

N. Nagaosa

Quantum Field Theory in Condensed Matter Physics

凝聚态物理学中的量子场论

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Preface

Why is quantum field theory of condensed matter physics necessary?

Condensed matter physics deals with a wide variety of topics, ranging from gas to liquids and solids, as well as plasma, where owing to the interplay between the motions of a tremendous number of electrons and nuclei, rich varieties of physical phenomena occur. Quantum field theory is the most appropriate "language", to describe systems with such a large number of degrees of freedom, and therefore its importance for condensed matter physics is obvious. Indeed, up to now, quantum field theory has been successfully applied to many different topics in condensed matter physics. Recently, quantum field theory has become more and more important in research on the electronic properties of condensed systems, which is the main topic of the present volume.

Up to now, the motion of electrons in solids has been successfully described by focusing on one electron and replacing the Coulomb interaction of all the other electrons by a mean field potential. This method is called mean field theory, which made important contributions to the explanation of the electronic structure in solids, and led to the classification of insulators, semiconductors and metals in terms of the band theory. It might be said that also the present achievements in the field of semiconductor technology rely on these foundations.

In the mean field approximation, effects that arise due to the correlation of the motions of many particles, cannot be described. It has been treated in a perturbative way under the assumption that its effect is small. However, recently, many systems that cannot be described in this standard way have been discovered, and it became clear that a new world opened its doors. Connected to these new aspects of condensed matter physics, the most fundamental problem of quantum theory – the duality between the particle picture and the wave picture – appeared in a very striking way. This particle-wave duality appears in the framework of many-particle quantum field theory as a canonical conjugate relation between the particle number and the quantum mechanical phase.

From this point of view, in systems where the strong repulsive force between the particles fixes the particle number, as is the case, for example, for the Mott insulator and the Wigner crystal, the charge density and the spin

density waves are stabilized and the system shows its particle-like face. On the other hand, when the motions of the particles lead to coherence of the quantum mechanical phase, as is the case in superconductors and superfluids, the phase is fixed and becomes visible, and the system shows its wave-like face. The competition between both appears in low-dimensional systems and mesoscopic systems in a very clear manner. Problems like the quantum Hall effect, high-temperature superconductors, organic conductors, metal-insulator transition, superconductor-insulator transition, can all be grasped from this point of view.

The new problems that arise due to this competition are given in the following three points.

(i) Quantum phase transition or quantum critical phenomena – In contrast to the phase transition at finite temperature due to the competition between energy and entropy, these are phase transitions that occur at the absolute zero temperature or low temperature due to quantum fluctuations.

(ii) Novel ground states and low-energy excitations – New types of quantum states have been discovered, such as non-Fermi liquids in relation to high-temperature superconductors, and incompressible quantum liquids in relation to the quantum Hall system. Their elementary excitations, the spinon and the holon, are anyons obeying fractional statistics.

(iii) The quantal phase and its topological properties – The topological aspects of the quantal phase, including the topological defects, show up in the physical properties of solids. Especially, when due to some kind of constraint a gauge field is introduced, phenomena that are also discussed in quantum chromodynamics reappear with some modifications in condensed matter physics.

The present book has been written for graduate students and researchers who are not necessarily specialists in quantum field theory. Starting with a short review of quantum mechanics, the framework of quantum field theory is introduced and applied to problems that are uppermost in the present research in condensed matter physics.

In Chap. 1, most basic principles are reviewed. Topics that are not only important in single-particle quantum mechanics but also in quantum field theory are recalled, namely, canonical conjugate relation, symmetry and the conservation law, and the variation principle. This analogy between single-particle quantum mechanics and quantum field theory can be efficiently applied when quantization is performed using path integral methods, as presented in Chap. 2. The coordinate and momentum in the single-particle problem correspond in the many-particle system to the phase and the amplitude of the quantum field. A similar analogy can be applied for the gauge field and the spin system. In Chap. 3, phase transitions are discussed, being characteristic of field theories, because they cannot occur in systems with only a small number of degrees of freedom. This topic is one fundamental concept of modern condensed matter physics and is developed further to systems where it is

difficult to define an order parameter. As examples, the Kosterlitz–Thouless transition, being a topological phase transition that will reappear later on in a different context, and the problem of colour-confinement in gauge theory, are discussed.

After these preliminaries, starting from Chap. 4, explicit applications of quantum field theory to condensed matter physics are discussed. The content of Chap. 4 is a warming up, where representative examples of a fermionic system and a bosonic system are presented, namely the classical RPA theory of an electron gas and the Bogoliubov theory of superfluidity. It is demonstrated that the method of path integrals provides the clearest formulation of the problems. In Chap. 5, many different problems related to superconductors are discussed. Problems that have so far been treated independently, namely the renormalization of the Coulomb interaction, collective modes and gauge invariance in BCS theory, are discussed in a unified approach. In the second part of Chap. 5, the Josephson junction and the two-dimensional superconductor are discussed, being an issue of current interest. In Chap. 6, the new quantum state of the (fractional) quantum Hall liquid is discussed within the framework of the Chern–Simons gauge field.

Of course, it is not possible to discuss all the applications of quantum field theory here; therefore, our intention is to reveal their common structure and ideas that provide the tools necessary for further studies.

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Tokyo, January 1999

Naoto Nagaosa

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1. Review of Quantum Mechanics and Basic Principles of Field Theory

The content of this chapter is nothing but a review of the most basic principles. Starting with the quantum mechanics of a single-particle system, then the canonical conjugate relations, the relation between symmetries and conservation laws, the description of multi-particles systems using field theory, finally gauge invariance and the gauge field will be introduced, all being fundamental concepts that built the basis for the whole following discussion. The reader should reconfirm the universality of the quantum mechanical description and get a taste of the efficiency of an analogy.

1.1 Single-Particle Quantum Mechanics

We start by recalling some facts about single-particle quantum mechanics. All points that will be mentioned here will again become important when proceeding to quantum field theory.

The equation of motion of the single-particle system is given by the Schrödinger equation:

$$i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t} = \hat{H} \psi(\mathbf{r}, t) = \left[\frac{\hat{\mathbf{p}}^2}{2m} + V(\hat{\mathbf{r}}) \right] \psi(\mathbf{r}, t) . \quad (1.1.1)$$

$\psi(\mathbf{r}, t)$ is the so-called wave function, depending on the space coordinates \mathbf{r} and the time t . \hat{H} is the so-called Hamiltonian operator, creating a new wave function $\hat{H}\psi(\mathbf{r}, t)$ by acting on the wave function $\psi(\mathbf{r}, t)$. In what follows, operators are assigned by a hat, except for obvious cases where this notation will be omitted. $\hat{\mathbf{p}}$ and $\hat{\mathbf{r}}$ are three-component vector operators that represent the momentum and space coordinate of the particle, respectively. $\hat{\mathbf{p}}^2/2m$ is the kinetic energy, $V(\hat{\mathbf{r}})$ the potential energy, and its sum is the total energy of the particle, called the Hamiltonian operator \hat{H} . Equation (1.1.1) signifies that the time development of the wave function is determined by the Hamiltonian operator \hat{H} . By defining the exponential $\exp(\hat{A})$ of an operator by

$$\exp(\hat{A}) = \sum_{n=0}^{\infty} \frac{1}{n!} (\hat{A})^n , \quad (1.1.2)$$

its solution can be written as

$$\psi(\mathbf{r}, t) = \exp\left(-\frac{i}{\hbar} \hat{H} t\right) \psi(\mathbf{r}, 0) . \quad (1.1.3)$$

In quantum mechanics, the wave function is interpreted in terms of probability. The square of the absolute value of the wave function

$$P(\mathbf{r}, t) = |\psi(\mathbf{r}, t)|^2 \quad (1.1.4)$$

is interpreted as the probability of detecting the particle at time t at the coordinate \mathbf{r} . Therefore, because the sum (integral) of the probability over the whole space is 1, we obtain the normalization condition of the wave function:

$$\int d^3\mathbf{r} P(\mathbf{r}, t) = \int d^3\mathbf{r} |\psi(\mathbf{r}, t)|^2 = 1 . \quad (1.1.5)$$

We will now explain the matrix formulation of quantum mechanics. We interpret the function $f(\mathbf{r})$ as a vector in the Hilbert space (the vector space of functions) and write $|f\rangle$ for the state that the function represents. Doing so, the operator \hat{A} acting on the vectors in this space generates a new vector, which is a linear transformation. Therefore, it corresponds to a matrix. Furthermore, to every vector $|f\rangle$, there exists the conjugate vector $\langle f|$, being specified as the so-called ket- and bra-vector, respectively. Thinking in components, the bra-vector $\langle f|$ can be regarded as the transposed and complex conjugate of the ket-vector $|f\rangle$. The inner product $\langle g | f \rangle$ in this vector space is defined by

$$\langle g | f \rangle = \int d^3\mathbf{r} g^*(\mathbf{r}) f(\mathbf{r}) = \langle f | g \rangle^* . \quad (1.1.6)$$

The matrix element $\langle g | \hat{A} | f \rangle$ of the operator (the matrix) \hat{A} is given by

$$\langle g | \hat{A} | f \rangle = \langle g | \hat{A} f \rangle = \int d^3\mathbf{r} g^*(\mathbf{r}) \hat{A} f(\mathbf{r}) . \quad (1.1.7)$$

In order to give a more concrete picture of the considerations made so far, we introduce now an orthonormal basis $|i\rangle, i = 1, 2, 3, \dots$, of the Hilbert space. (We wrote $i = 1, 2, 3, \dots$; however, the basis is not necessarily a countable set. In general, when the volume of the system is infinite, the set of basis vectors is uncountable. In these cases, the sum \sum_i over the set labelled by i must be replaced by an integral.) Because the basis is orthonormal, the orthonormality condition

$$\langle i | j \rangle = \delta_{i,j} \quad (1.1.8)$$

and the completeness condition

$$\sum_i |i\rangle\langle i| = \hat{1} \quad (1.1.9)$$

hold. Here, the so-called Kronecker delta $\delta_{i,j}$ is defined to equal 1 when $i = j$, and to be zero otherwise. $\hat{1}$ is the identity matrix; in other words, the identity operator. In this basis, the vector $|f\rangle$ can be represented by its components:

$$|f\rangle = \sum_i |i\rangle\langle i|f\rangle, \quad \langle f| = \sum_i \langle f|i\rangle\langle i|. \quad (1.1.10)$$

Furthermore, the component representation of $\hat{A}|f\rangle$ is given by

$$\begin{aligned} \hat{A}|f\rangle &= \left(\sum_i |i\rangle\langle i| \right) \hat{A} \left(\sum_j |j\rangle\langle j| \right) |f\rangle \\ &= \sum_{i,j} |i\rangle\langle i|\hat{A}|j\rangle\langle j|f\rangle \end{aligned} \quad (1.1.11)$$

and (1.1.7) can be written as

$$\langle g|\hat{A}|f\rangle = \sum_{i,j} \langle g|i\rangle\langle i|\hat{A}|j\rangle\langle j|f\rangle. \quad (1.1.12)$$

We define the Hermitian conjugate \hat{A}^\dagger of \hat{A} by requiring that

$$\langle g|\hat{A}|f\rangle = \langle \hat{A}^\dagger g|f\rangle \quad (1.1.13)$$

holds for every $|f\rangle$ and $|g\rangle$. Comparing the inner product of the conjugate of

$$|\hat{A}^\dagger g\rangle = \sum_{j,i} |j\rangle\langle j|\hat{A}^\dagger|i\rangle\langle i|g\rangle \quad (1.1.14)$$

with $|f\rangle$ and

$$\langle \hat{A}^\dagger g|f\rangle = \sum_{j,i} \langle g|i\rangle\langle j|\hat{A}^\dagger|i\rangle^* \langle j|f\rangle \quad (1.1.15)$$

with (1.1.13), we obtain

$$\langle j|\hat{A}^\dagger|i\rangle = \langle i|\hat{A}|j\rangle^*. \quad (1.1.16)$$

This is nothing but the usual definition of the Hermitian conjugation of a matrix. In the case that \hat{A} and \hat{A}^\dagger are equal $\hat{A} = \hat{A}^\dagger$, \hat{A} is called a Hermitian operator. In quantum mechanics, all physical quantities are represented in terms of Hermitian operators.

We now introduce the eigenvalue a and the eigenstate $|a\rangle$ of the Hermitian operator \hat{A} :

$$\hat{A}|a\rangle = a|a\rangle. \quad (1.1.17)$$

By taking the inner product with $|a\rangle$

$$\langle a|\hat{A}|a\rangle = a\langle a|a\rangle \quad (1.1.18)$$

we can deduce that at the left-hand side due to hermiticity

$$\langle a|\hat{A}|a\rangle = \langle \hat{A}^\dagger a|a\rangle = \langle \hat{A}a|a\rangle = a^*\langle a|a\rangle \quad (1.1.19)$$

holds, and obtain $a = a^*$. Therefore, we conclude that the eigenvalue a is real. Furthermore, for $a \neq a'$ with

$$\langle a'|\hat{A} = a'\langle a'| \quad (1.1.20)$$

from (1.1.19) we can deduce that

$$\langle a'|\hat{A}|a\rangle = a\langle a'|a\rangle = a'\langle a'|a\rangle \quad (1.1.21)$$

and conclude that $\langle a'|a\rangle = 0$. This signifies that the eigenstates of a Hermitian operator with different eigenvalues are orthogonal to each other. Therefore, by a suitable normalization it is possible to build an orthonormal basis using the eigenstates of an Hermitian operator by orthogonalizing in eigenspaces belonging to the same eigenvalue.

Naturally, the space coordinate $\hat{\mathbf{r}}$ is a Hermitian operator. Every component \hat{r}_α of $\hat{\mathbf{r}}$ acts on $f(\hat{\mathbf{r}})$

$$\hat{r}_\alpha f(\mathbf{r}) = r_\alpha f(\mathbf{r}) \quad (1.1.22)$$

creating a new function. Notice that on the right-hand side, r_α is no longer an operator, but the α -component of the function \mathbf{r} . The generalization of (1.1.22) is

$$V(\hat{\mathbf{r}})f(\mathbf{r}) = V(\mathbf{r})f(\mathbf{r}) \quad (1.1.23)$$

with $V(\hat{\mathbf{r}})$ being the potential energy of equation (1.1.1). With (1.1.22) we write

$$\begin{aligned} \langle g|\hat{r}_\alpha|f\rangle &= \int d^3\mathbf{r} g^*(\mathbf{r})\hat{r}_\alpha f(\mathbf{r}) = \int d^3\mathbf{r} g^*(\mathbf{r})r_\alpha f(\mathbf{r}) = \int d^3\mathbf{r} [r_\alpha g(\mathbf{r})]^* f(\mathbf{r}) \\ &= \int d^3\mathbf{r} [\hat{r}_\alpha g(\mathbf{r})]^* f(\mathbf{r}) = \langle \hat{r}_\alpha g|f\rangle . \end{aligned} \quad (1.1.24)$$

It should be clear from these equations that \hat{r}_α is Hermitian.

We introduce now the state $|\mathbf{r}\rangle$ being the eigenstate with eigenvalue \mathbf{r} of the operator $\hat{\mathbf{r}}$:

$$\hat{\mathbf{r}}|\mathbf{r}\rangle = \mathbf{r}|\mathbf{r}\rangle . \quad (1.1.25)$$

Because $\langle \mathbf{r}'|\mathbf{r}\rangle = 0$ for $\mathbf{r} \neq \mathbf{r}'$,

$$\langle \mathbf{r}'|\mathbf{r}\rangle = \delta(\mathbf{r} - \mathbf{r}') , \quad (1.1.26)$$

with an appropriate choice of the normalization. Here we have introduced the so-called delta function $\delta(\mathbf{r} - \mathbf{r}')$, defined to be zero for $\mathbf{r} \neq \mathbf{r}'$, and infinite at $\mathbf{r} = \mathbf{r}'$, and to give the value 1 when integrated over $\mathbf{r} - \mathbf{r}'$ in a region containing the origin. Furthermore, $|\mathbf{r}\rangle$ and $\langle\mathbf{r}|$ fulfil the completeness relation

$$\int d^3\mathbf{r} |\mathbf{r}\rangle\langle\mathbf{r}| = \hat{1} . \quad (1.1.27)$$

The reader not familiar with the delta function is referred to the Appendices A and B. As mentioned there, we can introduce a vector space on a discrete lattice. The components of a vector in this space are defined by the values of a function on the discrete lattice points. This vector space approaches the Hilbert space when the number of lattice points N_L becomes infinite, that is, when the lattice spacing Δx becomes zero. In this case, the sum $(\Delta x)^3 \sum_{\text{lattice points } i}$ approaches the three-dimensional integral appearing in (1.1.6). As a basis of the N_L -dimensional vector space, we define states that are zero at all lattice points except for the coordinate \mathbf{r}_i , where the value is defined to be $1/(\Delta x)^{3/2}$. Then we have

$$\langle\mathbf{r}_i|\mathbf{r}_j\rangle = \sum_k \frac{\delta_{\mathbf{r}_i, \mathbf{r}_k}}{(\Delta x)^{3/2}} \frac{\delta_{\mathbf{r}_k, \mathbf{r}_j}}{(\Delta x)^{3/2}} = \frac{\delta_{\mathbf{r}_i, \mathbf{r}_j}}{(\Delta x)^3}$$

and, furthermore,

$$(\Delta x)^3 \sum_i |\mathbf{r}_i\rangle\langle\mathbf{r}_i| = \hat{1} .$$

In the limit as $\Delta x \rightarrow 0$, these equations approach the equations of the inner product and the completeness relation of the basis \mathbf{r} mentioned above.

Now, owing to the completeness relation of the basis \mathbf{r} , we can write the inner product (1.1.6) as

$$\langle g|f\rangle = \int d^3\mathbf{r} \langle g|\mathbf{r}\rangle\langle\mathbf{r}|f\rangle \quad (1.1.28)$$

and obtain

$$\begin{aligned} f(\mathbf{r}) &= \langle\mathbf{r}|f\rangle , \\ g^*(\mathbf{r}) &= \langle g|\mathbf{r}\rangle . \end{aligned} \quad (1.1.29)$$

From this point of view, the wave function $\psi(\mathbf{r}, t)$ is nothing but the \mathbf{r} -component of the state vector $|\psi(t)\rangle$ of the Hilbert space written in the basis $|\mathbf{r}\rangle$.

Now, what about the momentum operator $\hat{\mathbf{p}}$? Here, we meet the very first example of the most fundamental relation in quantum mechanics, namely the canonical conjugation relation. A plane wave with wave number vector \mathbf{k} can

be expressed as $\psi_{\mathbf{k}}(\mathbf{r}) = (2\pi\hbar)^{-3/2} e^{i\mathbf{k}\cdot\mathbf{r}}$. Writing the plane wave as a function of \mathbf{r} , and using

$$\hat{\mathbf{p}} = \frac{\hbar}{i} \frac{\partial}{\partial \mathbf{r}} \quad (1.1.30)$$

we obtain

$$\hat{\mathbf{p}}\psi_{\mathbf{k}}(\mathbf{r}) = \hbar\mathbf{k}\psi_{\mathbf{k}}(\mathbf{r}) = \mathbf{p}\psi_{\mathbf{k}}(\mathbf{r}) \quad (1.1.31)$$

and therefore the relation $\mathbf{p} = \hbar\mathbf{k}$. We now define the following combination of $\hat{\mathbf{r}}$ and $\hat{\mathbf{p}}$:

$$[\hat{r}_{\alpha}, \hat{p}_{\beta}] = \hat{r}_{\alpha}\hat{p}_{\beta} - \hat{p}_{\beta}\hat{r}_{\alpha} \quad (1.1.32)$$

This is the so-called commutator of \hat{r}_{α} and \hat{p}_{α} , which is also an operator. Acting with this commutator on an arbitrary function $f(\mathbf{r})$, we obtain

$$\begin{aligned} [\hat{r}_{\alpha}, \hat{p}_{\beta}]f(\mathbf{r}) &= \left(\hat{r}_{\alpha} \frac{\hbar}{i} \frac{\partial}{\partial r_{\beta}} - \frac{\hbar}{i} \frac{\partial}{\partial r_{\beta}} \hat{r}_{\alpha} \right) f(\mathbf{r}) \\ &= \frac{\hbar}{i} \left\{ r_{\alpha} \frac{\partial f(\mathbf{r})}{\partial r_{\beta}} - \frac{\partial}{\partial r_{\beta}} (r_{\alpha} f(\mathbf{r})) \right\} = i\hbar \delta_{\alpha,\beta} f(\mathbf{r}) \end{aligned}$$

and therefore the identity

$$[\hat{r}_{\alpha}, \hat{r}_{\beta}] = i\hbar \delta_{\alpha,\beta} \quad (1.1.33)$$

This is the so-called commutation relation. It follows from (1.1.33) for $\alpha = \beta$ that $[\hat{r}_{\alpha}, \hat{p}_{\alpha}] = i\hbar$. This means that \hat{r}_{α} and \hat{p}_{α} are canonical conjugates of each other. This commutation relation, as well as (1.1.30), is the starting point for many very fundamental and wide conceptual developments that will be discussed in what follows. However, we first discuss some aspects of the eigenstates of $\hat{\mathbf{p}}$. We can interpret (1.1.31) as

$$\hat{\mathbf{p}}|\mathbf{p}\rangle = \mathbf{p}|\mathbf{p}\rangle, \quad (1.1.34)$$

$$\langle \mathbf{r} | \mathbf{p} \rangle = \psi_{\mathbf{p}/\hbar}(\mathbf{r}) = \frac{1}{(2\pi\hbar)^{3/2}} \exp \left(\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{r} \right) \quad (1.1.35)$$

$|\mathbf{p}\rangle$ also spans a basis; orthogonality can be shown with

$$\begin{aligned} \langle \mathbf{p}' | \mathbf{p} \rangle &= \int d^3\mathbf{r} \langle \mathbf{p}' | \mathbf{r} \rangle \langle \mathbf{r} | \mathbf{p} \rangle \\ &= \int \frac{d^3\mathbf{r}}{(2\pi\hbar)^3} \exp \left[\frac{i}{\hbar} (-\mathbf{p}' + \mathbf{p}) \cdot \mathbf{r} \right] = \delta(\mathbf{p} - \mathbf{p}') \end{aligned} \quad (1.1.36)$$

and, in the same manner, the completeness relation

$$\int d^3\mathbf{p} |\mathbf{p}\rangle \langle \mathbf{p}| = \hat{1} \quad (1.1.37)$$

by acting on it with $\langle \mathbf{r}' |$ and $|\mathbf{r}\rangle$ on the left- and right-hand sides:

$$\begin{aligned} \int d^3\mathbf{p} \langle \mathbf{r}' | \mathbf{p} \rangle \langle \mathbf{p} | \mathbf{r} \rangle &= \int \frac{d^3\mathbf{p}}{(2\pi\hbar)^3} \exp \left[\frac{i}{\hbar} \mathbf{p} \cdot (\mathbf{r}' - \mathbf{r}) \right] \\ &= \delta(\mathbf{r} - \mathbf{r}') = \langle \mathbf{r}' | \mathbf{r} \rangle . \end{aligned} \quad (1.1.38)$$

Equations (1.1.26), (1.1.27), (1.1.36) and (1.1.37) are the basic relations of the Fourier analysis, because

$$f(\mathbf{r}) = \langle \mathbf{r} | f \rangle = \int d^3\mathbf{p} \langle \mathbf{r} | \mathbf{p} \rangle \langle \mathbf{p} | f \rangle = \int \frac{d^3\mathbf{p}}{(2\pi\hbar)^{3/2}} e^{i\mathbf{p} \cdot \mathbf{r}/\hbar} \langle \mathbf{p} | f \rangle \quad (1.1.39)$$

is the Fourier representation of $f(\mathbf{r})$ in terms of $\langle \mathbf{p} | f \rangle = F(\mathbf{p})$, and the inversion of this Fourier transformation can be written as

$$F(\mathbf{p}) = \langle \mathbf{p} | f \rangle = \int d^3\mathbf{r} \langle \mathbf{p} | \mathbf{r} \rangle \langle \mathbf{r} | f \rangle = \int \frac{d^3\mathbf{r}}{(2\pi\hbar)^{3/2}} e^{-i\mathbf{p} \cdot \mathbf{r}/\hbar} f(\mathbf{r}) . \quad (1.1.40)$$

We conclude that the Fourier transformation is the basis transformation that links the two basis sets (coordinate sets) $|\mathbf{r}\rangle$ and $|\mathbf{p}\rangle$ in the Hilbert space. (Explanations about the Fourier transformation can be found in Appendix A.)

We now return to the commutation relation and discuss its meaning in more detail. First, Heisenberg's uncertainty principle can be deduced from (1.1.33). We consider now the expectation values $\hat{r}_\alpha = \langle \psi | \hat{r}_\alpha | \psi \rangle$ and $\hat{p}_\alpha = \langle \psi | \hat{p}_\alpha | \psi \rangle$ of \hat{r}_α and \hat{p}_α in the state $|\psi\rangle$. As mentioned earlier, the interpretation of quantum mechanics is only possible in terms of probabilities, and the observed values of \hat{p}_α and \hat{r}_α should follow a probability distribution around each expectation value. The width of this distribution can in some way be understood as the uncertainty, and in order to make it precise, we define the so-called variation in the following manner:

$$\begin{aligned} \langle (\Delta \hat{r}_\alpha)^2 \rangle &= \langle (\hat{r}_\alpha - \langle \hat{r}_\alpha \rangle)^2 \rangle = \langle \hat{r}_\alpha^2 \rangle - \langle \hat{r}_\alpha \rangle^2 , \\ \langle (\Delta \hat{p}_\alpha)^2 \rangle &= \langle (\hat{p}_\alpha - \langle \hat{p}_\alpha \rangle)^2 \rangle = \langle \hat{p}_\alpha^2 \rangle - \langle \hat{p}_\alpha \rangle^2 . \end{aligned} \quad (1.1.41)$$

We now introduce the Schwarz inequality. With λ being an arbitrary complex parameter

$$\begin{aligned} \langle |\Delta \hat{r}_\alpha + \lambda \Delta \hat{p}_\alpha|^2 \rangle &= \langle (\Delta \hat{r}_\alpha)^2 \rangle + \lambda^* \langle \Delta \hat{r}_\alpha \Delta \hat{p}_\alpha \rangle + \lambda \langle \Delta \hat{p}_\alpha \Delta \hat{r}_\alpha \rangle \\ &\quad + |\lambda|^2 \langle (\Delta \hat{p}_\alpha)^2 \rangle , \end{aligned} \quad (1.1.42)$$

we can deduce the Schwarz inequality from the fact that this expression must be positive, therefore

$$\langle (\Delta \hat{r}_\alpha)^2 \rangle \langle (\Delta \hat{p}_\alpha)^2 \rangle \geq |\langle \Delta \hat{r}_\alpha \Delta \hat{p}_\alpha \rangle|^2 . \quad (1.1.43)$$

We make the following decomposition:

$$\Delta\hat{r}_\alpha\Delta\hat{p}_\alpha = \frac{1}{2}\{\Delta\hat{r}_\alpha, \Delta\hat{p}_\alpha\} + \frac{1}{2}[\Delta\hat{r}_\alpha, \Delta\hat{p}_\alpha] , \quad (1.1.44)$$

where $\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$ is the so-called anti-commutator. Recalling that both $\Delta\hat{r}_\alpha$ and $\Delta\hat{p}_\alpha$ are Hermitian, it follows that the Hermitian conjugate of the first term on the right-hand side of the above equation is

$$\{\Delta\hat{r}_\alpha, \Delta\hat{p}_\alpha\}^\dagger = \{\Delta\hat{r}_\alpha, \Delta\hat{p}_\alpha\} . \quad (1.1.45)$$

Therefore, its expectation value is real. On the other hand, the second term equals

$$\frac{1}{2}[\Delta\hat{r}_\alpha, \Delta\hat{p}_\alpha] = \frac{1}{2}[\hat{r}_\alpha, \hat{p}_\alpha] = \frac{i\hbar}{2} \quad (1.1.46)$$

and is therefore complex. Finally, we obtain

$$|\langle\Delta\hat{r}_\alpha\Delta\hat{p}_\alpha\rangle|^2 = \frac{1}{4}\langle\{\Delta\hat{r}_\alpha, \Delta\hat{p}_\alpha\}\rangle^2 + \frac{\hbar^2}{4} \geq \frac{\hbar^2}{4} \quad (1.1.47)$$

and, in combination with (1.1.43),

$$\langle(\Delta\hat{r}_\alpha)^2\rangle\langle(\Delta\hat{p}_\alpha)^2\rangle \geq \frac{\hbar^2}{4} . \quad (1.1.48)$$

This is Heisenberg's uncertainty principle. Normally, we forget about the numerical factor and just write

$$\Delta\hat{r}_\alpha\Delta\hat{p}_\alpha \gtrsim \hbar . \quad (1.1.49)$$

No state exists that is an eigenstate of both \hat{r}_α and \hat{p}_α , which means that it is impossible to determine \hat{r}_α and \hat{p}_α simultaneously, and the product of the uncertainty must be larger than a number of the order of the Planck constant.

We can deduce the following physical picture from the uncertainty principle. As can be seen in (1.1.1), the Hamiltonian is the sum of the kinetic energy $\hat{p}^2/2m$ and the potential energy $V(\hat{r})$. In classical mechanics, because it is possible to determine \mathbf{p} and \mathbf{r} simultaneously, the ground state is given by $\mathbf{p} = 0$ and $\mathbf{r} = \mathbf{r}_0$ (being the minimum of $V(\mathbf{r})$). In quantum mechanics, it follows from (1.1.49) that if we require $\mathbf{p} = 0$, then \mathbf{r} is totally undetermined, and the gain of the potential energy is lost; on the other hand, if we require $\mathbf{r} = \mathbf{r}_0$, then \mathbf{p} is totally undetermined, and the kinetic term becomes large.

Therefore, owing to the uncertainty principle, \hat{r}_α and \hat{p}_α have a strained relationship with each other. Let us make this more concrete. We start by considering the one-dimensional harmonic oscillator with Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 . \quad (1.1.50)$$

Writing Δx for the width of the ground state $|0\rangle$ in coordinate space, and Δp in momentum space, we can estimate the expectation value of the Hamiltonian or, in other words, the energy, by

$$E = \langle 0 | \hat{H} | 0 \rangle \sim \frac{(\Delta p)^2}{2m} + \frac{1}{2} m \omega^2 (\Delta x)^2 . \quad (1.1.51)$$

We now insert the equation $\Delta p \propto \hbar/\Delta x$, obtained from the uncertainty relation:

$$E \sim \frac{\hbar^2}{2m(\Delta x)^2} + \frac{1}{2} m \omega^2 (\Delta x)^2 . \quad (1.1.52)$$

This is only a function of Δx . Calculating the minimum by $\partial E/\partial(\Delta x) = 0$, we obtain

$$\Delta x_0 \sim \left(\frac{\hbar}{m\omega} \right)^{1/2} . \quad (1.1.53)$$

This is the scale that lies behind the Hamiltonian (1.1.50), which can be seen as the compromise point between two competing tendencies, namely the kinetic energy requiring $\Delta p = 0$, and the potential energy requiring $\Delta x = 0$.

Inserting Δx_0 in (1.1.52), it is easy to calculate the zero point energy:

$$E_0 \sim \hbar\omega .$$

In much the same manner this calculation can also be performed for the hydrogen atom with the Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} - \frac{e^2}{|\hat{r}|} . \quad (1.1.54)$$

Inserting $|p| \propto \hbar/r$ and $|r| \propto r$, we obtain

$$E \sim \frac{\hbar^2}{2mr^2} - \frac{e^2}{r} . \quad (1.1.55)$$

Again, by calculating the minimum $\partial E/\partial r = 0$ we obtain

$$r \sim r_0 = \frac{\hbar^2}{me^2} \quad (1.1.56)$$

and

$$E_0 \sim -R_H = -\frac{me^4}{2\hbar^2} . \quad (1.1.57)$$

Here, r_0 is the so-called Bohr radius, and R_H is the Rydberg energy. We could argue that the electron of the hydrogen atom does not fall into the nucleus and that the atom does not collapse owing to the uncertainty principle.