

Quantum Field Theory in Condensed Matter Physics

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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 begin 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 function) 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 $\langle \mathbf{r}|$ fulfill 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 $1/(\Delta)^{3/2}$. 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,

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

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 ex-

ample of the most fundamental relation in quantum mechanics, namely the canonical conjugate relation. A plane wave with wave number \mathbf{k} can be expressed as $\psi_{\mathbf{k}}(\mathbf{r}) = (2\pi\hbar)^{-3/2} e^{i\mathbf{k}\mathbf{r}}$. 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 $\hat{\mathbf{r}}_\alpha$ and $\hat{\mathbf{p}}_\alpha$, which is also an operator. Acting with this commutator on an arbitrary function $f(\mathbf{r})$, we obtain

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

and therefore the identity

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

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 follow. 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

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

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 (coordinates 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 $\hat{\mathbf{p}}^2/2m$ and the potential energy $V(\hat{\mathbf{r}})$. 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

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

Inserting $|\mathbf{p}| \propto \hbar/r$ and $|\mathbf{r}| \propto r$, 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.

Another important aspect that is related to the canonical conjugation relation are

symmetry operations. We start with the Taylor expansion:

$$\begin{aligned} f(\mathbf{r} + \mathbf{a}) = & f(\mathbf{r}) + \left(\mathbf{a} \cdot \frac{\partial}{\partial \mathbf{r}} \right) f(\mathbf{r}) + \frac{1}{2} \left(\mathbf{a} \cdot \frac{\partial}{\partial \mathbf{r}} \right)^2 f(\mathbf{r}) \\ & + \frac{1}{3!} \left(\mathbf{a} \cdot \frac{\partial}{\partial \mathbf{r}} \right)^3 f(\mathbf{r}) + \dots \end{aligned} \quad (1.1.58)$$

Using the definition (1.1.2) of the exponential of an operator, we can write this as

$$f(\mathbf{r} + \mathbf{a}) = e^{\mathbf{a} \cdot \frac{\partial}{\partial \mathbf{r}}} f(\mathbf{r}) \equiv \hat{U}(\mathbf{a}) f(\mathbf{r}) \quad (1.1.59)$$

where $\hat{U}(\mathbf{a})$ acts like a translation operator about \mathbf{a} and, using (1.1.30), can be written as

$$\hat{U}(\mathbf{a}) = e^{\frac{i}{\hbar} \mathbf{a} \cdot \hat{\mathbf{p}}} \quad (1.1.60)$$

It follows that $[\hat{U}(\mathbf{a})]^\dagger = \hat{U}(-\mathbf{a}) = [\hat{U}(\mathbf{a})]^{-1}$, and therefore $\hat{U}(\mathbf{a})$ is a unitary operator. An operator written in the exponential, as in the case here for $\hat{\mathbf{p}}$, which induces a symmetry operation, is called a generator.

In (1.1.59) we consider a linear operation on the function $f(\mathbf{r})$. Next we consider a linear transformation on the operator $V(\hat{\mathbf{r}})$. We start by writing down the conclusion:

$$V(\hat{\mathbf{r}} + \mathbf{a}) = \hat{U}(\mathbf{a}) V(\hat{\mathbf{r}}) [\hat{U}(\mathbf{a})]^\dagger = \hat{U}(\mathbf{a}) V(\hat{\mathbf{r}}) \hat{U}(-\mathbf{a}) \quad (1.1.61)$$

The meaning of this equation becomes evident by acting on a function $f(\mathbf{r})$

$$\begin{aligned} [\hat{U}(\mathbf{a}) V(\hat{\mathbf{r}}) \hat{U}(-\mathbf{a})] f(\mathbf{r}) &= [\hat{U}(\mathbf{a}) V(\hat{\mathbf{r}})] f(\mathbf{r} - \mathbf{a}) \\ &= \hat{U}(\mathbf{a}) [V(\mathbf{r}) f(\mathbf{r} - \mathbf{a})] = V(\mathbf{r} + \mathbf{a}) f(\mathbf{r}) = V(\hat{\mathbf{r}} + \mathbf{a}) f(\mathbf{r}) \end{aligned} \quad (1.1.62)$$

Since $f(\mathbf{r})$ is arbitrary, we obtain (1.1.61). Furthermore, because the operator $\hat{U}(\mathbf{a})$ depends only on $\hat{\mathbf{p}}$,

$$\hat{U}(\mathbf{a}) \hat{\mathbf{p}} \hat{U}(-\mathbf{a}) = \hat{\mathbf{p}} \quad (1.1.63)$$

can be proved easily. Therefore, the kinetic energy is invariant:

$$\hat{U}(\mathbf{a}) \frac{\hat{\mathbf{p}}^2}{2m} [\hat{U}(\mathbf{a})]^\dagger = \frac{\hat{\mathbf{p}}^2}{2m} \quad (1.1.64)$$

Let us suppose that the system is invariant under translation. In our case, this means that the potential is independent of the position, $V(\hat{\mathbf{r}} + \mathbf{a}) = V(\hat{\mathbf{r}})$. Then, we can write

$$\hat{U}(\mathbf{a}) \hat{H} [\hat{U}(\mathbf{a})]^{-1} = \hat{H} \quad (1.1.65)$$

Since \mathbf{a} is an arbitrary real vector, we can choose it infinitesimally small and write

the power series

$$\hat{U}(\pm \mathbf{a}) \simeq \hat{1} \pm \frac{i}{\hbar} \mathbf{a} \cdot \hat{\mathbf{p}}. \quad (1.1.66)$$

Then we obtain from (1.1.65)

$$[\mathbf{a} \cdot \hat{\mathbf{p}}, \hat{H}] = 0. \quad (1.1.67)$$

Because \mathbf{a} is an arbitrary infinitesimal vector, we can conclude

$$[\hat{p}_\alpha, \hat{H}] = 0. \quad (1.1.68)$$

Conversely, it is possible to deduce (1.1.65) from (1.1.68). In order to do so, let λ be an arbitrary real parameter, then we define

$$\hat{H}(\lambda) = \hat{U}(\lambda \mathbf{a}) \hat{H} \hat{U}(-\lambda \mathbf{a}) \quad (1.1.69)$$

Differentiating with respect to λ , with

$$\frac{\partial \hat{U}(\pm \lambda \mathbf{a})}{\partial \lambda} = \pm \frac{i}{\hbar} \mathbf{a} \cdot \hat{\mathbf{p}} \hat{U}(\pm \lambda \mathbf{a}) = \frac{i}{\hbar} \hat{U}(\pm \lambda \mathbf{a}) \mathbf{a} \cdot \hat{\mathbf{p}} \quad (1.1.70)$$

we obtain

$$\frac{\partial \hat{H}(\lambda)}{\partial \lambda} = \frac{i}{\hbar} \hat{U}(\lambda \mathbf{a}) [\mathbf{a} \cdot \hat{\mathbf{p}}, \hat{H}] \hat{U}(-\lambda \mathbf{a}). \quad (1.1.71)$$

Owing to (1.1.68), the right-hand side is zero, therefore $\hat{H}(\lambda)$ does not depend on λ , and we regain (1.1.65) from $\hat{H}(1) = \hat{H}(0)$.

In this way, the symmetry of a system can be interpreted as the fact that the generator of the symmetry operation commutes with the Hamiltonian. And indeed, the commutator with the Hamiltonian has the important meaning of the time development of the physical quantity. To be complete, we will now review the Heisenberg picture. Equation (1.1.3) describes the time evolution of the wave function ψ . This is the so-called Schrödinger picture. On the other hand, the formal description where the wave function is time-independent, and the operators change in time, is called the Heisenberg picture. Explicitly, using (1.1.3), from

$$\begin{aligned} \langle \psi(t) | \hat{A} | \psi(t) \rangle &= \langle \psi(0) | \exp\left(\frac{i}{\hbar} \hat{H} t\right) \hat{A} \exp\left(-\frac{i}{\hbar} \hat{H} t\right) | \psi(0) \rangle \\ &= \langle \psi(0) | \hat{A}_H(t) | \psi(0) \rangle \end{aligned} \quad (1.1.72)$$

we obtain the following definition:

$$\hat{A}_H(t) = \exp\left(\frac{i}{\hbar} \hat{H} t\right) \hat{A} \exp\left(-\frac{i}{\hbar} \hat{H} t\right) \quad (1.1.73)$$

We obtain the Heisenberg equation of motion as

$$\begin{aligned}\frac{d\hat{A}_H(t)}{dt} &= \exp\left(\frac{i}{\hbar}\hat{H}t\right) \frac{i}{\hbar}[\hat{H}, \hat{A}] \exp\left(-\frac{i}{\hbar}\hat{H}t\right) \\ &= \frac{i}{\hbar}[\hat{H}, \hat{A}_H(t)]\end{aligned}\tag{1.1.74}$$

Of course, the time evolution of the Hamiltonian itself is given by

$$\hat{H}_H(t) = \hat{H}\tag{1.1.75}$$

and is therefore time independent. This is nothing but the energy conservation law in quantum mechanics.

Returning to the discussion of symmetry, we obtain from (1.1.68)

$$\frac{d\hat{p}_\alpha(t)}{dt} = \frac{i}{\hbar}[\hat{H}, \hat{p}_\alpha(t)] = 0\tag{1.1.76}$$

We see that \hat{p}_α does not change in time and therefore is a conserved quantity. The symmetry operation in the $\hat{\mathbf{r}}$ coordinate is written in terms of the canonical conjugate $\hat{\mathbf{p}}$ as a symmetry generator, and this symmetry leads to a conservation law for $\hat{\mathbf{p}}$. When we proceed to quantum field theory, this will be seen to be related to the Noether theorem.

1.2 Many-Particle Quantum Mechanics: Second Quantization

In this section, we consider the many-particle case. In this case the wave function is a function of the time t and $3N$ -dimensional coordinate space (for a moment, we omit the spin dependence)

$$\langle \mathbf{r}_1, \dots, \mathbf{r}_N | \psi(t) \rangle = \psi(\mathbf{r}_1, \dots, \mathbf{r}_N, t)\tag{1.2.1}$$

Unlike classical mechanics, in many-particle quantum mechanics it is impossible in principle to distinguish particles of the same species. We cannot think about indistinguishable particles as rigid bodies; however, it should be possible to get an idea of it with the following metaphor.

Think about a luminous advertisement screen. By switching the lamps on and off at every point of the surface, it is possible to create a moving picture. Places that are illuminated have more energy than the other places, and therefore there should be a particle. A state with N particles at $\mathbf{r}_1 \cdots \mathbf{r}_N$ should correspond to the state where N lights are illuminated. In this metaphor, it is clear that it is not possible to distinguish the particles. The particle appears as an illuminated lamp, and it is not possible to

trace back the way of it as rigid body.

In mathematical language, this means that exchanging the order of $\mathbf{r}_1 \cdots \mathbf{r}_N$ does not lead to a new state, but should lead to the very same state again. Explicitly, taking care also of the statistics when exchanging \mathbf{r}_i with \mathbf{r}_j , we obtain

$$\begin{aligned} & \psi(\mathbf{r}_1, \cdots, \mathbf{r}_j, \cdots, \mathbf{r}_i, \cdots, \mathbf{r}_N) \\ &= \begin{cases} +\psi(\mathbf{r}_1, \cdots, \mathbf{r}_i, \cdots, \mathbf{r}_j, \cdots, \mathbf{r}_N) & (\text{boson}) \\ -\psi(\mathbf{r}_1, \cdots, \mathbf{r}_i, \cdots, \mathbf{r}_j, \cdots, \mathbf{r}_N) & (\text{fermion}) \end{cases}. \end{aligned} \quad (1.2.2)$$

However, as the reader might have realized, we now have a little problem with the interpretation of the wave function. Of course,

$$P(\mathbf{r}_1, \cdots, \mathbf{r}_N; t) = |\psi(\mathbf{r}_1, \cdots, \mathbf{r}_N; t)|^2 \quad (1.2.3)$$

is the probability of finding at time t the N particles at $\mathbf{r}_1 \cdots \mathbf{r}_N$. However, the image that we have in mind in the single-particle case, namely that $\psi(\mathbf{r}, t)$ is the complex wave amplitude at the position \mathbf{r} in the three-dimensional physical space, is ruined because we now have to think mathematically about a $3N$ -dimensional space. The answer to the question whether in the many-particle case it is still possible to think about a wave function in the physical three-dimensional space is given by the so-called method of second quantization.

For a detailed discussion of the second quantization the reader is referred to [1]. Here, we proceed in a heuristic way. Let us return to the single-particle case. We decompose the single-particle wave function $\psi(\mathbf{r}, t)$ in an orthonormal basis $\phi_n(\mathbf{r})$

$$\psi(\mathbf{r}, t) = \sum_n a_n(t) \phi_n(\mathbf{r}) \quad (1.2.4)$$

The whole time dependence is given by the expansion coefficients $a_n(t)$. Inserting (1.2.4) into the Schrödinger equation, we obtain

$$i\hbar \sum_n \frac{da_n(t)}{dt} \phi_n(\mathbf{r}) = \sum_n a_n(t) \hat{H} \phi_n(\mathbf{r}) \quad (1.2.5)$$

Multiplying by $\phi_n^*(\mathbf{r})$ and integrating over \mathbf{r} , we obtain

$$i\hbar \frac{da_n(t)}{dt} = \sum_m \langle \phi_n | \hat{H} | \phi_m \rangle a_m(t). \quad (1.2.6)$$

The complex conjugate of this equation is given by

$$i\hbar \frac{da_n^*(t)}{dt} = - \sum_m a_m^*(t) \langle \phi_m | \hat{H} | \phi_n \rangle, \quad (1.2.7)$$

where $\hat{H}^\dagger = \hat{H}$ has been used.

These equations determine the time development of the expansion coefficients $a_n(t)$. We will now modify them a little. In order to do so, we must think about the energy expectation value \hat{H} in the state $|\psi(t)\rangle$:

$$\langle \hat{H} \rangle = \langle \psi(t) | \hat{H} | \psi(t) \rangle = \sum_{n,m} a_n^*(t) a_m(t) \langle \phi_n | \hat{H} | \phi_m \rangle \quad (1.2.8)$$

Using this expression we can write for (1.2.6) and (1.2.7), respectively

$$\frac{da_n(t)}{dt} = \frac{\partial \langle \hat{H} \rangle}{\partial (i\hbar a_n^*)} \quad (1.2.9)$$

and

$$\frac{d(i\hbar a_n^*(t))}{dt} = -\frac{\partial \langle \hat{H} \rangle}{\partial a_n}. \quad (1.2.10)$$

Here, we see that these equations are formally analogous to Hamilton's canonical equation with the correspondences $a_n \leftrightarrow x$ and $i\hbar a_n^* \leftrightarrow p$. However, of course the expansion coefficients a_n and a_n^* are not dynamical variables of the system.

The idea of second quantization is to promote a_n and a_n^* to operators and to interpret $N_n = N|a_n|^2 = Na_n a_n^*$ as physical quantities of the system. Originally, in single-particle quantum mechanics, N_n is N times the probability of detecting the particle when the same experiment is performed N times. Then, N is the number of experiments, and therefore in principle this experiment can be performed in single particle quantum mechanics.

On the other hand, consider a system with N non-interacting particles where only one experiment is performed, and where the number of particles in the single particle state n is observed to be \hat{N}_n . Since both experiments described above are different, N_n and \hat{N}_n are different quantities - repeating number, or observed number of particles. Experience tells us that these two numbers often agree. Admitting this, the number N_n appearing in the single particle system after performing N experiments will be promoted to the observable (physical quantity) $\hat{N} = \hat{A}_n^\dagger \hat{A}_n$ in the N -particle system. At the same time,

$$\begin{aligned} \sqrt{N} a_n &\rightarrow \hat{A}_n, \\ \sqrt{N} a_n^* &\rightarrow \hat{A}_n^\dagger \end{aligned} \quad (1.2.11)$$

are promoted to operators. Taking into account also that the energy expectation value \hat{H} is multiplied by N , it is clear from (1.2.9) and (1.2.10) that \hat{A}_n and $i\hbar \hat{A}_n^*$ are canonical conjugate variables. Therefore, we suppose that they fulfill the same commutation relation as \hat{r} and \hat{p} :

$$[\hat{A}_n, i\hbar \hat{A}_n^\dagger] = i\hbar \quad (1.2.12)$$

Further generalizing (1.2.12), we obtain

$$\begin{aligned} [\hat{A}_n, i\hbar\hat{A}_m^\dagger] &= i\hbar\delta_{n,m}, \\ [[\hat{A}_n, \hat{A}_m] &= [i\hbar\hat{A}_n^\dagger, i\hbar\hat{A}_m^\dagger] = 0. \end{aligned} \quad (1.2.13)$$

From these commutation relations it can be understood that \hat{A}_n^\dagger , and \hat{A}_n are creating and annihilating one particle in the state n , respectively. We write $|N_n\rangle$ for the many-particle state where N_n particles are in the single-particle state n . Then, the following equation holds:

$$\hat{N}_n|N_n\rangle = N_n|N_n\rangle \quad (1.2.14)$$

Acting with \hat{N}_n on the state $\hat{A}_n^\dagger|N_n\rangle$, we obtain

$$\begin{aligned} \hat{N}_n\hat{A}_n^\dagger|N_n\rangle &= ([\hat{N}_n, \hat{A}_n^\dagger] + \hat{A}_n^\dagger\hat{N}_n)|N_n\rangle \\ &= (N_n + 1)\hat{A}_n^\dagger|N_n\rangle \end{aligned} \quad (1.2.15)$$

Here, we used a variation of equation (1.2.13)

$$[\hat{N}_n, \hat{A}_n^\dagger] = [\hat{A}_n^\dagger\hat{A}_n, \hat{A}_n^\dagger] = \hat{A}_n^\dagger[\hat{A}_n, \hat{A}_n^\dagger] = \hat{A}_n^\dagger \quad (1.2.13')$$

From (1.2.15) it follows that the particle number eigenvalue of the state $\hat{A}_n^\dagger|N_n\rangle$ is given by $N_n + 1$, and therefore \hat{A}_n^\dagger is an operator that increases the particle number by one. In the same way, it can be seen that \hat{A}_n is an operator that decreases the particle number by one. Starting from the state $|N_n = 0\rangle$, we can create the states $N_n = 0, 1, 2, \dots$ by acting on it successively with \hat{A}_n^\dagger . The particle picture arises because the particle number eigenvalue N_n counts discrete integer numbers.

On the other hand, what might the wave picture be? In order to understand it, we define the field operators $\hat{\psi}(\mathbf{r})$ and $\hat{\psi}^\dagger(\mathbf{r})$

$$\begin{aligned} \hat{\psi}(\mathbf{r}) &= \sum_n \hat{A}_n \phi_n(\mathbf{r}), \\ \hat{\psi}^\dagger(\mathbf{r}) &= \sum_n \hat{A}_n^\dagger \phi_n(\mathbf{r}), \end{aligned} \quad (1.2.16)$$

Using the commutator relation (1.2.13) and the fact that $\{\phi_n(\mathbf{r})\}$ is an orthonormal basis of single-particle states, we obtain

$$\begin{aligned} [\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')] &= \sum_{n,m} [\hat{A}_n, \hat{A}_m^\dagger] \phi_n(\mathbf{r}) \phi_m^*(\mathbf{r}') \\ &= \sum_n \langle \mathbf{r}|n\rangle \langle n|\mathbf{r}'\rangle = \langle \mathbf{r}|\mathbf{r}'\rangle = \delta(\mathbf{r} - \mathbf{r}') \end{aligned} \quad (1.2.17)$$

and

$$[\hat{\psi}(\mathbf{r}), \hat{\psi}(\mathbf{r}')] = [\hat{\psi}^\dagger(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')] = 0 \quad (1.2.18)$$

$n(\mathbf{r}) = \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})$ is the particle density at the position \mathbf{r} , $\hat{\psi}^\dagger(\mathbf{r})$ is the creation operator of a particle at position \mathbf{r} , and $\hat{\psi}(\mathbf{r})$ is the annihilation operator of a particle at position \mathbf{r} . By promoting the wave functions $\psi(\mathbf{r})$ and $\psi^*(\mathbf{r})$ to operators $\hat{\psi}(\mathbf{r})$ and $\hat{\psi}^*(\mathbf{r})$, we regain the picture of wave functions in the three-dimensional physical space, and also the metaphor of the luminous advertisement screen works well. More precisely, the position coordinate $\hat{\mathbf{r}}$ is degraded from an operator to a label \mathbf{r} defining the position of the light, and instead operators switching the light on ($\hat{\psi}^\dagger(\mathbf{r})$) and off ($\hat{\psi}(\mathbf{r})$) emerge. A particle is described as the excitation of a field that is created and annihilated.

We now introduce the phase operator $\hat{\theta}_n$ describing the interference of a wave by

$$\begin{aligned}\hat{A}_n^\dagger &= (\hat{N}_n)^{1/2} e^{-\frac{i}{\hbar} \hat{\theta}_n}, \\ \hat{A}_n &= e^{\frac{i}{\hbar} \hat{\theta}_n} (\hat{N}_n)^{1/2}.\end{aligned}\tag{1.2.19}$$

We show that by assuming the canonical conjugation relations of \hat{N} and $\hat{\theta}_n$

$$[\hat{N}_n, \hat{\theta}_n] = i\hbar\tag{1.2.20}$$

the commutation relation (1.2.12) is obtained. In order to do so, we define

$$\hat{N}_n(\lambda) = \exp\left(\frac{i}{\hbar} \lambda \hat{\theta}_n\right) \hat{N}_n \exp\left(-\frac{i}{\hbar} \lambda \hat{\theta}_n\right)\tag{1.2.21}$$

Then, the following equation holds:

$$[\hat{A}_n, \hat{A}_n^\dagger] = \hat{N}_n(1) - \hat{N}_n(0) = \int_0^1 \frac{d\hat{N}_n(\lambda)}{d\lambda} d\lambda.\tag{1.2.22}$$

On the other hand, owing to (1.2.20), we obtain

$$\frac{d\hat{N}_n(\lambda)}{d\lambda} d\lambda = \frac{i}{\hbar} \exp\left(\frac{i}{\hbar} \lambda \hat{\theta}_n\right) [\hat{\theta}_n, \hat{N}_n] \exp\left(-\frac{i}{\hbar} \lambda \hat{\theta}_n\right) = 1\tag{1.2.23}$$

and therefore (1.2.12).

Now, having introduced the particle number operator \hat{N}_n and its canonical conjugate, the phase $\hat{\theta}_n$, it is necessary to stress the following. Obviously, \hat{N}_n is a Hermitian operator; however, exactly speaking, $\hat{\theta}_n$ is not Hermitian. In order to see this, we notice that owing to (1.2.22)

$$\exp\left(\frac{i}{\hbar} \lambda \hat{\theta}_n\right) \hat{N}_n \exp\left(-\frac{i}{\hbar} \lambda \hat{\theta}_n\right) = \hat{N}_n + 1\tag{1.2.24}$$

holds, and for a general integer number m

$$\begin{aligned} \exp\left(\frac{i}{\hbar}\lambda\hat{\theta}_n\right)(\hat{N}_n)^m\exp\left(-\frac{i}{\hbar}\lambda\hat{\theta}_n\right) &= \left[\exp\left(\frac{i}{\hbar}\lambda\hat{\theta}_n\right)\hat{N}_n^m\exp\left(-\frac{i}{\hbar}\lambda\hat{\theta}_n\right)\right]^m \\ &= (\hat{N}_n + 1)^m \end{aligned} \quad (1.2.25)$$

holds. For a general function $g(N)$ we obtain

$$\exp\left(\frac{i}{\hbar}\lambda\hat{\theta}_n\right)g(\hat{N}_n)\exp\left(-\frac{i}{\hbar}\lambda\hat{\theta}_n\right) = g(\hat{N}_n + 1). \quad (1.2.26)$$

This means that $\hat{U} = \exp(\frac{i}{\hbar}\lambda\hat{\theta}_n)$ is a linear operator acting on \hat{N}_n , just like $\hat{U}(\mathbf{a})$ in (1.1.60). If $\hat{\theta}_n$ were Hermitian, then \hat{U} would be a unitary operator with $\hat{U}^\dagger\hat{U} = \hat{U}\hat{U}^\dagger = 1$. However, this identity is not true. This can be seen from (1.2.26): \hat{U}^\dagger increases N_n by one, \hat{U} decreases N_n by one. Acting with \hat{U} on the vacuum state with no particles $|N_n = 0\rangle$ we obtain $\hat{U}|N_n = 0\rangle = 0$. Acting on this equation with \hat{U}^\dagger we obtain of course $\hat{U}^\dagger\hat{U}|N_n = 0\rangle = 0$. However, because of $\hat{U}\hat{U}^\dagger|N_n = 0\rangle = \hat{U}|N_n = 1\rangle = |N_n = 0\rangle \neq 0$ we have just demonstrated that $\hat{U}^\dagger\hat{U} \neq \hat{U}\hat{U}^\dagger$. Therefore, we conclude that because the particle number N_n is bounded from below, $\hat{\theta}$ is not Hermitian. However, when only states with $N_n \gg 1$ are considered, the existence of a lower bound can be neglected, and $\hat{\theta}$ can be regarded to be Hermitian.

Next, we deduce the Hamiltonian occurring after second quantization. Continuing in a heuristic manner as above, we declare in (1.2.8) $\langle\hat{H}\rangle$ to be an operator again and write

$$\hat{H} = \sum_{n,m} \hat{A}_n^\dagger \langle\phi_n|\hat{H}_1|\phi_m\rangle \hat{A}_m \quad (1.2.27)$$

Here, \hat{H}_1 is the single-particle Hamiltonian, being an operator in the sense that it acts on single-particle wave functions $\phi^*(\mathbf{r})$ and $\phi_m(\mathbf{r})$. \hat{H} is an operator because \hat{A}_n^\dagger and \hat{A}_m are operators; however, $\dagger\langle\phi_n|\hat{H}_1|\phi_m\rangle$ is a simple complex number.

Equation (1.2.27) can also be expressed in terms of the field operators $\hat{\psi}^\dagger(\mathbf{r})$ and $\hat{\psi}(\mathbf{r})$:

$$\hat{H} = \int^3 d\mathbf{r} \hat{\psi}^\dagger(\mathbf{r}) \hat{H}_1 \hat{\psi}(\mathbf{r}). \quad (1.2.28)$$

The Heisenberg equation of motion of $\hat{\psi}$ is given by

$$i\hbar \frac{\partial \hat{\psi}(\mathbf{r}, t)}{\partial t} = [\hat{\psi}(\mathbf{r}), \hat{H}] = \hat{H}_1 \hat{\psi}(\mathbf{r}, t). \quad (1.2.29)$$

If $\hat{\psi}(\mathbf{r})$ were a single-particle wave function, then this equation would be the Schrödinger equation (1.1.1); however, again we mention that $\hat{\psi}(\mathbf{r})$ is an operator, and the above equation describes the time evolution of this operator in the Heisenberg picture, which leads to a totally different meaning.

In the framework of second quantization, it is also possible to express the interaction between particles in terms of $\hat{\psi}(\mathbf{r})$ and $\hat{\psi}^\dagger(\mathbf{r})$. We mention only the result

$$\sum_{i < j} v(\mathbf{r}_i - \mathbf{r}_j) \rightarrow \frac{1}{2} \int d^3\mathbf{r} d^3\mathbf{r}' \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') v(\mathbf{r} - \mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}). \quad (1.2.30)$$

The Hamiltonian is then the sum of \hat{H} in (1.2.28) and the right-hand side of (1.2.30), and the equation of motion of the field operator is

$$i\hbar \frac{\partial \hat{\psi}(\mathbf{r}, t)}{\partial t} = \hat{H}_1 \hat{\psi}(\mathbf{r}, t) + \left[\int d^3\mathbf{r}' \hat{\psi}^\dagger(\mathbf{r}', t) v(\mathbf{r} - \mathbf{r}') \hat{\psi}(\mathbf{r}', t) \right] \hat{\psi}(\mathbf{r}, t) \quad (1.2.31)$$

Comparing this expression with (1.2.29), we notice that owing to the interaction, a non-linear term emerges. Because this is not the Schrödinger equation, but the Heisenberg equation, there is no conflict with the superposition principle of quantum mechanics.

Finally, we mention the case of fermions. The whole discussion so far is valid for the case when all particles obey Bose statistics. For fermions, all the commutator relations (1.2.12), (1.2.13), (1.2.17) and (1.2.18) must be replaced by the anti-commutator relations. By doing so, the Hamiltonian (1.2.28), (1.2.30) and the equation of motion of the field (1.2.31) are valid as they stand.

In the case when the particles have a spin degree of freedom, the \mathbf{r} coordinate must be extended to (\mathbf{r}, σ) [σ is the spin component, for example the eigenvalue S_z of the spin in the z direction]. The discussion of the phase of the fermions is not that simple compared with the bosonic case. This question will be examined in Chap. 5.

1.3 The Variation Principle and the Noether Theorem

We return to a single-particle system. The Heisenberg equation of motion, describing the time evolution of a particle at position $\hat{\mathbf{r}}$ having momentum $\hat{\mathbf{p}}$, is given by

$$i\hbar \frac{d}{dt} \hat{\mathbf{r}}(t) = [\hat{\mathbf{r}}(t), \hat{H}] = i\hbar \left. \frac{\partial H(\mathbf{r}, \mathbf{p})}{\partial \mathbf{p}} \right|_{\substack{\mathbf{r}=\hat{\mathbf{r}}(t) \\ \mathbf{p}=\hat{\mathbf{p}}(t)}}, \quad (1.3.1)$$

$$i\hbar \frac{d}{dt} \hat{\mathbf{p}}(t) = -[\hat{\mathbf{p}}(t), \hat{H}] = i\hbar \left. \frac{\partial H(\mathbf{r}, \mathbf{p})}{\partial \mathbf{r}} \right|_{\substack{\mathbf{r}=\hat{\mathbf{r}}(t) \\ \mathbf{p}=\hat{\mathbf{p}}(t)}}. \quad (1.3.2)$$

Here, $H(\mathbf{r}, \mathbf{p})$ is a function of \mathbf{r} and \mathbf{p} , from which the Hamiltonian \hat{H} is obtained by substituting $\mathbf{r} \rightarrow \hat{\mathbf{r}}(t)$ and $\mathbf{p} \rightarrow \hat{\mathbf{p}}(t)$. The above equation has the same structure as

the classical canonical equations of the Hamiltonian:

$$\frac{d}{dt}\mathbf{r}(t) = \frac{\partial H(\mathbf{r}(t), \mathbf{p}(t))}{\partial \mathbf{p}(t)} \quad (1.3.1')$$

$$\frac{d}{dt}\mathbf{p}(t) = -\frac{\partial H(\mathbf{r}(t), \mathbf{p}(t))}{\partial \mathbf{r}(t)} \quad (1.3.2')$$

Here, we return for a moment to classical mechanics and use the variation principle of analytical mechanics:

$$L(\mathbf{r}, \dot{\mathbf{r}}; \mathbf{p}) = \mathbf{p} \cdot \dot{\mathbf{r}} - H(\mathbf{r}, \mathbf{p}) \quad (1.3.3)$$

We define the action S as

$$S = \int dt L(\mathbf{r}(t), \dot{\mathbf{r}}(t); \mathbf{p}(t)) \quad (1.3.4)$$

The variation of S in \mathbf{r} and \mathbf{p} is given by

$$\begin{aligned} \delta S &= \int dt \left\{ \delta \mathbf{r}(t) \cdot \frac{\partial L}{\partial \mathbf{r}(t)} + \delta \dot{\mathbf{r}}(t) \cdot \frac{\partial L}{\partial \dot{\mathbf{r}}(t)} + \delta \mathbf{p}(t) \cdot \frac{\partial L}{\partial \mathbf{p}(t)} \right\} \\ &= \int dt \left\{ \delta \mathbf{r}(t) \cdot \left[\frac{\partial L}{\partial \mathbf{r}(t)} - \frac{d}{dt} \frac{\partial L}{\partial \dot{\mathbf{r}}(t)} \right] + \delta \mathbf{p}(t) \cdot \frac{\partial L}{\partial \mathbf{p}(t)} \right\}. \end{aligned} \quad (1.3.5)$$

(The reader unfamiliar with the variation principle or functional derivative is referred to Appendix A.2.) By requiring that the variation δS must be zero for arbitrary transformations $\delta \mathbf{r}(t)$ and $\delta \mathbf{p}(t)$, we obtain directly (1.3.1') and (1.3.2').

So, what might be the variation principle corresponding to the field equation (1.2.31)? We know already the analogy $\hat{\mathbf{r}} \leftrightarrow \hat{\psi}(\mathbf{r})$ and $\hat{\mathbf{p}} \leftrightarrow i\hbar\hat{\psi}^\dagger(\mathbf{r})$. From (1.3.3) we can deduce that the Lagrangian must be

$$L(\{\psi(\mathbf{r})\}, \{\dot{\psi}(\mathbf{r})\}, \{\psi^\dagger(\mathbf{r})\}) = \int i\hbar\psi^\dagger(\mathbf{r})\dot{\psi}(\mathbf{r})d\mathbf{r} - H(\psi(\mathbf{r}), \psi^\dagger(\mathbf{r})). \quad (1.3.6)$$

We write for the Lagrange density \mathcal{L}

$$\begin{aligned} \mathcal{L}(\{\phi_A(x)\}, \{\partial_\mu \phi_A(x)\}) &= i\hbar\psi^\dagger(\mathbf{r}, t)\dot{\psi}(\mathbf{r}, t) \\ &\quad - \frac{\hbar^2}{2m}[\nabla\psi^\dagger(\mathbf{r}, t)][\nabla\psi(\mathbf{r}, t)] - V(\mathbf{r})\psi^\dagger(\mathbf{r}, t)\psi(\mathbf{r}, t) \\ &\quad - \frac{1}{2} \int d\mathbf{r}' \psi^\dagger(\mathbf{r}, t)\psi^\dagger(\mathbf{r}', t)v(\mathbf{r} - \mathbf{r}')\psi(\mathbf{r}', t)\psi(\mathbf{r}, t) \end{aligned} \quad (1.3.7)$$

We now introduce the combined notation x for the space coordinate \mathbf{r} and the time coordinate t , defining the x^μ components to be (t, \mathbf{r}) . The space-time coordinates with lower index x_μ are defined to be $(f, -\mathbf{r})$. The partial differential operator ∂_μ corresponding to these coordinate components is given by $\partial_\mu = \partial/\partial x^\mu = (\partial/\partial t, \nabla)$.

We wrote the label A to distinguish between different complex fields $\varphi_A(x)$; in the present case we write $\varphi_{A=1} = \psi(\mathbf{r}, t)$ and $\varphi_{A=2} = \psi^\dagger(\mathbf{r}, t)$. The action S can be expressed in terms of L or \mathcal{L} as

$$\begin{aligned} S &= \int dt L(\{\varphi_A(x)\}, \{\partial_\mu \varphi_A(x)\}) \\ &= \int d^4x \mathcal{L}(\{\varphi_A(x)\}, \{\partial_\mu \varphi_A(x)\}) \end{aligned} \quad (1.3.8)$$

As in (1.3.5), by taking the variation

$$\begin{aligned} \delta S &= \int d^4x \left\{ \delta \varphi_A(x) \frac{\delta S}{\delta \varphi_A(x)} + \delta(\partial_\mu \varphi_A(x)) \frac{\delta S}{\delta(\partial_\mu \varphi_A(x))} \right\} \\ &= \int d^4x \delta \varphi_A(x) \left\{ \frac{\delta S}{\delta \varphi_A(x)} - \partial_\mu \left(\frac{\delta S}{\delta(\partial_\mu \varphi_A(x))} \right) \right\} \end{aligned} \quad (1.3.9)$$

and requiring that $\delta S = 0$, we obtain

$$\frac{\delta S}{\delta \varphi_A(x)} - \partial_\mu \left(\frac{\delta S}{\delta(\partial_\mu \varphi_A(x))} \right) = 0 \quad (1.3.10)$$

From (1.3.7), for the case $A = 2$ we obtain

$$\begin{aligned} i\hbar \dot{\psi}(\mathbf{r}, t) - V(\mathbf{r})\psi(\mathbf{r}, t) - \int d\mathbf{r}' \psi^\dagger(\mathbf{r}', t) v(\mathbf{r} - \mathbf{r}') \psi(\mathbf{r}', t) \\ - \nabla \cdot \left\{ -\frac{\hbar^2}{2m} \nabla \psi(\mathbf{r}, t) \right\} = 0 \end{aligned}$$

By rearranging this equation, we regain equation (1.2.31).

Next, we examine the symmetry operations in quantum field theory. Corresponding to the transformation $\hat{\mathbf{r}} \rightarrow \hat{\mathbf{r}} + \boldsymbol{\alpha}$ in single-particle quantum mechanics, we consider the transformation

$$\varphi_A(x) \rightarrow \varphi'_A(x) = \varphi_A(x) + \delta \varphi_A(x) \quad (1.3.11)$$

$$\partial_\mu \varphi_A(x) \rightarrow \partial_\mu \varphi'_A(x) = \partial_\mu \varphi_A(x) + \partial_\mu (\delta \varphi_A(x)) \quad (1.3.12)$$

As an explicit example, we consider a phase transformation with constant phase of the field operator

$$\begin{aligned} \varphi_1(x) = \psi(x) &\rightarrow \psi'(x) = e^{-ia} \psi(x) \simeq \psi(x) - ia\psi(x) \\ \varphi_2(x) = \psi^\dagger(x) &\rightarrow \psi'^\dagger(x) = e^{+ia} \psi^\dagger(x) \simeq \psi^\dagger(x) + ia\psi^\dagger(x) \end{aligned} \quad (1.3.13)$$

Under the transformation (1.3.11) and (1.3.12), the action S that we assume now to

be bounded to a space-time region Ω transforms as

$$\begin{aligned}
S \rightarrow S' &= \int_{\Omega} d^4x \mathcal{L}(\{\varphi_A(x) + \delta\varphi_A(x)\}, \{\partial_{\mu}\varphi_A(x) + \partial_{\mu}(\delta\varphi_A(x))\}) \\
&= S + \int_{\Omega} d^4x \left\{ \delta\varphi_A(x) \frac{\delta S}{\delta\varphi_A(x)} + \partial_{\mu}(\delta\varphi_A(x)) \frac{\delta S}{\delta(\partial_{\mu}\varphi_A(x))} \right\} \\
&= S + \int_{\Omega} d^4x \delta\varphi_A(x) \left[\frac{\delta S}{\delta\varphi_A(x)} - \partial_{\mu} \left(\frac{\delta S}{\delta(\partial_{\mu}\varphi_A(x))} \right) \right] \\
&\quad + \int_{\Omega} d^4x \partial_{\mu} \left[\frac{\delta S}{\delta(\partial_{\mu}\varphi_A(x))} \delta\varphi_A(x) \right]
\end{aligned} \tag{1.3.14}$$

Assuming that ϕ_A obeys the equation of motion (1.3.10), only the third term of the previous expression contributes to the transformation of S . In the case that the action S is invariant under the transformation (1.3.11) and (1.3.12), in every arbitrary region Ω , we obtain

$$\partial_{\mu} \left[\frac{\delta S}{\delta(\partial_{\mu}\varphi_A(x))} \delta\varphi_A(x) \right] = 0. \tag{1.3.15}$$

Defining a current J^{μ} as

$$J^{\mu} \propto \frac{\delta S}{\delta(\partial_{\mu}\varphi_A(x))} \delta\varphi_A(x) \tag{1.3.16}$$

then (1.3.15) becomes the current conservation law.

$$\partial_{\mu} J^{\mu} = 0 \tag{1.3.17}$$

We just deduced the Noether theorem (in its simplest form). “The invariance of the action S shows up in the symmetry under the transformation, and from this symmetry a current conservation law can be deduced.” In the explicit example (1.3.13), the transformation of the action integral S under the phase transformation α can be written via the chain rule with ψ^{\dagger} and ψ as

$$J^{\mu} = \frac{\delta S}{\delta(\partial_{\mu}\psi^{\dagger}(x))} \frac{\partial\delta\psi^{\dagger}(x)}{\partial\alpha} + \frac{\delta S}{\delta(\partial_{\mu}\psi(x))} \frac{\partial\delta\psi(x)}{\partial\alpha} \tag{1.3.18}$$

Because the action is the integral in space and time of the Lagrangian density (1.3.7), we obtain

$$\begin{aligned}
J^0 &= \frac{\delta S}{\delta\dot{\psi}^{\dagger}(x)} i\psi^{\dagger}(x) + \frac{\delta S}{\delta\dot{\psi}(x)} (-i\psi(x)) \\
&= 0 + i\hbar\psi^{\dagger}(x)(-i\psi(x)) \\
&= \hbar\psi^{\dagger}(x)\psi(x) = \hbar n(x) \quad (\mu = 0)
\end{aligned} \tag{1.3.19}$$

$$\begin{aligned}
J^\alpha &= \frac{\delta S}{\delta (\partial_\alpha \psi^\dagger(x))} i\psi^\dagger(x) + \frac{\delta S}{\delta (\partial_\alpha \psi(x))} (-i\psi(x)) \\
&= \left(-\frac{\hbar^2}{2m} \partial_\alpha \psi(x) \right) i\psi^\dagger(x) + \left(-\frac{\hbar^2}{2m} \partial_\alpha \psi^\dagger(x) \right) (-i\psi(x)) \\
&= \frac{\hbar^2}{2mi} \left\{ \psi^\dagger(x) \partial_\alpha \psi(x) - [\partial_\alpha \psi^\dagger(x)] \psi(x) \right\} \\
&= \hbar j^\alpha(x) \quad (\mu = \alpha = 1, 2, 3)
\end{aligned} \tag{1.3.20}$$

Here, $n(x)$ is the particle density, $\mathbf{j}(x)$ is the particle current density, and (1.3.17) becomes the well-known continuity equation:

$$\frac{\partial n(x)}{\partial t} + \nabla \cdot \mathbf{j}(x) = 0 \tag{1.3.21}$$

The number of particles $N_V(t)$ in a three-dimensional volume V is given by

$$N_V(t) = \int_V n(\mathbf{r}, t) d^3\mathbf{r} \tag{1.3.22}$$

and owing to (1.3.21), its time derivative is given by

$$\frac{dN_V(t)}{dt} = \int_V \frac{\partial n(\mathbf{r}, t)}{\partial t} d^3\mathbf{r} = - \int_V \nabla \cdot \mathbf{j}(\mathbf{r}, t) d^3\mathbf{r} = - \int_{\partial V} d\mathbf{S} \cdot \mathbf{j}(\mathbf{r}, t) \tag{1.3.23}$$

Here, we re-expressed the volume integral as a surface integral by using Gauss's theorem. For the case when V is the whole space, $N_V(t)$ becomes the total particle number $N(t)$, and dV becomes the boundary at infinity, where $\mathbf{j}(\mathbf{r}, t)$ is zero and therefore the surface integral vanishes. We conclude that the total particle number $N(t)$ obeys the conservation law $dN(t)/dt = 0$. The conservation law in N that we obtained from the symmetry in the phase is analogous to the conservation law for p that we deduced from the translational symmetry in x .

Last, we discuss the generators of transformations in field theory. Up to now, we have performed functional derivatives of ψ , ψ^\dagger , N and \mathbf{j} in a formal manner, ignoring the fact that we are dealing with operators. Now, we need to recall the properties of operators. We define $\hat{U}(\{\delta\psi(x)\})$ as follows:

$$\begin{aligned}
\hat{U}(\{\delta\psi\}) &= \exp \left[\frac{i}{\hbar} \int d\mathbf{r} \hat{H}(\mathbf{r}) \delta\psi(\mathbf{r}) \right] \\
&\equiv \exp \left[\frac{i}{\hbar} \hat{Q}(\{\delta\psi\}) \right]
\end{aligned} \tag{1.3.24}$$

We define $\hat{\Pi}(\mathbf{r})$ to be the canonical conjugate of $\hat{\psi}$

$$\hat{\Pi}(\mathbf{r}) = \frac{\delta S}{\delta (\partial_t \hat{\psi}(\mathbf{r}))} \quad (1.3.25)$$

and assume the commutation relation

$$[\hat{\psi}(\mathbf{r}), \hat{\Pi}(\mathbf{r}')] = i\hbar \delta(\mathbf{r} - \mathbf{r}') \quad (1.3.26)$$

From (1.3.7) we obtain

$$\hat{\Pi}(\mathbf{r}) = i\hbar \hat{\psi}^\dagger(\mathbf{r}) \quad (1.3.27)$$

and therefore (1.3.26) is identical to (1.2.17).

It is possible to show that

$$\hat{U}(\{\delta\psi(\mathbf{r})\})\hat{\psi}(\mathbf{r})\hat{U}(\{-\delta\psi(\mathbf{r})\}) = \hat{\psi}(\mathbf{r}) + \delta\psi(\mathbf{r}) \quad (1.3.28)$$

holds. The proof corresponds to the discussion concerning (1.1.69)-(1.1.71). Starting with the definition

$$\hat{\psi}(\mathbf{r}; \lambda) = \hat{U}(\{\lambda\delta\psi(\mathbf{r})\})\hat{\psi}(\mathbf{r})\hat{U}(\{-\lambda\delta\psi(\mathbf{r})\}) \quad (1.3.29)$$

we obtain

$$\begin{aligned} \frac{\partial \hat{\psi}(\mathbf{r}; \lambda)}{\partial \lambda} &= \frac{i}{\hbar} \exp \left[\frac{i}{\hbar} \lambda \hat{Q}(\{\delta\psi\}) \right] [\hat{Q}(\{\delta\psi\}), \hat{\psi}(\mathbf{r})] \\ &\quad \times \exp \left[-\frac{i}{\hbar} \lambda \hat{Q}(\{\delta\psi\}) \right] \end{aligned} \quad (1.3.30)$$

and

$$[\hat{Q}(\{\delta\psi\}), \hat{\psi}(\mathbf{r})] = \int d\mathbf{r}' [\hat{\Pi}(\mathbf{r}'), \hat{\psi}(\mathbf{r})] \delta\psi(\mathbf{r}') = -i\hbar \delta\psi(\mathbf{r}) \quad (1.3.31)$$

Because $\delta\psi(\mathbf{r})$ is simply a function, (1.3.30) becomes

$$\frac{\partial \hat{\psi}(\mathbf{r}; \lambda)}{\partial \lambda} = \delta\psi(\mathbf{r}) \quad (1.3.32)$$

Integrating this equation in λ from zero to one, we obtain (1.3.28). Therefore, (1.3.24) acts on $\hat{\psi}(\mathbf{r})$ by shifting it by $\delta\psi(\mathbf{r})$, and therefore it is clear that $\hat{\Pi}$ given in (1.3.25) is the generator of the transformation.

1.4 Quantization of the Electromagnetic Field

2. Quantization with Path Integral Methods

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A. Appendix

A.1 Fourier Transformation

A.2 Functionals and the Variation Principle

A.3 Quantum Statistical Mechanics

References

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