceived as particularly abstract. This is probably due to the fact that one was introduced to it at the beginning of physics courses and it now seems familiar.

[12] This is also why we chose the symbol $\cong$ to distinguish between an abstract ket and its representation as a column vector.

1. It is not known at this point how the ket $|\Psi\rangle$ is formulated in detail[13]; it is just an *abstract notation*, comparable to the designation of a vector by the symbol **a**. Similarly, the form of the operator A_{abstract} is not known at this point; this is comparable to the use of the abstract symbol $\mathbb{A}$ for a general matrix.[14]
2. For the sake of a better distinction, we have denoted the nature of the operators in (11.15) and (11.16) by an index. But it is quite common[15] to use the same symbol for the operators in different concrete and abstract representations, that is to write simply A in all three equations:

$$A\Psi(x) = a\Psi(x);\ A\mathbf{c} = a\mathbf{c}; A|\Psi\rangle = a|\Psi\rangle. \tag{11.17}$$

   Strictly speaking, this is evidently wrong, because A refers to quite different mathematical objects e.g. in the expressions $A\Psi(x)$ and $A|\Psi\rangle$. That this 'nonchalant' notation is rather ambiguous may seem annoying, but it is widespread and can, if one is used to it, even be quite practical. Of course, it must be clear from the context what is precisely meant where necessary.
   In the algebraic approach, we introduced the symbol $\cong$ to emphasize the difference between an abstract ket and its representation as a column vector. In the following, we will relax this rule and often use $=$ instead of $\cong$, thus following common practice.
3. The relationship between $\Psi(x)$ and $|\Psi\rangle$ will be addressed in Chap. 12.

The following paragraph is merely a repetition of the facts already discussed in the preceding (even-numbered) chapters. We recall that the adjoint (of a column vector) means the transposed and complex conjugated vector. The adjoint[16] of a ket is a *bra*:

$$(|\Psi\rangle)^\dagger \equiv \langle\Psi| \tag{11.18}$$

(accordingly, the adjoint of a column vector is the row vector with complex conjugate elements). The adjoint of an operator A is written as $A^\dagger$, where $AA^\dagger = A^\dagger A$ holds. Because the application of an operator A to a ket $|\Psi\rangle$ gives another ket, one also writes

$$A|\Psi\rangle \equiv |A\Psi\rangle. \tag{11.19}$$

The adjoint of a number is its complex conjugate $c^\dagger = c^*$. In particular, we have for the scalar product $\langle f|g\rangle$:

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[13] It is in any case not a column vector (even if this idea sometimes proves to be helpful).

[14] To avoid misunderstandings: **a** is an abstract or general *column vector*, whereas $|\Psi\rangle$ is an *abstract state* which can be represented, where appropriate, as a column vector, but for which also other representations exist. Quite analogously, $\mathbb{A}$ denotes a general matrix and A_{abstract} an abstract operator, which can, where appropriate, be represented as a matrix.

[15] However, there are books that distinguish them quite consistently.

[16] Note that here 'adjoint' means the Hermitian adjoint $a^\dagger$, as always in non-relativistic quantum mechanics. In relativistic quantum mechanics, one uses instead the Dirac adjoint $a^\dagger \gamma_o$.

$$\langle f \mid g\rangle^\dagger = \langle f \mid g\rangle^* = \langle g \mid f\rangle. \tag{11.20}$$

In the adjoint of a compound expression, the order of the constituents is reversed. We give some examples for the adjoint:

$$\begin{gathered}(c\,|\Psi\rangle)^\dagger = c^*\,\langle\Psi| = \langle\Psi|\,c^* \\ (A\,|\Psi\rangle)^\dagger = |A\Psi\rangle^\dagger = \langle A\Psi| = \langle\Psi|\,A^\dagger \\ \langle\Phi\,|A|\,\Psi\rangle^\dagger = \left\langle\Psi\,\middle|A^\dagger\middle|\,\Phi\right\rangle.\end{gathered} \tag{11.21}$$

Expressions of the form $\langle\varphi\,|A|\,\psi\rangle$ are called *matrix elements* . Finally, we note again the equations defining a Hermitian operator: In the formulation with integrals, we have

$$\int \Psi_1^* A\Psi_2 \mathrm{d}V = \int (A\Psi_1)^*\,\Psi_2 \mathrm{d}V. \tag{11.22}$$

With $\int f^* g dV = \langle f\ |g\rangle$, this is written in the bra-ket notation as

$$\begin{aligned}\int \Psi_1^* A\Psi_2 \mathrm{d}V &= \langle\Psi_1\ |A\Psi_2\rangle = \langle\Psi_1\,|A|\,\Psi_2\rangle \\ \int (A\Psi_1)^*\,\Psi_2 \mathrm{d}V &= \langle A\Psi_1\ |\Psi_2\rangle = \left\langle\Psi_1\,\middle|A^\dagger\middle|\,\Psi_2\right\rangle.\end{aligned} \tag{11.23}$$

Comparing the right-hand sides exhibits a familiar result: For a Hermitian operator, it holds that $A = A^\dagger$; the operator is self-adjoint.[17]

Experience shows that it is rather difficult to imagine something quite abstract (only kidding!). So here, we give the hint to think of a column (row) vector in the case of a ket (bra), and of a matrix in the case of an operator (and not to forget that this is an *auxiliary notion*). In this way, many 'calculation rules' and statements become quite familiar, e.g. the rule that operators do not commute in general—which applies also to matrices.

Although the relation between e.g. $\Psi(x)$ and $|\Psi\rangle$ still needs to be clarified, we can 'play around' a little with the abstract notation. As an example, we consider a CONS $\{\varphi_n(x)\}$. From the expansion theorem, it follows for each wavefunction $\Psi(x)$ that

$$\Psi(x) = \sum\nolimits_n c_n \varphi_n(x). \tag{11.24}$$

With

$$c_m = \int \varphi_m^*(x)\Psi(x)\mathrm{d}x = \langle\varphi_m\ |\Psi\rangle, \tag{11.25}$$

we find due to

$$\int \varphi_m^*(x)\varphi_n(x)\mathrm{d}x = \delta_{nm} \tag{11.26}$$

[17] In fact, there may be a difference between self-adjoint and Hermitian (see Chap. 13 and Appendix I, Vol. 1). Among the problems considered here, this difference is not noticeable.

the equation

$$\begin{aligned}\langle\Psi\ |\Psi\rangle = \int \Psi^*(x)\Psi(x)\mathrm{d}x \underset{(11.24)}{=} \int \sum_{n,m} c_n^* c_m \varphi_n^*(x)\varphi_m(x)\mathrm{d}x \underset{(11.26)}{=} \\ \underset{(11.26)}{=} \sum_n c_n^* c_n \underset{(11.25)}{=} \sum_n \langle\Psi\ |\varphi_n\rangle\langle\varphi_n\ |\Psi\rangle .\end{aligned} \tag{11.27}$$

Comparing the right-hand and left-hand sides, we obtain the completeness relation in the abstract notation

$$\sum_n |\varphi_n\rangle\langle\varphi_n| = 1, \tag{11.28}$$

i.e. a result which we knew already from the algebraic approach.

11.4 Concrete: Abstract

Finally, we make a remark about the relationship of the abstract formulation to concrete representations.

In the algebraic approach, the 'de-abstracting' of kets is not problematic. We can associate (and have done so occasionally) a ket to a representation as a column vector such as e.g. $|h\rangle \cong \begin{pmatrix} 1 \\ 0 \end{pmatrix}$. Since we formulate operators in this approach as sums over dyadic products, the concrete representation of operators may be easily formulated. Thus, there are no difficulties with the algebraic formulation at this level.

The situation is similar in the analytical approach when we have a discrete spectrum. Again, as we have just explored, we can represent states and operators that depend on local variables by vectors and matrices.

In order to illustrate these relationships through examples, we start with a Hamiltonian $H = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})$ with a discrete and nondegenerate spectrum. We want to derive the matrix representation and the abstract formulation for the stationary SEq. (Similar considerations for the time-dependent SEq can be found in the exercises.) The eigenvalue problem (stationary SEq) reads

$$H\psi(\mathbf{r}) = E\psi(\mathbf{r}) . \tag{11.29}$$

The eigenfunctions $\varphi_n(\mathbf{r})$ and the eigenvalues E_n of the Hamiltonian are known:

$$H\varphi_n(\mathbf{r}) = E_n\varphi_n(\mathbf{r}); n = 1, 2, \ldots \tag{11.30}$$

Every state $\psi(\mathbf{r})$ can be written as a linear combination of the eigenfunctions (which form a CONS):

$$\psi(\mathbf{r}) = \sum_n c_n\varphi_n(\mathbf{r}); c_n = \int \varphi_n^*(\mathbf{r})\,\psi(\mathbf{r})\ \mathrm{d}V. \tag{11.31}$$

In the matrix representation, we represent the state by the column vector of the coefficients c_n:

$$\mathbf{c} = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \end{pmatrix} \tag{11.32}$$

We identify as follows:

$$\varphi_1(\mathbf{r}) \to \begin{pmatrix} 1 \\ 0 \\ \vdots \end{pmatrix}; \varphi_2(\mathbf{r}) \to \begin{pmatrix} 0 \\ 1 \\ \vdots \end{pmatrix} \text{ etc.} \tag{11.33}$$

Now we have to replace H by a matrix. For this, we repeat the above reasoning by inserting (11.31) into (11.29), multiplying by $\varphi_m^*(\mathbf{r})$, and integrating:

$$\sum\nolimits_n c_n \int \varphi_m^*(\mathbf{r}) H \varphi_n(\mathbf{r}) \, dV = E \sum\nolimits_n c_n \int \varphi_m^*(\mathbf{r}) \varphi_n(\mathbf{r}) \, \mathrm{d}V. \tag{11.34}$$

On the left-hand side, we employ (11.30), and on both sides we make use of the orthonormality of the eigenfunctions. It follows that

$$E_m c_m = E c_m. \tag{11.35}$$

In other words, the Hamiltonian H is replaced by a diagonal matrix H_{matrix}:

$$H_{\text{matrix}} = \begin{pmatrix} E_1 & 0 & \dots \\ 0 & E_2 & \dots \\ \vdots & \vdots & \ddots \end{pmatrix} \tag{11.36}$$

and the stationary SEq in the matrix representation reads

$$H_{\text{matrix}} \mathbf{c} = E \mathbf{c}. \tag{11.37}$$

From this equation, we can reconstruct (11.29)—but as said above, only if we know the eigenfunctions $\varphi_n(\mathbf{r})$ which do not appear in (11.37).

In order to arrive at the abstract notation, we interpret the vector $\begin{pmatrix} 1 \\ 0 \\ \vdots \end{pmatrix}$ as a representation of the ket $|\varphi_1\rangle$, and analogously for the other components. Then it follows that

$$|\varphi_1\rangle \langle\varphi_1| \cong \begin{pmatrix} 1 \\ 0 \\ \vdots \end{pmatrix} \begin{pmatrix} 1 & 0 & \dots \end{pmatrix} = \begin{pmatrix} 1 & 0 & \dots \\ 0 & 0 & \dots \\ \vdots & \vdots & \ddots \end{pmatrix}, \tag{11.38}$$

and we find for the abstract representation of the Hamiltonian[18]:

$$H_{\text{abstract}} = \sum\nolimits_n |\varphi_n\rangle \langle\varphi_n| E_n. \tag{11.39}$$

11.5 Exercises

1. Show that the equation
$$\sum_i c_i A_{ji} = a c_j \tag{11.40}$$
may be written in the matrix representation as
$$\mathbb{A}\mathbf{c} = a\mathbf{c} \tag{11.41}$$
with the matrix $\{A_{ji}\} \equiv \mathbb{A}$ and the column vector $\mathbf{c}$. Is the equation valid also for non-square matrices?
2. Do the functions of one variable which are continuous in the interval [0, 1] form a Hilbert space?
3. The space $l^{(2)}$ consists of all vectors $|\varphi\rangle$ with infinitely many components (coordinates) $c_1, c_2, \ldots$, such that
$$\||\varphi\rangle\|^2 = \sum_n |c_n|^2 < \infty. \tag{11.42}$$
Show that also the linear combination of two vectors $|\varphi\rangle$ and $|\chi\rangle$ belongs to this space, and that the scalar product $\langle\varphi\,|\chi\rangle$ is defined.
4. Given the operator A and the equation
$$i\frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle = A\,|\psi\rangle, \tag{11.43}$$
which condition must A fulfill so that the norm of $|\psi\rangle$ is conserved?
5. Given the operator A, derive the equation
$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\langle A\rangle = \langle[A, H]\rangle + i\hbar\langle\dot{A}\rangle \tag{11.44}$$
in the bra-ket formalism.
6. Given a Hamiltonian H with a discrete and nondegenerate spectrum, (a) in the formulation with space variables, and (b) as an abstract operator; what is in each case the matrix representation of the time-dependent SEq?

[18] This form is called *spectral representation*; we discuss it in more detail in Chap. 13.