



# **Models of Quantum Matter**

*A First Course on Integrability  
and the Bethe Ansatz*

Hans-Peter Ecker

OXFORD GRADUATE TEXTS

# MODELS OF QUANTUM MATTER



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A First Course on Integrability and the Bethe Ansatz

Hans-Peter Eckle

*Humboldt Study Centre  
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*Für Irene*



# Preface

Why study Bethe ansatz? The Bethe ansatz provides one of the very few methodologies to calculate the physical properties of models for strongly interacting quantum matter *non-perturbatively*. Arguably it is the only such method we have which is exact. This means, once we have set up the model, there are no approximations or further assumptions necessary: we can exactly compute physically relevant properties of the model. There is, furthermore, an infinite set of conserved quantities: the quantum mechanical model is integrable.

This makes the search for quantum models which are amenable to an exact solution by the Bethe ansatz methodology so important and rewarding. Even if—as is sometimes, but *certainly* not always, the case—the model with an exact solution is not the most physically relevant one, the exact solution will provide important benchmarks for other models that may occasionally be closer to physical reality, but do not admit an exact solution. Hence, for a plethora of cases, the Bethe ansatz solution provides valuable insight into the physics of strongly interacting quantum matter.

Since Hans Bethe provided the eponymous method to solve the Heisenberg quantum spin chain, many more models of low-dimensional quantum systems have been found to be integrable by the Bethe ansatz.

Moreover, these models and their integrability have been and continue to play an influential role in many subfields of physics, which include classical and quantum statistical mechanics, quantum field theory, and quantum many-particle and condensed matter physics, the latter in recent times especially in connection with modern developments in physics on the nanometre scale and in low dimensions. Quantum optics has also benefited from studying integrable models, especially in investigations of ultracold Bosonic and Fermionic quantum gases and Bose–Einstein condensates in artificial crystals of light, the so-called optical lattices. Recently in string theory and cosmology there is a hype of activity involving conjectures of Bethe ansatz integrability in the framework of the celebrated anti-de-Sitter space/conformal field theory (AdS/CFT) correspondence.

Of course, Bethe ansatz and integrability are discussed in Mathematical Physics, but there is also an ongoing cross-fertilization with various subfields of pure Mathematics.

Some prominent examples of integrable models include: various variants of the Heisenberg quantum spin chain whose physical realizations are probed by neutron scattering; the Hubbard model and its variants which inter alia have been discussed in connection with high-temperature superconductivity; the Kondo model which has recently seen a renaissance because of the development of tunable quantum dots; interacting Bose and Fermi gases which can now be produced in very pure and tunable form in optical lattices.

But, what is the Bethe ansatz? In its original form, devised by Bethe, it is an ingeniously guessed form for the wave function of a one-dimensional quantum system. However, why this wave function is correct and even exact remained an open question which has only been answered much later through the algebraic form of the Bethe ansatz. This method enables us to construct an integrable quantum model in one dimension from a two-dimensional statistical mechanical model. The construction reveals the reason for quantum integrability and delivers the infinite set of conserved quantities together with the wave function which Bethe guessed. In our exposition of the Bethe ansatz methodology, we shall therefore start, somewhat unhistorically, but more systematically, with the algebraic Bethe ansatz.

Who is this book for? Interestingly, a look at Richard Feynman's last blackboards (Paz, 1989) reveals that he may well have been interested. In one of his last publications (1988), Feynman in fact wrote:

‘I got really fascinated by these  $(1 + 1)$ -dimensional models that are solved by the Bethe ansatz and how mysteriously they jump out at you and work and you don't know why. I am trying to understand all this better.’ Cited after Batchelor (2007).

In view of the exciting developments in Bethe ansatz of the last two decades, Richard Feynman's fascination would certainly have continued.

The most helpful prerequisites for present readers are a good grounding in quantum mechanics, statistical mechanics, and the basics of quantum many-particle theory, especially second quantization. However, we shall comprehensively discuss the necessary tools and background in part I of the book. Through this approach, the book should be smoothly accessible for Master's students who look for an area of specialization as well as for beginning graduate students. Moreover, to paraphrase Paul Halmos (in the preface of his book on Measure Theory (Halmos, 1978)), the novice to the Bethe ansatz methodology should *not* be discouraged if she or he finds that she or he does not have the prerequisites to read the preliminaries. After all, as Max Born reminds us, where would quantum physics be if Werner Heisenberg had been discouraged that he did not know what a matrix was when he developed the matrix form of quantum mechanics?

The book grew out of lecture notes the author prepared for an invited graduate lecture series at the Indian Institute of Science in Bangalore in 1995, summer school courses at the University of Jyväskylä in Central Finland in 1997 (on *Bethe Ansatz Methods in Many-Body Physics*) and 1999 (on *Conformal Invariance in Statistical Physics*), a graduate course at the same University which, together with an amiable group of students, made the extremely cold Finnish winter of 1999 actually an enjoyable experience, and postgraduate courses at the University of New South Wales in Sydney in 2000, and within the Mathematics–Physics  $\mathcal{MP}^2$  Platform at Göteborg University in 2009, as well as summer school lectures in Turkey: 2013 in Turunç, 2014 in Izmir and 2013 in Ireland in Dungarven under the auspices of the School of Theoretical Physics of the Dublin Institute for Advanced Studies.

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I learned coordinate Bethe ansatz from and during a fruitful collaboration with Ferenc Woynarovich. We both were initiated to the algebraic Bethe ansatz by Tuong Truong.

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# Introduction

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*A journey of a thousand miles begins with a single step.*

– Lao Tzu

This brief introductory chapter's purpose is to direct you, the reader, quickly to those places in the book where you can find general introductory information that may be helpful for an overview of and the orientation within the book. It is deliberately kept short to avoid redundancies.

The general motivation for the writing of the book and the main targeted readerships as well as the levels of sophistication assumed and detail aimed at in the presentation of the various parts of the book are outlined in the preface. There, we also attempt a delineation of an assessment of the relevance of the book's topics for current and potential future research.

The list of contents, by its nature in the form of key words and key phrases, provides a more comprehensive orientation of all the topics treated and their mutual dependence.

The book is divided into six major parts and, including this short introductory chapter, into twenty chapters. Each part and each chapter begins with a description detailing their respective subject matter. The part descriptions supply the bigger picture, while the outlines at the beginnings of each chapter point more specifically to the topics treated. Wherever this seemed to be helpful, we have attempted to supply further signposts about what we have achieved and where we plan to go from there.

At various places, we also remark on the depth with which the topics are treated, what may have been left out or will only be mentioned in passing, the relation to other parts and chapters and the book's intentions as a whole, and where to find alternative and further specialized treatments of these topics.

In order to supply a rough overview, let us briefly summarize the major parts of the book and their interrelationship.

Part I ranges from the fundamental concepts and tools required for an understanding of strongly interacting quantum matter to the fundamental models that represent the physical systems of strongly interacting quantum matter. In this book, we want to investigate selected aspects of these models with a particular emphasis on the uses of the exact methodology of the Bethe ansatz and of quantum integrability.

Part II is devoted to the quantum inverse scattering method and the algebraic Bethe ansatz that demonstrate the quantum integrability of certain one-dimensional strongly interacting quantum models and provide their exact solution. Our approach makes decisive use of the intimate connection between these models and two-dimensional

models of classical statistical mechanics. The concrete models we shall be enlisting in this part are the Heisenberg quantum spin chain as one-dimensional quantum model and the six-vertex model as two-dimensional classical statistical model.

In part III, we introduce the coordinate Bethe ansatz, the original approach Bethe used to solve the Heisenberg quantum spin chain. Since this approach does not allow us to understand why the models are quantum integrable, we shall address it only after we discuss the algebraic Bethe ansatz and the quantum inverse scattering method. The coordinate Bethe ansatz approach is, however, still extremely useful. We demonstrate this again for the Heisenberg quantum spin chain and also for a gas of Bosons interacting via  $\delta$ -function potentials in one dimension.

Part IV is concerned with strongly interacting quantum models where the fundamental constituents have internal degrees of freedom. Our examples, the one-dimensional gas of Fermions interacting via  $\delta$ -function potentials, the one-dimensional Hubbard model, and the Kondo model of a magnetic impurity interacting with conduction electrons, are all electronic models where there is only one internal degree of freedom in addition to the particle degree of freedom, which is electronic spin. We shall find that these models can be solved by two interconnected Bethe ansätze. The method is thus called *nested* Bethe ansatz.

Thus far, the Bethe ansatz methods discussed were mainly investigating the low-lying and therefore zero temperature properties of the quantum models. In part V we examine how to extend the Bethe ansatz to finite temperatures. Again, our quantum models of choice will be the Heisenberg quantum spin chain and also the Bose gas interacting via  $\delta$ -function potentials in one dimension.

In part VI, the final part of the book, we relinquish another assumption we made or had to make in order to find solutions of the Bethe ansatz equations, equations which generally hold for a finite system. So far, we usually considered the thermodynamic limit, the limit of an infinite system size. This limit allowed us to rewrite the Bethe ansatz equations as linear integral equations for certain densities whose solutions characterized solutions of the Bethe ansatz equations, but only, of course, for the thermodynamic limit. The Bethe ansatz for finite systems attempts to find corrections to the Bethe ansatz solutions and physical quantities, e.g. the ground state energy of the thermodynamic limit that takes into account the finiteness of a system. Again, we inquire into how this can be achieved using the Heisenberg quantum spin chain as our exemplary model system.

The focus of this book is on selected concepts, methods, and mathematical techniques in the area of strongly interacting quantum matter systems, especially the various Bethe ansatz techniques discussed. We hope that these techniques will prove useful in future research in the area of strongly interacting quantum matter. We also hope that some physical insight will be gained from the models of quantum matter used as examples to demonstrate the concepts and techniques and will provide guidance for the understanding of other systems not treated here.

For the most part, we shall use natural units where the speed of light, Boltzmann's, and Planck's constants are

$$c = k \equiv k_B = \hbar = 1, \tag{1.1}$$

except when including the constants explicitly will render the results more transparent.

# Part 1

## Methods and Models in the Theory of Quantum Matter

*Cannot we be content with experiment alone? No, that is impossible; that would be a complete misunderstanding of the true character of science. The man of science must work with method. Science is built up of facts, as a house is built of stones; but an accumulation of facts is no more a science than a heap of stones is a house.*

– Henri Poincaré (1854–1912)

This first part of the book presents an overview of the most important methods indispensable for an understanding of the theory of strongly interacting quantum matter. Moreover, we introduce a selection of quantum mechanical many-particle models and the related concepts that form the background of the theory of quantum matter, especially in view of the quantum integrable models, whose exact Bethe ansatz solutions are discussed in later parts of the book. These methods and models are relevant also in many other parts of theoretical and mathematical physics. It is therefore recommended that readers review this material to judge how familiar they are with it.

These chapters, however, do not treat and do not attempt to treat their topics in a fully comprehensive manner. There is always a lot more that could be covered. In fact, there is a vast literature specifically devoted to these topics. Nevertheless, we attempt as clear and comprehensible a treatment as possible of the aspects we cover with the intention to render those aspects that we do cover self-contained. Where a self-contained treatment is beyond the limitations of this book, we provide appropriate hints to the literature specially devoted to these topics.

More specifically, in chapter 2, basic facts are reviewed from the quantum mechanics of many-particle systems, in particular leading from the Hilbert spaces representing quantum many-particle systems to a discussion of second quantization, which is the language most useful to formulate the models of strongly interacting quantum matter.

Moreover, in chapter 3 we address the quantum mechanical theory of angular momentum, especially for many quantum particles, which is indispensable for an understanding of the magnetic properties of the models of strongly interacting quantum

matter. These magnetic properties will be at the centre of much of our discussion of quantum integrable models and their exact Bethe ansatz solutions.

Quantum many-particle theory is, of course, resting on the foundations of equilibrium statistical mechanics, especially quantum statistical mechanics. But classical statistical mechanics also will be necessary to appreciate the developments of quantum models that are integrable by the Bethe ansatz method. An examination of the methods and results of equilibrium statistical mechanics, both classical and quantum, will therefore be a useful addition in this first part of the book, and which we take up in chapter 4.

Among the most fascinating phenomena of many-particle systems, again classical and quantum, phase transitions and critical phenomena occupy a prominent place. Their theoretical description is challenging and requires an arsenal of sophisticated and innovative methods that are outlined in chapter 5, where we also analyse the approach to the thermodynamic limit of systems of finite size.

There is an intimate connection between quantum field theory and (classical) statistical mechanics on which much of the quantum inverse scattering method and the algebraic Bethe ansatz is founded. Chapter 6 offers an introduction to this immensely useful connection, which will also play a central role in the subsequent chapter.

Bethe ansatz calculations for finite systems, being rather more involved than those in the thermodynamic limit, produce results that can be directly compared to predictions based on the conformal symmetry of two-dimensional classical statistical mechanics. In order to fully appreciate this connection, chapter 7 offers an introduction into basic aspects of the conformal symmetry of critical systems.

While the chapters described so far were mainly concerned with methods useful for a thorough appreciation of the Bethe ansatz methodologies examined in later parts of the book, chapter 8 of this first part introduces the physical background of a selection of models of strongly interacting quantum matter together with methods to investigate and understand them. The selection criteria have been whether appropriate versions of the models exhibit quantum integrability and are solvable by Bethe ansatz. The quantum many-particle models considered range from the Bose fluid to models of itinerant as well as localized magnetism and to the Fermi liquid and ultimately to models of strong light-matter interaction.

## 2

# Quantum Many-Particle Systems and Second Quantization

---

*One of the principal objects of theoretical research is to find the point of view from which the subject appears in the greatest simplicity.*

Josiah Willard Gibbs (1839–1903)

This chapter reviews some aspects of the quantum mechanics of systems composed of many particles (many-body or many-particle systems), which will prove useful for the later developments in this book. We mainly concentrate on the foundations of quantum many-particle physics leading to the formalism of *second quantization* as a convenient language for the formulation of the properties of the many-particle systems of quantum matter.

Many-particle quantum systems can be described by a many-particle Schrödinger equation, whose corresponding wave function depends on the configuration of the particles, e.g. their positions  $\mathbf{r}_i$  and possibly further quantum numbers, e.g. the spin quantum numbers  $\sigma_i$  of the particles. In practice this approach is very cumbersome even for quite modest numbers of particles, let alone for the macroscopic numbers of particles of quantum statistical mechanics and condensed matter physics. *Second quantization* is a formulation or language of many-particle quantum mechanics that helps to minimize the technical complications of practical calculations for many-particle systems.

It is also the appropriate language of other branches of theoretical physics, most notably quantum field theory (see, for example Lancaster and Blundell, 2014).

Two examples illustrate the usefulness of second quantization. In quantum field theory as well as many applications of many-particle physics and condensed matter physics, the number of particles is variable, i.e. particles can be created as well as destroyed.<sup>1</sup> Moreover, the Schrödinger equation, and hence the wave function, for a

<sup>1</sup> As we shall see, the concept of creating and annihilating particles is a rather abstract one, especially for Fermions, i.e. particles for which the Pauli exclusion principle applies. Richard Feynman, in his Nobel prize acceptance speech (Feynman, 1965), alludes to this in a personal reminiscence: ‘I remember that when someone had started to teach me about creation and annihilation operators, that this operator creates an electron, I said, “how do you create an electron? It disagrees with the conservation of charge”, and in that way, I blocked my mind from learning a very practical scheme of calculation.’

system of  $N = 10^{24}$  particles is different from those of a system of  $N = 10^{24} - 1$  particles. Yet, we expect both systems to exhibit the same macroscopic physics. In the language of second quantization, which is specifically adapted to accommodate variable numbers of particles, we can cope easily with both situations as detailed work in this chapter and in chapter 4 on equilibrium statistical mechanics shows, as well as throughout many other chapters of this book.

Second quantization is a standard topic of quantum many-particle theory and treatments can be found in many books wholly or partly devoted to this topic. A classic reference devoted to the method of second quantization is Berezin (1966). Some standard references are the corresponding chapters of Abrikosov *et al.* (1975), Fetter and Walecka (2003), Mahan (2000), and Negele and Orland (1998). More recent work includes Nazarov and Danon (2013), Altland and Simons (2010), and Coleman (2015). Of course, all of these works treat many more topics in the theory of quantum many-particle physics.

In particular, applications of the method of second quantization can be found in the cited works and in later chapters of this book, where we shall make ample use of the language of second quantization. In this chapter, however, we concentrate on the formalism, demonstrating its power with only a few elementary examples.

Section 2.1 of this chapter constructs the Hilbert spaces, the tensor product spaces, and the Fock spaces, appropriate for the states of the many-particle system and then section 2.2, selects from these Hilbert spaces the symmetrized many-particle states of the many-particle Hilbert space that describe Bosons, where any number of particles can occupy the same quantum state and the antisymmetrized many-particle states that describe Fermions, where at most one particle can occupy the same quantum state.

This construction of Hilbert spaces is more general: for any quantum system composed of subsystems, a Hilbert space can be constructed in the way we describe. Therefore, we initially keep the discussion more general before we focus again on Hilbert spaces composed of (many) quantum particles.

For the following few sections, we focus on the Bosonic case, before eventually also discussing Fermions. In section 2.3, we introduce creation and annihilation operators for Bosons. These operators are the main objects in which the formalism of second quantization is expressed.

The creation and annihilation operators can be expressed in different orthonormal and complete bases. The transformations of the creation and annihilation operators between different abstract orthonormal and complete bases are derived in section 2.4, while in section 2.5 the creation and annihilation operators in the position basis, then called quantum field operators, are introduced as one of the most important examples.

Section 2.6 is devoted to the introduction of one-particle operators, section 2.7 to two-particle operators in the formalism of second quantization.

An elementary introduction of second quantization starts from the time-dependent single-particle Schrödinger equation of basic quantum mechanics. How this can be achieved is demonstrated for Bosons in section 2.8 and for Fermions in section 2.10.

Section 2.9 finally returns to Fermions, introducing creation and annihilation operators for the Fermionic case.

The penultimate section of this chapter, 2.11 demonstrates explicitly the equivalence of the many-particle wave function and the formalism of second quantization, while the final section 2.12 of this chapter touches on the issue of the correct ordering of creation and annihilation operators, i.e. the normal ordering.

As a prelude to the formalism, we start with an elementary exercise: the quantum treatment of the single particle one-dimensional harmonic oscillator in terms of creation and annihilation operators, sometimes also called ladder operators. In this exercise we are reminded of important notions that help illuminate the more formal treatment of the rest of this chapter. Moreover, the algebraic structure encountered here will reappear many times in this and in later chapters. Hence, it may be quite a good idea to go through this elementary exercise to gain confidence for the more involved later developments.

**EXERCISE 2.1 Quantum mechanical harmonic oscillator** The Hamiltonian of the one-dimensional harmonic oscillator of a mass  $m$  and frequency  $\omega$  is given in terms of the position operator  $x$  and the momentum operator  $p = -i\frac{d}{dx}$  satisfying the canonical commutation relation

$$[x, p] = i \tag{2.1}$$

as

$$\mathcal{H} = \frac{1}{2m}p^2 + \frac{m\omega^2}{2}x^2. \tag{2.2}$$

Among the many ways to solve the Schrödinger equation of the harmonic oscillator, a particularly elegant, and fruitful, way deconstructs the Hamiltonian (2.2) into operators, the creation and annihilation operator, respectively

$$a^\dagger = \sqrt{\frac{m\omega}{2}} \left( x - i\frac{1}{m\omega}p \right) \quad \text{and} \quad a = \sqrt{\frac{m\omega}{2}} \left( x + i\frac{1}{m\omega}p \right). \tag{2.3}$$

- Show, using the ladder operators  $a$  and  $a^\dagger$ , that the canonical commutation relation  $[x, p] = i$  becomes

$$[a, a^\dagger] = 1 \tag{2.4}$$

and the Hamiltonian (2.2)

$$\mathcal{H} = \omega \left( a^\dagger a + \frac{1}{2} \right). \tag{2.5}$$

- Furthermore, show that, if  $\lambda$  is the eigenvalue corresponding to the normalized eigenstate  $|\lambda\rangle$  of the operator  $\Lambda = a^\dagger a$ , then

$$a|\lambda\rangle = c_\lambda|\lambda - 1\rangle \tag{2.6}$$

$$a^\dagger|\lambda\rangle = d_\lambda|\lambda + 1\rangle. \quad (2.7)$$

- Calculate the coefficients  $c_\lambda$  and  $d_\lambda$ .
- Prove that  $\lambda \geq 0$  and that  $\lambda = 0$  must be an eigenvalue. What is, hence, the spectrum of eigenvalues of  $\Lambda$  and  $H$ , respectively? Show that this implies for the ground state  $a|0\rangle = 0$ .
- Use the representation (2.3) of the ladder operators as differential operators to solve the Schrödinger equation for the ground state corresponding to  $\lambda = 0$ , i.e. determine the ground state wave function  $\langle x|0\rangle$ .
- Determine the wave function of the first excited state by applying the creation operator  $a^\dagger$  once to the ground state wave function.

The results obtained thus far suggest that the operator  $\Lambda$  can be interpreted as an operator counting the number of excitations of the harmonic oscillator. In order to make this even more suggestive let us change the notation and replace  $\Lambda$  by  $n$  and  $|\lambda\rangle$  by  $|n\rangle$ . Furthermore, as we shall see in more detail in this chapter, these results suggest an interpretation of the excitations of the harmonic oscillator as *particles* or *quasiparticles*. The state with no particles  $|0\rangle$  then corresponds to the vacuum state.

- Show with the help of (2.6) and (2.7) that the properly normalized state of  $n$  excitations or  $n$  particles is

$$|n\rangle = \frac{1}{\sqrt{n!}} \left(a^\dagger\right)^n |0\rangle. \quad (2.8)$$

- Finally, to appreciate how fruitful this algebraic treatment of the harmonic oscillator is, calculate the expectation values of the first few powers of the position operator in the state  $|n\rangle$ , let us say  $x$ ,  $x^2$ ,  $x^3$ , and  $x^4$ .
- Hint: Prove first that the number operator  $n = a^\dagger a$ , and hence the Hamiltonian  $\mathcal{H} = \omega \left(a^\dagger a + \frac{1}{2}\right)$ , are Hermitian operators and that therefore the corresponding eigenstates, which are non-degenerate (why?), are orthogonal.

With this exercise at the back of our minds, we can now start to develop the formalism of second quantization by first constructing a Hilbert space appropriate for a quantum many-particle system.

## 2.1 Many-particle Hilbert spaces

The formalism of ‘second quantization’<sup>2</sup> provides an elegant and economic way to describe a physical system containing a great, possibly indeterminate, number of

<sup>2</sup> The name is a trifle unfortunate and originates from the interpretation of the algebra of ladder operators (see exercise 2.1). These operators and their corresponding quantum excitations can be viewed as discrete ‘quantized’ units. It must be emphasized, however, that ‘second’ quantization is a representation of quantum mechanics particularly suitable for problems involving many particles. It is *not* a quantizing an already quantized theory. However, to be able to distinguish representations, we shall in places also have to use the equally unfortunate epithet ‘first’ quantization.

particles. It describes particles as quanta of a quantum field and is, hence, at the heart of the modern understanding of quantum mechanics and quantum field theory.

We assume that the solution of the quantum problem for one particle is known, i.e. we assume that

- there is a one-particle Hilbert space (quantum state space)  $\mathcal{H}_1$ , with, especially, the scalar product  $\langle \phi | \psi \rangle$  of states  $|\psi\rangle, |\phi\rangle \in \mathcal{H}_1$  from this Hilbert space;
- this means in particular, that the one-particle Schrödinger eigenvalue problem has been solved for the single particle Hamiltonian  $\mathcal{H}$ :

$$\mathcal{H}|\lambda\rangle = \epsilon_\lambda|\lambda\rangle, \quad (2.9)$$

where  $|\lambda\rangle \in \mathcal{H}_1$  is a normalized eigenstate and  $\epsilon_\lambda$  the corresponding eigenvalue;

- furthermore, the time evolution of the particle is determined by the unitary operator (ignoring the possibility of an explicitly time-dependent Hamiltonian)

$$U(t) = e^{-i\mathcal{H}t}, \quad (2.10)$$

- lastly, observables such as position  $\mathbf{r}$ , momentum  $\mathbf{p}$ , angular momentum  $\mathbf{L}$ , etc., of the single particle problem have been determined.

Second quantization is a formalism permitting to construct quantities that correspond to a system composed of an arbitrary, indeterminate number of such quantum particles under the assumption that the statements above for a single particle hold true.

The basis of the formalism consists in constructing Hilbert spaces and states for an arbitrary number of particles from the Hilbert space and states of a single particle.

### 2.1.1 Composite Hilbert space of two systems A and B

As mentioned in the introduction to this chapter, we begin with a more general point of view. Assume that there are two quantum systems  $A$  and  $B$  which may but need not be individual quantum particles. For instance, system  $A$  could denote a microscopic system, while system  $B$  could represent a macroscopic measurement apparatus. Their respective Hilbert spaces are  $\mathcal{H}^A$  and  $\mathcal{H}^B$ . We are interested in the composite quantum system  $AB$ .

We can construct a Hilbert space for the composite quantum system in two different ways. Both ways begin by forming a space of all ordered pairs of states taken from the Hilbert spaces  $\mathcal{H}^A$  and  $\mathcal{H}^B$

$$\mathcal{M} \equiv \mathcal{H}^A \times \mathcal{H}^B = \left\{ F | F = (f^A, f^B), f^A \in \mathcal{H}^A, f^B \in \mathcal{H}^B \right\} \quad (2.11)$$

which can be made into a composite Hilbert space by choosing a scalar product in two different ways.

### 2.1.1.1 *Tensor product Hilbert space*

The first construction is achieved through the introduction of a tensor product Hilbert space  $\mathcal{H}^{AB}$  of two Hilbert spaces  $\mathcal{H}^A$  and  $\mathcal{H}^B$ , whose dimensions  $\dim \mathcal{H}^A$  and  $\dim \mathcal{H}^B$  need not be the same,

$$\mathcal{H}^{AB} = \mathcal{H}^A \otimes \mathcal{H}^B \quad (2.12)$$

with dimension  $\dim \mathcal{H}^{AB} = (\dim \mathcal{H}^A)(\dim \mathcal{H}^B)$ . With respect to the composite Hilbert space  $\mathcal{H}^{AB}$ , the Hilbert spaces  $\mathcal{H}^A$  and  $\mathcal{H}^B$  are called factor spaces.

It should be emphasized that already the Hilbert space of a single particle can be a tensor product space as the example of the spin-orbit Hilbert space of a single particle shows where

$$\mathcal{H}_{\text{spin-orbit}} = \mathcal{H}_{\text{orbit}} \otimes \mathcal{C}^2 \quad (2.13)$$

is the tensor product of the orbital Hilbert space  $\mathcal{H}_{\text{orbit}}$  of the particle with its two-dimensional spin state space  $\mathcal{C}^2$ .

Now the construction of the tensor product Hilbert space  $\mathcal{H}^{AB}$  proceeds as follows. For each pair of states  $f^A \equiv |\psi^A\rangle \in \mathcal{H}^A$  and  $f^B \equiv |\varphi^B\rangle \in \mathcal{H}^B$  there is a (formal) product state  $F$  for which different notations are in use

$$F \equiv |\psi^{AB}\rangle \equiv |\psi^A\rangle \otimes |\varphi^B\rangle \equiv |\psi^A\rangle |\varphi^B\rangle \equiv |\psi^A, \varphi^B\rangle \equiv |\psi, \varphi\rangle. \quad (2.14)$$

These notations, going from left to right, emphasize less and less that the states belong to, in general, different Hilbert spaces. Hence, their use requires more and more caution and a clear understanding of their meaning in particular situations.

The composite states are linear in each of their factors separately, i.e.

$$|\psi^A\rangle \otimes (\lambda |\varphi_1^B\rangle + \mu |\varphi_2^B\rangle) = \lambda |\psi^A\rangle \otimes |\varphi_1^B\rangle + \mu |\psi^A\rangle \otimes |\varphi_2^B\rangle, \quad (2.15)$$

$$(\lambda |\psi_1^A\rangle + \mu |\psi_2^A\rangle) \otimes |\varphi^B\rangle = \lambda |\psi_1^A\rangle \otimes |\varphi^B\rangle + \mu |\psi_2^A\rangle \otimes |\varphi^B\rangle \quad (2.16)$$

with complex numbers  $\lambda$  and  $\mu$ .

The scalar product between composite states is formed in a space-wise manner by

$$\langle \psi^A | \langle \varphi^B | \cdot | \xi^A \rangle | \zeta^B \rangle = \langle \psi^A | \xi^A \rangle \langle \varphi^B | \zeta^B \rangle. \quad (2.17)$$

In order to obtain a composite Hilbert space  $\mathcal{H}^{AB}$  large enough to contain states that cannot be written as pure product states, i.e. states of the form

$$|\psi_1^A\rangle \otimes |\phi_1^B\rangle + |\psi_2^A\rangle \otimes |\phi_2^B\rangle \quad (2.18)$$

we need to consider the linear span (also called linear hull) of the space  $\mathcal{M}$ . This is achieved by taking bases of the factor Hilbert spaces  $\mathcal{H}^A$  and  $\mathcal{H}^B$ , e.g.  $\{|r^A\rangle\}$  and  $\{|m^B\rangle\}$ , to form a basis of the composite Hilbert space  $\mathcal{H}^{AB}$

$$\{|r^A\rangle \otimes |m^B\rangle\}, \quad (2.19)$$

a so-called (tensor) product basis, in the sense that all states of the form

$$|\psi^{AB}\rangle = \sum_{n,m} c_{n,m} |r^A\rangle \otimes |m^B\rangle \quad (2.20)$$

with complex numbers  $c_{n,m}$  as expansion coefficients, i.e. the linear span of  $\mathcal{M}$ , define the composite Hilbert space  $\mathcal{H}^{AB}$ .

Since an orthonormal basis in  $\mathcal{H}^{AB}$  satisfies, using (2.17),

$$\langle r^A, m^B | p^A, q^B \rangle = \langle r^A | p^A \rangle \langle m^B | q^B \rangle = \delta_{np} \delta_{mq}, \quad (2.21)$$

that is, the basis of the composite Hilbert space is orthonormal if the bases of the factor states are orthonormal, we obtain for the scalar product of two states of the form (2.20)

$$\langle \psi_1^{AB} | \psi_2^{AB} \rangle = \sum_{n,m} c_{nm}^{(1)*} c_{nm}^{(2)}, \quad (2.22)$$

which completes the construction of the composite Hilbert space  $\mathcal{H}^{AB}$ .

Using the notion of a product Hilbert space  $\mathcal{H}^{AB}$ , we are now in a position to introduce in a formal way an important notion at the heart of many investigations in quantum physics. It is the notion of *quantum entanglement*, which goes back to important publications by Einstein, Podolsky, and Rosen 1935, and especially by Schrödinger (1935). A composite state in  $\mathcal{H}^{AB}$  is called entangled if it cannot be represented as a product state but only as a superposition of product states, as in (2.20).

Examples of composite states that cannot be written as product states are the so-called *Bell states*

$$|\Phi_{\pm}^{AB}\rangle = \frac{1}{\sqrt{2}} \left( |0^A, 0^B\rangle \pm |1^A, 1^B\rangle \right) \quad (2.23)$$

$$|\Psi_{\pm}^{AB}\rangle = \frac{1}{\sqrt{2}} \left( |0^A, 1^B\rangle \pm |1^A, 0^B\rangle \right), \quad (2.24)$$

which are states in the composite Hilbert space

$$\mathcal{H}^{AB} = \mathcal{H}_2^A \otimes \mathcal{H}_2^B \quad (2.25)$$

where the factor states describe two-level systems or so-called qubits. These states are maximally entangled states. Details about maximally entangled states and entanglement measures in general can be found in Audretsch (2007).

### 2.1.1.2 Composite Hilbert space as a direct sum

However, a different way is also possible to construct a composite Hilbert space from the Hilbert spaces  $\mathcal{H}^A$  and  $\mathcal{H}^B$  of the two quantum systems  $A$  and  $B$ . The starting point is again the space  $\mathcal{M}$  of ordered pairs of states given in (2.11).

However, now we define the scalar product of two states  $F = (f^A, f^B) \equiv |\psi^{AB}\rangle \equiv (|\psi^A\rangle, |\psi^B\rangle)$  and  $G = (g^A, g^B) \equiv |\varphi^{AB}\rangle \equiv (|\varphi^A\rangle, |\varphi^B\rangle)$  from  $\mathcal{M}$  as

$$F \cdot G = f^A \cdot g^A + f^B \cdot g^B \equiv \langle \psi^{AB} | \varphi^{AB} \rangle \equiv \langle \psi^A | \varphi^A \rangle + \langle \psi^B | \varphi^B \rangle. \quad (2.26)$$

This definition of a scalar product for the space  $\mathcal{M}$  makes it into a composite Hilbert space  $\tilde{\mathcal{H}}^{AB}$  different from the tensor product Hilbert space  $\mathcal{H}^{AB}$  we constructed in the previous section. This composite Hilbert space is called a direct sum space and is denoted

$$\tilde{\mathcal{H}}^{AB} = \mathcal{H}^A \oplus \mathcal{H}^B. \quad (2.27)$$

In order to avoid possible confusion, we mention that multiplication by a complex number  $\lambda$  is to be understood component-wise

$$\lambda F = (\lambda f^A, \lambda f^B) = \lambda |\psi^{AB}\rangle = (\lambda |\psi^A\rangle, \lambda |\psi^B\rangle), \quad (2.28)$$

in contrast to the tensor product Hilbert space  $\mathcal{H}^{AB}$  where

$$\lambda |\psi^{AB}\rangle = (\lambda |\psi^A\rangle) |\psi^B\rangle = |\psi^A\rangle (\lambda |\psi^B\rangle) = \lambda |\psi^A\rangle |\psi^B\rangle. \quad (2.29)$$

We encounter this important kind of space later under the name of Fock space when we discuss situations involving particle production and destruction and, hence, need a Hilbert space with a variable number of particles.

There we shall also need the notion of orthogonality for states from different Hilbert spaces that can be conveniently defined using a direct sum of these spaces. We extend the vectors  $f^A \in \mathcal{H}^A$  and  $g^B \in \mathcal{H}^B$  to the space  $\mathcal{H} = \mathcal{H}^A \oplus \mathcal{H}^B$  by defining

$$F_0 \equiv (f^A, 0), \quad (2.30)$$

$$G_0 \equiv (0, g^B). \quad (2.31)$$

Calculating the scalar product (2.26) of these two special vectors of  $\mathcal{H}$ , we discover the important result

$$F_0 \cdot G_0 = f^A \cdot 0 + 0 \cdot g^B = 0, \quad (2.32)$$

namely, that states from different subspaces of a direct sum Hilbert space are orthogonal to each other.

### 2.1.2 Case of many distinguishable particles

The construction of a composite Hilbert space consisting of the Hilbert spaces of two subsystems, discussed in the previous section, can easily be generalized to the case of many subsystems. From now on we focus on the case of many subsystems where each subsystem is a single quantum particle. In constructing the many-particle Hilbert space, let us assume for the time being that the particles are *distinguishable*. Of course, in quantum physics, we encounter many situations where particles are indeed distinguishable, e.g. the electron and proton forming a hydrogen atom are distinguishable quantum particles.

The Hilbert space of a system composed of *exactly*  $N$  particles is given by the tensor product Hilbert space of  $N$  copies of the single-particle Hilbert space  $\mathcal{H}_1$  with dimension  $\dim \mathcal{H}_1$ :

$$\mathcal{H}_1^{\otimes N} \equiv \prod_{i=1}^N \otimes \mathcal{H}_1 \equiv \underbrace{\mathcal{H}_1 \otimes \mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_1}_N \quad (2.33)$$

The states of this Hilbert space are formed from linear combinations of product states of the form (cp. (2.14))

$$|\varphi_1, \varphi_2, \dots, \varphi_N\rangle = |\varphi_1\rangle |\varphi_2\rangle \dots |\varphi_N\rangle, \quad |\varphi_i\rangle \in \mathcal{H}_1. \quad (2.34)$$

Such a state vector represents a state of the system where the first particle is in state  $|\varphi_1\rangle$ , the second in the state  $|\varphi_2\rangle, \dots$ , and the  $N$ th in the state  $|\varphi_N\rangle$ . Crucially, we note that the states of different particles may coincide, i.e. that the possibility

$$|\varphi_i\rangle = |\varphi_j\rangle \quad (2.35)$$

for particles  $i \neq j$  must be taken into account.

The scalar product in  $\mathcal{H}_1^{\otimes N}$  is defined by generalizing (2.17)

$$\langle \varphi_1, \varphi_2, \dots, \varphi_N | \psi_1, \psi_2, \dots, \psi_N \rangle = \langle \varphi_1 | \psi_1 \rangle \langle \varphi_2 | \psi_2 \rangle \cdots \langle \varphi_N | \psi_N \rangle. \quad (2.36)$$

In order to be able to consider a state with zero particles, we formally introduce a one-dimensional Hilbert space  $\mathcal{V}$ , the *vacuum* space,

$$\mathcal{V} \equiv \mathcal{H}_1^{\otimes 0} \quad (2.37)$$

which contains only one normalized basis state, the zero particle or vacuum state  $|0\rangle$ , i.e.  $\langle 0|0\rangle = 1$ .

To each basis of  $\mathcal{H}_1$ , there corresponds a basis of  $\mathcal{H}_1^{\otimes N}$ . Explicitly this statement means that, if a set of orthonormal vectors  $|k\rangle$  ( $k = 1, \dots, \dim \mathcal{H}_1 \equiv M$ ) spans the one-particle Hilbert space  $\mathcal{H}_1$ , then the set of vectors

$$|k_1, k_2, \dots, k_M\rangle = |k_1\rangle|k_2\rangle \dots |k_M\rangle \quad (2.38)$$

forms an orthonormal basis of  $\mathcal{H}_1^{\otimes n}$ , i.e. with complex numbers  $c_k$ , we have for each single-particle state  $|\varphi\rangle$

$$|\varphi\rangle = \sum_{k=1}^M c_k |k\rangle. \quad (2.39)$$

The number of single-particle basis states  $|k\rangle$ , i.e.  $\dim \mathcal{H}_1 = M$ , depends on the concrete single-particle problem at hand and may be finite or infinite, or there can be a continuous dependence, e.g. for a free particle described by a plane wave of continuous momentum  $p$ . In the latter case, the sum in (2.39) will be replaced by an integral over the appropriate range of the continuous variable  $k$ .

If the number of particles of the system is indeterminate, the states of the system are obtained by superposition of states that correspond to each possible value of  $N$ . The state space is the direct sum of all state spaces  $\mathcal{H}_1^{\otimes N}$  for  $N = 0, 1, 2, \dots$ :

$$\mathcal{H} = \mathcal{H}_1^{\otimes 0} \oplus \mathcal{H}_1^{\otimes 1} \oplus \mathcal{H}_1^{\otimes 2} \oplus \dots \equiv \sum_{N=0}^{\infty} \mathcal{H}_1^{\otimes N}. \quad (2.40)$$

The state space  $\mathcal{H}$  is defined by its subspaces  $\mathcal{H}_1^{\otimes N}$ . More precisely, if  $|\varphi^{(N)}\rangle$  denotes an arbitrary state vector of  $\mathcal{H}_1^{\otimes N}$ , then a state in  $\mathcal{H}$  is defined as an infinite series of states with particle numbers  $N = 0, 1, 2, \dots$  which we can formally write as a sum (cp. section 2.1.1.2)

$$\left( |\varphi^{(0)}\rangle, |\varphi^{(1)}\rangle, \dots, |\varphi^{(N)}\rangle, \dots \right) \equiv |\varphi^{(0)}\rangle + |\varphi^{(1)}\rangle + \dots + |\varphi^{(N)}\rangle + \dots \quad (2.41)$$

and the scalar product of this state with another state  $|\psi^{(0)}\rangle + |\psi^{(1)}\rangle + \dots + |\psi^{(N)}\rangle + \dots$  of  $\mathcal{H}$  is given by

$$\sum_{N=0}^{\infty} \langle \varphi^{(N)} | \psi^{(N)} \rangle \quad (2.42)$$

where the scalar products  $\langle \varphi^{(N)} | \psi^{(N)} \rangle$  are calculated according to equation (2.36). The vacuum state for  $N = 0$  is here denoted by  $|\varphi^{(0)}\rangle = \alpha|0\rangle$ , for some complex number  $\alpha$ .

Using the notation of (2.38), the set of states of the form

$$|0\rangle, |k\rangle, |k_1, k_2\rangle, \dots, |k_1, k_2, \dots, k_N\rangle, \dots \quad (2.43)$$

is a complete orthonormal basis of  $\mathcal{H}$ , i.e.

$$\begin{aligned} \langle 0|0\rangle &= 1, \\ \langle k|k'\rangle &= \delta_{kk'}, \\ \langle k_1, k_2|k'_1, k'_2\rangle &= \delta_{k_1 k'_1} \delta_{k_2 k'_2}, \\ &\dots \end{aligned} \quad (2.44)$$

and

$$\begin{aligned} |0\rangle\langle 0| &= \mathbb{I}, \\ \sum_k |k\rangle\langle k| &= \mathbb{I}, \\ \sum_{k_1, k_2} |k_1, k_2\rangle\langle k_1, k_2| &= \mathbb{I}, \\ &\dots \end{aligned} \quad (2.45)$$

### 2.1.3 Case of many indistinguishable particles

At the microscopic level, quantum particles of the same kind, e.g. two electrons or two Helium atoms, are indistinguishable, except for possible inner degrees of freedom of the particles, e.g. spin.

For a system of  $N$  indistinguishable particles, also called identical particles, the Hamiltonian  $\mathcal{H}$  depends on the dynamical and internal degrees of freedom of all particles. However, indistinguishability implies that the Hamiltonian cannot change if the degrees of freedom of two arbitrary particles  $i$  and  $j$  are exchanged

$$\mathcal{H} = \mathcal{H}(1, 2, \dots, i, \dots, j, \dots, N) = \mathcal{H}(1, 2, \dots, j, \dots, i, \dots, N), \quad (2.46)$$

where the labels  $1, 2, \dots, i, \dots, j, \dots, N$  represent the degrees of freedom of the particles, e.g. their momenta, positions, and internal degrees of freedom, e.g. spin.

The corresponding many-particle state

$$|\varphi\rangle = |\varphi_1, \varphi_2, \dots, \varphi_N\rangle = |\varphi_1\rangle|\varphi_2\rangle \dots |\varphi_N\rangle \quad (2.47)$$

of this assembly of  $N$  indistinguishable quantum particles is, under exchange of two arbitrary particles, either totally symmetric or totally antisymmetric. This can be seen by acting with the operator exchanging two arbitrary particles,  $i$  and  $j$ , on a state of  $N$  identical particles

$$\mathcal{T}_{ij}|\varphi_1, \varphi_2, \dots, \varphi_i, \dots, \varphi_j, \dots, \varphi_N\rangle = |\varphi_1, \varphi_2, \dots, \varphi_j, \dots, \varphi_i, \dots, \varphi_N\rangle \quad (2.48)$$

$$= \eta_{ij}|\varphi_1, \varphi_2, \dots, \varphi_i, \dots, \varphi_j, \dots, \varphi_N\rangle, \quad (2.49)$$

which produces a state that may not be physically different from the original state, so that there can only be a phase factor

$$\eta_{ij} = e^{i\alpha_{ij}}. \quad (2.50)$$

Moreover, because of

$$\mathcal{T}_{ji} = \mathcal{T}_{ij} \quad (2.51)$$

we have

$$\mathcal{T}_{ij}^2 = 1 \quad (2.52)$$

and, hence

$$\eta_{ij} = \pm 1. \quad (2.53)$$

Lastly, the phase factor must be the same for all pairs  $(i, j)$  of particles because the exchange operators, and thus the phases, satisfy

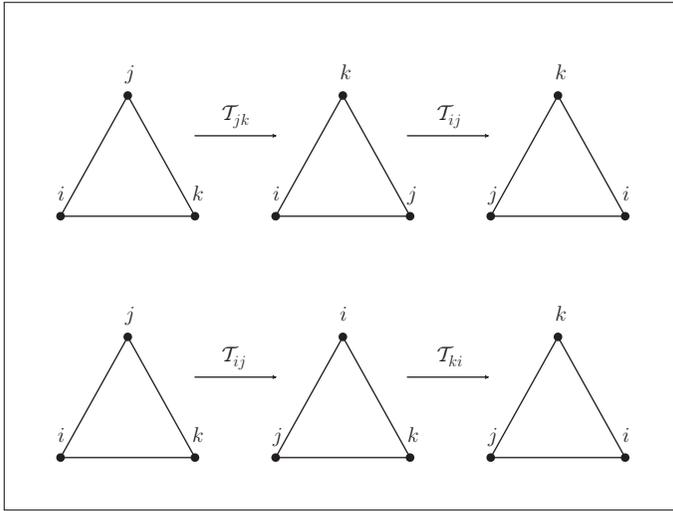
$$\mathcal{T}_{ij}\mathcal{T}_{jk} = \mathcal{T}_{ki}\mathcal{T}_{ij} \quad \text{and} \quad \eta_{ij}\eta_{jk} = \eta_{ki}\eta_{ij}, \quad (2.54)$$

hence

$$\eta_{jk} = \eta_{ki} = \eta = \pm 1 \quad (2.55)$$

the phase factors are the same for all pairs of particles because the choice of particles  $i$ ,  $j$ , and  $k$  has been arbitrary.

The validity of (2.54) is easiest seen graphically (Figure 2.1).



**Figure 2.1** Action of two pairs of particle exchange operators leading to the same final state.

These results imply that there are only two types of quantum particles:

- $\eta = +1$  particles whose states are symmetrical under particle exchange,
- $\eta = -1$  particles whose states are antisymmetrical under particle exchange.

### 2.1.3.1 Pauli exclusion principle

As an immediate consequence of the restriction of the eigenvalues of the transposition operator to only two allowed values  $\eta = \pm 1$ , (2.55), we obtain an important result that is connected to Wolfgang Pauli's name: the exclusion principle in its form for many-particle systems.

While the case  $\eta = +1$  imposes no restriction on the many-particle state

$$|\varphi\rangle = |\varphi_1, \varphi_2, \dots, \varphi_i, \dots, \varphi_j, \dots, \varphi_N\rangle = |\varphi_1\rangle|\varphi_2\rangle \dots |\varphi_i\rangle \dots |\varphi_j\rangle \dots |\varphi_N\rangle \quad (2.56)$$

if two single-particle states in it are equal, e.g.  $|\varphi_i\rangle = |\varphi_j\rangle$ , the case  $\eta = -1$  implies that the many-particle state  $|\varphi\rangle$  vanishes if two single-particle states in it are equal.

Many-particle states with  $\eta = +1$  under exchange of single-particle states describe systems of Bose particles, or Bosons. Many-particle states with  $\eta = -1$  under exchange of single-particle states describe systems of Fermi particles, or Fermions. These two possibilities are the only two possibilities for quantum particles under ordinary circumstances (with an exception). The two kinds of particles show clearly distinct properties.

Thus we can state the famous Pauli exclusion principle:

- The probability for a many-particle state to contain two or more Fermions in the same single-particle state vanishes.

- In other words, it is impossible that two Fermions in a many-Fermion state coincide in all quantum variables, e.g. in position and spin quantum number.
- There can be at most one Fermion in each single-particle state of a many-Fermion state.

Such a many-particle state is, however, quite possible for Bosons, as we have seen. A many-particle Bosonic state can contain an arbitrary number of Bosons, described by equal single-particle states.

A few further remarks are in order at this stage.

- In another important contribution, Wolfgang Pauli (1940) proved by his famous spin-statistics theorem that Bosons carry integer spin,  $s = 0, 1, 2, \dots$ , while Fermions carry half-integer spin,  $s = 1/2, 3/2, \dots$ .
- The following sections discuss the drastic consequences of this distinction. Furthermore, the two types of particle exhibit very different statistical behaviour as we discuss in chapter 4. This fact is also the reason for the name of the famous theorem Pauli proved.
- Note that the spin-statistics theorem depends on the spatial dimension. It presupposes three (or more) space dimensions. In lower dimensions, the behaviour of particles under exchange may offer much richer possibilities. This has been demonstrated by Leinaas and Myrheim (1977) and has been a major research area of theoretical physics of low-dimensional systems ever since. The postulated particles of fractional statistics, called anyons, play a major role in the physics of the quantum Hall effect. For recent reviews of anyons in relation to the quantum Hall effect, see Stern (2008) and Stern (2010).

.....  
**EXERCISE 2.2 Consequence of the indistinguishability of particles** For this exercise we first need to show that any permutation  $\mathcal{P}$  of the permutation group  $S_N$  is a unitary operator, i.e.

$$\mathcal{P}^\dagger = \mathcal{P}^{-1}. \tag{2.57}$$

Reminder: Permutations are defined as arrangements of the numbers  $(1, 2, \dots, N)$  in a particular sequence and written as  $\mathcal{P} = (p_1, p_2, \dots, p_N)$ . The number of arrangements of  $N$  numbers  $(1, 2, \dots, N)$  is  $a(N) = N!$ . The permutations of  $N$  numbers form a group  $S_N$  with  $\mathcal{I} = (1, 2, \dots, N)$  as identity element. A pair of numbers  $p_i$  and  $p_j$  in the permutation  $\mathcal{P}$  for which  $p_i > p_j$  form an inversion. A permutation with an even number of inversions is called even, a permutation with an odd number of inversions is called odd. Each permutation is thus characterized by

$$\chi(\mathcal{P}) = e^{\mathcal{J}(\mathcal{P})} = \pm 1 \tag{2.58}$$

where  $\mathcal{J}(\mathcal{P})$  is the number of inversions and  $\chi(\mathcal{P}) = +1$  for an even,  $\chi(\mathcal{P}) = -1$  for an odd permutation.

The indistinguishability of quantum particles means that there can be *no* observable  $\mathcal{O}$  of the many-particle system that can be used to distinguish the particles.

Express this requirement as a relation between the observable  $\mathcal{O}$  and an arbitrary permutation  $\mathcal{P} \in S_N$ . You may want to start from the expressions for the expectation values of the observable  $\mathcal{O}$  in an arbitrary many-particle state  $|\psi\rangle$  and the permuted state  $\mathcal{P}|\psi\rangle$ .

.....

## 2.2 Occupation number representation: Bosons and Fermions

The states in  $\mathcal{H}_1^{\otimes N}$  and  $\mathcal{H} = \sum_N \mathcal{H}_1^{\otimes N}$  behave in complicated ways under the exchange of pairs of particles. To describe this behaviour would require the full representation theory of the permutation group  $S_N$ . However, as we have seen, for indistinguishable particles, we only need to consider many-particle states that are symmetric or antisymmetric under particle exchange, which corresponds to two simple one-dimensional representations of the permutation group. Only those states which remain either completely unchanged or only change by an overall sign, corresponding to  $\eta = \pm 1$ , are physically relevant.

In order to project out the physically relevant basis states, we introduce symmetrization  $\mathcal{S}$  and antisymmetrization  $\mathcal{A}$  operators for a fixed number  $N$  of particles. The symmetrization operator  $\mathcal{S}$  produces states which automatically satisfy  $\eta = 1$  by permuting the basis states to form a *permanent*

$$\mathcal{S}|k_1, k_2, \dots, k_N\rangle = \frac{1}{\sqrt{N!N_1! \dots N_M!}} \sum_{\mathcal{P}} |k_{i_1}, k_{i_2}, \dots, k_{i_N}\rangle \quad (2.59)$$

where the sum is taken over the  $N!$  permutations of the basis states  $|k_{i_1}\rangle, \dots, |k_{i_N}\rangle$ . The factor  $1/\sqrt{N!}$  normalizes the sum consisting of  $N!$  terms.

As discussed, not all single-particle basis states in the many-particle basis state must be different (cf. the discussion with respect to 2.35). In order not to overcount basis states for which this happens, we introduce the factors  $N_l!$  for  $l = 1, \dots, M$  with  $M \leq N$ , the numbers  $N_l$  counting the basis states in  $|k_1, k_2, \dots, k_N\rangle$  which are equal.  $M = N$  corresponds to all basis states being different, i.e. all  $N_l = 1$ . The numbers  $N_l$ , which here appear for normalization purposes, will obtain a physical interpretation as occupation numbers of the corresponding states and, thus, play an important role in the following developments.

Similarly, we introduce an antisymmetrization operator  $\mathcal{A}$

$$\mathcal{A}|k_1, k_2, \dots, k_N\rangle = \frac{1}{\sqrt{N!}} \sum_{\mathcal{P}} (-1)^{\mathcal{P}} |k_{i_1}, k_{i_2}, \dots, k_{i_N}\rangle, \quad (2.60)$$

where the sum is over all  $N!$  permutations  $\mathcal{P}$  of  $1, 2, \dots, N$ . As opposed to the symmetrized state, (2.59), we can disregard multiple single-particle states because their contribution to (2.60) vanishes by construction as is required from an antisymmetrical many-particle state.

The real space wave function  $\langle \mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N | \mathcal{A} | k_1, k_2, \dots, k_N \rangle$  then becomes a determinant, called the Slater determinant,

$$\langle \mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N | \mathcal{A} | k_1, k_2, \dots, k_N \rangle = \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_1(\mathbf{r}_1) & \varphi_2(\mathbf{r}_1) & \cdots & \varphi_N(\mathbf{r}_1) \\ \varphi_1(\mathbf{r}_2) & \varphi_2(\mathbf{r}_2) & \cdots & \varphi_N(\mathbf{r}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \varphi_1(\mathbf{r}_N) & \varphi_2(\mathbf{r}_N) & \cdots & \varphi_N(\mathbf{r}_N) \end{vmatrix} \quad (2.61)$$

where  $\varphi_i(\mathbf{r}_j) = \langle \mathbf{r}_j | k_i \rangle$ .

## 2.2.1 Fock spaces for Bosons and Fermions

We now come back to our goal to deal with systems where the number of particles is indeterminate, potentially even infinite. In order to achieve this, we recall that the notion of a composite Hilbert space as a direct sum introduced in section 2.1.1.2 allowed us to construct a composite Hilbert space  $\mathcal{H}$  for an indeterminate number of particles as a direct sum of composite tensor product Hilbert spaces  $\mathcal{H}_1^{\otimes N}$  each for a fixed number  $N = 0, 1, 2, \dots$  of particles (cf. 2.40)

$$\mathcal{H} = \mathcal{H}_1^{\otimes 0} \oplus \mathcal{H}_1^{\otimes 1} \oplus \mathcal{H}_1^{\otimes 2} \oplus \dots \equiv \sum_{N=0}^{\infty} \mathcal{H}_1^{\otimes N}. \quad (2.62)$$

This Hilbert space can be symmetrized or antisymmetrized by performing the corresponding operation on all many-particle basis states for a fixed number  $N$  of particles, as described in section 2.1.2. The Hilbert spaces  $\mathcal{S}\mathcal{H}$  and  $\mathcal{A}\mathcal{H}$  constructed in this way are subspaces of  $\mathcal{H}$ , called Fock spaces, describing Bosonic and Fermionic many-particle spaces where the numbers of Bosons and Fermions are indeterminate.

The many-particle states (2.59) and (2.60) for  $N = 0, 1, 2, \dots$  form bases of the respective Fock spaces, which can be characterized by the sequence of occupation numbers  $N_l$  and written as

$$|\phi\rangle = (\mathcal{S}/\mathcal{A}) | k_1, k_2, \dots, k_N \rangle \equiv | N_1, N_2, \dots \rangle = | \{N\} \rangle \quad (2.63)$$

with  $N_l = 0, 1, 2, \dots$  for Bosons ( $\mathcal{S}$ ), and  $N_l = 0, 1$  for Fermions ( $\mathcal{A}$ ). The occupation numbers  $N_l$  completely characterize the state  $|\phi\rangle$ . Viewed as a state in the Fock space, the state  $|\phi\rangle$  has an infinite number of occupation number levels labelled by  $l = 1, 2, \dots, \infty$ . Nevertheless, each state  $|\phi\rangle$  contains a fixed number of particles

$$N = \sum_{l=1}^{\infty} N_l. \quad (2.64)$$

However, an important new feature the construction of the Fock spaces generates is that the total number of particles in these spaces is not fixed any more as it was in each tensor product many-particle Hilbert space. It is now rather a dynamic variable whose corresponding operator we obtain in the following section.

The states  $|\phi\rangle$  form a complete orthonormal set of many-particle states

$$\langle N_1, N_2, \dots | N'_1, N'_2, \dots \rangle = \delta_{N_1 N'_1} \delta_{N_2 N'_2} \dots \quad (2.65)$$

and

$$\sum_{N_1, N_2, \dots} |N_1, N_2, \dots\rangle \langle N'_1, N'_2, \dots| = \mathbb{I}. \quad (2.66)$$

---

**EXERCISE 2.3 Properties of symmetrization and antisymmetrization operators** Show that the symmetrization and antisymmetrization operators have the following properties:

- $S$  and  $\mathcal{A}$  are Hermitian operators.
  - $S$  and  $\mathcal{A}$  are idempotent, i.e.  $S^2 = S$  and  $\mathcal{A}^2 = \mathcal{A}$ .
  - $S$  and  $\mathcal{A}$  are orthogonal, i.e.  $S\mathcal{A} = \mathcal{A}S = 0$ .
- 

In the following, we treat the cases of Bosons and Fermions separately, beginning in the next section with the Bose case.

## 2.3 Creation and annihilation operators for Bosons

This section concentrates on the Bosonic case while Fermions are discussed in section 2.9.

On the Fock space  $\mathcal{S}\mathcal{H}$ , we define an operator  $a_i^\dagger$  acting on occupation level  $i$  of the state  $|\phi\rangle$  as

$$a_i^\dagger |\phi\rangle = \sqrt{N_i + 1} |\phi'\rangle = \sqrt{N_i + 1} |N_1, \dots, N_i + 1, \dots\rangle. \quad (2.67)$$

This operator, called a creation operator, creates a particle in the occupation level  $i$  of the many-particle state  $|\phi\rangle$ . It is important to note that, while  $|\phi\rangle$  is a many-particle state with  $N$  particles, the state  $|\phi'\rangle$  is a many-particle state with  $N + 1$  particles. However, both states are states in the direct sum Hilbert or Fock space  $\mathcal{S}\mathcal{H}$ . The Fock space  $\mathcal{S}\mathcal{H}$

has been constructed expressly for the purpose of accommodating the action of creation operators  $a_i^\dagger$  for  $i = 1, 2, \dots$

Similarly, we define an operator  $a_i$

$$a_i|\phi\rangle = \sqrt{N_i}|\phi''\rangle = \sqrt{N_i}|N_1, \dots, N_i - 1, \dots, N_l\rangle \quad (2.68)$$

which annihilates a particle in the occupation level  $i$  of the many-particle state  $|\phi\rangle$ , and hence is called an annihilation operator. From these definitions it is easy to demonstrate that  $a_i^\dagger$  and  $a_i$  are, as the notation suggests, mutually adjoint operators. Hence, the two definitions are not independent of each other and one would have sufficed since it implies the other.

The creation and annihilation operators  $a_i^\dagger$  and  $a_i$  permit a convenient representation of the many-particle state  $|\phi\rangle$ . By repeated application of the annihilation operator  $a_i$  for  $i = 1, 2, \dots$  all particles in a given state  $|\phi\rangle$  can be eliminated one by one and we arrive at an empty, no-particle, or vacuum, state

$$|vac\rangle = |0, 0, 0, 0, \dots\rangle \in \mathcal{S}\mathcal{H}. \quad (2.69)$$

This state has formally to be distinguished from the empty state  $|0\rangle \in \mathcal{H}^{\otimes 0}$ . One more application of an arbitrary annihilation operator  $a_i$

$$a_i|vac\rangle = a_i|0, 0, 0, 0, \dots\rangle = 0 \quad (2.70)$$

annihilates the vacuum state altogether.

On the other hand, applying creation operators  $a_i^\dagger$  for  $i = 1, 2, \dots$  on the vacuum state  $|vac\rangle$  we can built up any many-particle state  $|\phi\rangle$  one particle at a time. For example, a many-particle basis state with just one particle has the form

$$|1_\alpha\rangle = a_\alpha^\dagger|vac\rangle = |0, 0, \dots, 0, N_\alpha = 1, 0, \dots\rangle. \quad (2.71)$$

We shall call such a many-particle state a one-particle state to contrast it with the single-particle states  $|k\rangle$ . Later, we will also need two-particle states

$$|1_\alpha 1_\beta\rangle = a_\alpha^\dagger a_\beta^\dagger|vac\rangle = |0, 0, \dots, 0, N_\alpha = 1, 0, \dots, 0, N_\beta = 1, 0, \dots\rangle, \quad (2.72)$$

$$|2_\alpha\rangle = \frac{1}{\sqrt{2!}} \left(a_\alpha^\dagger\right)^2 |vac\rangle = |0, 0, \dots, 0, N_\alpha = 2, 0, \dots\rangle. \quad (2.73)$$

As shown in previous sections, Bosonic, as well as Fermionic, many-particle states are characterized by their behaviour under the exchange of pairs of particles. Building up a general many-particle basis state by repeated application of creation operators will have to be consistent with this symmetry under pairwise exchange of particles. This is guaranteed for Bosons by the commutation relations

$$[a_i, a_j] = [a_i^\dagger, a_j^\dagger] = 0, \quad [a_i, a_j^\dagger] = \delta_{ij} \quad (2.74)$$

which can be verified by evaluating the action of the commutators on an arbitrary many-particle state  $|\phi\rangle$ .

The general many-particle basis state in the Fock space  $\mathcal{S}\mathcal{H}$  can now be written with the help of the creation operators  $a_i^\dagger$  for  $i = 1, 2, \dots$

$$|\phi\rangle = |N_1, N_2, \dots, N_\alpha, \dots\rangle \quad (2.75)$$

$$= \frac{1}{\sqrt{N_1! N_2! \dots N_\alpha! \dots}} \left(a_1^\dagger\right)^{N_1} \left(a_2^\dagger\right)^{N_2} \dots \left(a_\alpha^\dagger\right)^{N_\alpha} \dots |vac\rangle \quad (2.76)$$

or, due to the commutation relations, in any other permuted order of the creation operators acting on the vacuum state.

From the definitions (2.67) and (2.68) we also obtain

$$a_i^\dagger a_i |\phi\rangle = N_i |\phi\rangle \quad (2.77)$$

and

$$a_i a_i^\dagger |\phi\rangle = (N_i + 1) |\phi\rangle. \quad (2.78)$$

This justifies the interpretation of the operator

$$n_i = a_i^\dagger a_i \quad (2.79)$$

as the operator that counts the number of particles in the occupation level  $i$  of the many-particle state  $|\phi\rangle$ , the particle number operator. The total particle number operator is thus

$$\mathcal{N} = \sum_{i=1}^{\infty} n_i = \sum_{i=1}^{\infty} a_i^\dagger a_i. \quad (2.80)$$

---

**EXERCISE 2.4 Bogoliubov transformation for Bosons** A canonical transformation of the form

$$b = ua + va^\dagger, \quad (2.81)$$

$$b^\dagger = ua^\dagger + va, \quad (2.82)$$

where  $u$  and  $v$  are real, is called a Bogoliubov transformation (after the mathematician and theoretical physicist Nikolai Bogoliubov).

Derive the condition under which the Bose commutation relations are preserved.

---

The following exercises furnish us with useful formulas for calculations involving Bosonic creation and annihilation operators.

However, let us start with a useful property of operator-valued functions, which are defined by a power series

$$f(\mathcal{O}) = \sum_{n=0}^{\infty} a(n)\mathcal{O}^n \tag{2.83}$$

with complex numbers  $a(n)$ .

.....  
**EXERCISE 2.5 Operator relation** Show that for operators  $\mathcal{O}$  and  $\mathcal{P}$  and an operator-valued function  $f(\mathcal{O})$ , defined by the power series (2.83), the equation

$$\mathcal{P}^{-1}f(\mathcal{O})\mathcal{P} = f(\mathcal{P}^{-1}\mathcal{O}\mathcal{P}) \tag{2.84}$$

holds.

This equation is particularly useful for the exponential function

$$f(\mathcal{O}) = e^{\mathcal{O}}, \tag{2.85}$$

for which it becomes

$$\mathcal{P}^{-1}e^{\mathcal{O}}\mathcal{P} = e^{(\mathcal{P}^{-1}\mathcal{O}\mathcal{P})}. \tag{2.86}$$

.....  
 The result of this exercise will prove useful for exercise 2.7.

Here are the first set of exercises that expound important relations for Bosonic creation and annihilation operators.

.....  
**EXERCISE 2.6 Functions of Bosonic creation and annihilation operators** A function  $f(b, b^\dagger)$  of the Bosonic operators  $b$  and  $b^\dagger$  is defined by its power series with respect to the two arguments, i.e.

$$f(b, b^\dagger) = \sum_{n,m=0}^{\infty} a(n, m)b^n(b^\dagger)^m \tag{2.87}$$

with complex numbers  $a(n, m)$ .

- Show that the following generalized commutator relations

$$bf(b, b^\dagger) - f(b, b^\dagger)b = \frac{\partial f(b, b^\dagger)}{\partial b^\dagger}, \tag{2.88}$$

$$b^\dagger f(b, b^\dagger) - f(b, b^\dagger) b^\dagger = -\frac{\partial f(b, b^\dagger)}{\partial b}. \quad (2.89)$$

are satisfied.

- Starting from the elementary commutation relation

$$bb^\dagger - b^\dagger b = 1 \quad (2.90)$$

prove first, by complete induction, the special case of, e.g., (2.88)

$$b(b^\dagger)^n - (b^\dagger)^n b = n(b^\dagger)^{n-1}. \quad (2.91)$$

- Show that the relations (2.88) and (2.89) imply

$$e^{-\alpha b^\dagger} b e^{\alpha b^\dagger} = b + \alpha, \quad (2.92)$$

$$e^{-\alpha b} b^\dagger e^{\alpha b} = b^\dagger - \alpha \quad (2.93)$$

for any complex number  $\alpha$ .

More generally, you may want to show that

$$U^\dagger b U = b + \alpha \quad (2.94)$$

$$U^\dagger b^\dagger U = b^\dagger + \alpha^* \quad (2.95)$$

with the unitary operator

$$U = e^{\alpha b^\dagger - \alpha^* b} = e^{-|\alpha|/2} e^{\alpha b^\dagger} e^{-\alpha^* b}. \quad (2.96)$$

**EXERCISE 2.7 Factorization of the exponential function** For this exercise the result of exercise 2.5 will prove useful.

Show that the exponential function of a sum of a creation and an annihilation operator can be factorized

$$e^{\alpha b^\dagger + \beta b} = e^{\alpha b^\dagger} e^{\beta b} e^{\frac{\alpha\beta}{2}} = e^{\beta b} e^{\alpha b^\dagger} e^{-\frac{\alpha\beta}{2}}. \quad (2.97)$$

**EXERCISE 2.8 Commutation with an exponential of  $b^\dagger b$**  Derive the formulas

$$e^{\alpha b^\dagger b} b e^{-\alpha b^\dagger b} = e^{-\alpha} b \quad (2.98)$$

$$e^{\alpha b^\dagger b} b^\dagger e^{-\alpha b^\dagger b} = e^{\alpha} b^\dagger \quad (2.99)$$

which can also be written in the form of commutation relations

$$b e^{-\alpha b^\dagger b} = e^{-\alpha} e^{-\alpha b^\dagger b} b \quad (2.100)$$

$$b^\dagger e^{-\alpha b^\dagger b} = e^{\alpha} e^{-\alpha b^\dagger b} b^\dagger. \quad (2.101)$$

.....

## 2.4 Basis transformation

The states  $|1_\alpha\rangle$  we constructed in (2.71), special cases of the many-particle states  $|\phi\rangle = |N_1, N_2, \dots\rangle$ , are one-particle states in the many-particle Fock space. These states are in themselves orthonormal and complete

$$\langle 1_\alpha | 1_\beta \rangle = \delta_{\alpha\beta}, \quad (2.102)$$

$$\sum_{\alpha} |1_\alpha\rangle\langle 1_\alpha| = \mathbb{I}, \quad (2.103)$$

and hence, they form a many-particle basis  $\{|1_\alpha\rangle\}$ . They are useful for a number of purposes where the fully general many-particle state  $|\phi\rangle$  would obscure the argument.

The creation and annihilation operators have been defined using the general many-particle state  $|\phi\rangle$ , but an equivalent definition makes use of only the one-particle states

$$a_\alpha^\dagger |0\rangle = |1_\alpha\rangle, \quad (2.104)$$

$$a_\alpha |1_\beta\rangle = \delta_{\alpha\beta} |0\rangle. \quad (2.105)$$

We now want to see how they transform under a basis transformation  $\{|1_\alpha\rangle\} \rightarrow \{|1_i\rangle\}$ .

Different basis states  $\{|1_\alpha\rangle\}$  and  $\{|1_i\rangle\}$  are mutually related via the completeness relations

$$|1_\alpha\rangle = \sum_i |1_i\rangle\langle 1_i | 1_\alpha\rangle, \quad (2.106)$$

$$|1_i\rangle = \sum_{\alpha} |1_\alpha\rangle\langle 1_\alpha | 1_i\rangle. \quad (2.107)$$

The creation and annihilation operators which use the specific one-particle basis states  $\{|1_\alpha\rangle\}$ , are transformed by the unitary transformations

$$a_i^\dagger = \sum_{\alpha} \langle 1_\alpha | 1_i\rangle a_\alpha^\dagger, \quad (2.108)$$

$$a_i = \sum_{\alpha} \langle 1_i | 1_\alpha\rangle a_\alpha, \quad (2.109)$$

such that in the new basis the corresponding relations

$$|1_i\rangle = a_i^\dagger |0\rangle, \quad (2.110)$$

$$|0\rangle = a_i |1_i\rangle \quad (2.111)$$

hold as expected.

The inverse transformations are

$$a_\alpha^\dagger = \sum_i \langle 1_i | 1_\alpha \rangle a_i^\dagger, \quad (2.112)$$

$$a_\alpha = \sum_i \langle 1_\alpha | 1_i \rangle a_i. \quad (2.113)$$

These relations for the creation and annihilation operators, together with the completeness relations in the different bases, are mutually consistent.

In the next section we exploit a particularly important case of basis transformation, which involves one-particle and two-particle basis states of well-defined position  $\mathbf{r}$

$$\{|1_\alpha\rangle\} = \{|\mathbf{r}\rangle\}, \quad (2.114)$$

where orthonormality and completeness take the form

$$\langle \mathbf{r} | \mathbf{r}' \rangle = \delta(\mathbf{r} - \mathbf{r}'), \quad (2.115)$$

$$\int d^3 r |\mathbf{r}\rangle \langle \mathbf{r}| = \mathbb{I} \quad (2.116)$$

The resulting operators are called quantum field creation and annihilation operators.

## 2.5 Quantum field operators

So far, the states have been states of an abstract Hilbert space, and, consequently, the creation and annihilation operators have been acting in abstract Hilbert spaces.

We now use for the following developments of investigating quantum field operators, as prepared in Section 2.4, the transformation to the particular position basis  $\{|\mathbf{r}\rangle\}$ , i.e. we deal with the creation and annihilation of particles at definite points  $\mathbf{r}$  in physical space. This can be achieved by introducing *quantum field operators* for creating and annihilating particles at position  $\mathbf{r}$  using the following transformations, which are special cases of the general transformations discussed earlier

$$a_\alpha^\dagger \rightarrow \psi^\dagger(\mathbf{r}) = \sum_\alpha \langle 1_\alpha | \mathbf{r} \rangle a_\alpha^\dagger = \sum_\alpha u_\alpha^*(\mathbf{r}) a_\alpha^\dagger, \quad (2.117)$$

and

$$a_\alpha \rightarrow \psi(\mathbf{r}) = \sum_\alpha \langle \mathbf{r} | 1_\alpha \rangle a_\alpha = \sum_\alpha u_\alpha(\mathbf{r}) a_\alpha, \quad (2.118)$$

where  $u_\alpha(\mathbf{r})$  is the wave function of the one-particle state  $|1_\alpha\rangle$ . The quantum field operators create and annihilate, respectively, a particle at position  $\mathbf{r}$

$$\psi^\dagger(\mathbf{r})|0\rangle = |\mathbf{r}\rangle, \quad (2.119)$$

$$\psi(\mathbf{r})|\mathbf{r}'\rangle = \delta(\mathbf{r} - \mathbf{r}')|0\rangle. \quad (2.120)$$

The inverse transformations are

$$a_\alpha^\dagger = \int d^3r \langle \mathbf{r} | 1_\alpha \rangle \psi^\dagger(\mathbf{r}) = \int d^3r u_\alpha(\mathbf{r}) \psi^\dagger(\mathbf{r}) \quad (2.121)$$

and

$$a_\alpha = \int d^3r \langle 1_\alpha | \mathbf{r} \rangle \psi(\mathbf{r}) = \int d^3r u_\alpha^*(\mathbf{r}) \psi(\mathbf{r}). \quad (2.122)$$

The number of particles at point  $\mathbf{r}$  in a small volume  $d^3r$  is

$$\psi^\dagger(\mathbf{r})\psi(\mathbf{r})d^3r = \rho(\mathbf{r})d^3r, \quad (2.123)$$

and, hence, the total number of particles

$$\mathcal{N} = \int d^3r \rho(\mathbf{r}) = \int d^3r \psi^\dagger(\mathbf{r})\psi(\mathbf{r}). \quad (2.124)$$

The commutators become

$$[\psi^\dagger(\mathbf{r}), \psi^\dagger(\mathbf{r}')] = 0, \quad (2.125)$$

$$[\psi(\mathbf{r}), \psi(\mathbf{r}')] = 0, \quad (2.126)$$

$$[\psi(\mathbf{r}), \psi^\dagger(\mathbf{r}')] = \delta(\mathbf{r} - \mathbf{r}'). \quad (2.127)$$

We close this section with an elementary example.

**Examples 1** *Free particle in a box* A simple but important example is provided by choosing the abstract one-particle basis  $\{|i\rangle\}$  in (2.108) and (2.109) to be the basis of momentum eigenstates  $\{|\mathbf{k}\rangle\}$  with

$$\mathbf{p}_i|\mathbf{k}\rangle = \mathbf{k}|\mathbf{k}\rangle, \quad (2.128)$$

$$\sum_{\mathbf{k}} |\mathbf{k}\rangle\langle\mathbf{k}| = \mathbb{I}, \quad (2.129)$$

$$\langle\mathbf{k}|\mathbf{k}'\rangle = \delta_{\mathbf{k}\mathbf{k}'}. \quad (2.130)$$

We obtain

$$a_{\mathbf{k}}^\dagger = \sum_{\alpha} \langle 1_{\alpha} | \mathbf{k} \rangle a_{\alpha}^\dagger = \sum_{\alpha} \int d^3 r \langle 1_{\alpha} | \mathbf{r} \rangle \langle \mathbf{r} | \mathbf{k} \rangle a_{\alpha}^\dagger = \int d^3 r \langle \mathbf{r} | \mathbf{k} \rangle \psi^\dagger(\mathbf{r}), \quad (2.131)$$

$$a_{\mathbf{k}} = \sum_{\alpha} \langle \mathbf{k} | 1_{\alpha} \rangle a_{\alpha} = \sum_{\alpha} \int d^3 r \langle \mathbf{k} | \mathbf{r} \rangle \langle \mathbf{r} | 1_{\alpha} \rangle a_{\alpha} = \int d^3 r \langle \mathbf{k} | \mathbf{r} \rangle \psi(\mathbf{r}), \quad (2.132)$$

where we have used (2.117) and (2.118). The functions

$$\langle \mathbf{r} | \mathbf{k} \rangle = (\langle \mathbf{k} | \mathbf{r} \rangle)^* = u_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} \quad (2.133)$$

where the wave vector  $\mathbf{k}$  is given by

$$\mathbf{k} = \frac{2\pi}{L} \begin{pmatrix} n_1 \\ n_2 \\ n_3 \end{pmatrix}, \quad n_i \in \mathbb{N}. \quad (2.134)$$

describe a free particle confined to a cubic volume  $V = L^3$  and subject to periodic boundary conditions. The final result for creation and annihilation operators is then given by

$$a_{\mathbf{k}}^\dagger = \int d^3 r e^{i\mathbf{k}\cdot\mathbf{r}} \psi^\dagger(\mathbf{r}), \quad (2.135)$$

and

$$a_{\mathbf{k}} = \int d^3 r e^{-i\mathbf{k}\cdot\mathbf{r}} \psi(\mathbf{r}), \quad (2.136)$$

respectively, with the inverse relations

$$\psi^\dagger(\mathbf{r}) = \frac{1}{V} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}} a_{\mathbf{k}}^\dagger, \quad (2.137)$$

$$\psi(\mathbf{r}) = \frac{1}{V} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} a_{\mathbf{k}}. \quad (2.138)$$

We will now express arbitrary operators in terms of creation and annihilation operators. In doing so, we distinguish operators acting on one, two,  $\dots$ ,  $N$  particles. The most important operators in practical situations are the one- and two-particle operators, to which the next two sections are devoted.

## 2.6 One-particle operators

The simplest operators to consider are additive one-particle operators. Recall that in first quantization an additive one-particle operator  $\mathbf{O}_1$  is given formally by its dependence on the dynamical variables of the particles, e.g. position operator  $\mathbf{r}$  and momentum operator

p. The additive one-particle operator is given by the sum over operators  $\mathbf{O}_i^{(1)}$ , each of which acts only on one particle

$$\mathbf{O}_1 = \sum_i \mathbf{O}_i^{(1)} \quad (2.139)$$

An example is the Hamiltonian of non-interacting particles in an external potential

$$\mathcal{H} = \sum_i \left( \frac{\mathbf{p}_i^2}{2m} + V(\mathbf{r}_i) \right) = \sum_i \mathcal{H}_i. \quad (2.140)$$

In order to make contact with the occupation number representation introduced in the previous discussion, we need to drop the particle index  $i$  of the operators  $\mathbf{O}_i^{(1)}$  and derive their action first on the abstract basis states discussed in sections 2.2 and especially 2.4, which are basis states where occupation levels are populated with particles (cf. (2.75)), especially one or two particles (cf. (2.71), (2.72), and (2.73)).

Let us assume now that there is a one-particle basis  $\{|1_\alpha\rangle\}$  in which the operators  $\mathbf{O}^{(1)}$  are diagonal with eigenvalues  $\omega_\alpha$

$$\mathbf{O}^{(1)}|1_\alpha\rangle = \omega_\alpha|1_\alpha\rangle, \quad (2.141)$$

as is, for instance, the case for momentum eigenstates of the momentum operator  $\mathbf{p}$  (see the example 2.2), then the one-particle operator becomes

$$\mathbf{O}_1 = \sum_\alpha \omega_\alpha N_\alpha = \sum_\alpha \omega_\alpha a_\alpha^\dagger a_\alpha. \quad (2.142)$$

In any other one-particle basis  $\{|1_i\rangle\}$  whose creation and annihilation operators are related to those of the one-particle basis  $\{|1_\alpha\rangle\}$  by (2.108) and (2.109) the second quantized form of the general operator (2.139) is then

$$\mathbf{O}_1 = \sum_{ij} \langle 1_i | \mathbf{O}^{(1)} | 1_j \rangle a_i^\dagger a_j. \quad (2.143)$$

In the real space or position basis  $\{|\mathbf{r}\rangle\}$ , the matrix elements in this expression can be written as

$$\langle 1_i | \mathbf{O}^{(1)} | 1_j \rangle = \int d^3 r d^3 r' u_i^*(\mathbf{r}) \langle \mathbf{r} | \mathbf{O}^{(1)} | \mathbf{r}' \rangle u_j(\mathbf{r}'), \quad (2.144)$$

which reduces for operators  $\mathbf{O}^{(1)}$  diagonal in this representation to

$$\langle 1_i | \mathbf{O}^{(1)} | 1_j \rangle = \int d^3 r u_i^*(\mathbf{r}) \mathbf{O}^{(1)}(\mathbf{r}, \mathbf{p}) u_j(\mathbf{r}), \quad (2.145)$$

Let us look at a few concrete examples.

### 2.6.1 Examples of one-particle operators

**Examples 2** *Position operator* The simplest example is arguably the position operator, i.e.  $\mathbf{O}_1 = \mathbf{R}$  and  $\mathbf{O}^{(1)} = \hat{\mathbf{r}}$ .<sup>3</sup> We use quantum field operators  $\psi^\dagger(\mathbf{r})$  and  $\psi(\mathbf{r})$  and the basis of position eigenstates  $\{| \mathbf{r} \rangle\}$  in the general expression (2.143) to obtain

$$\mathbf{R} = \int d^3 r d^3 r' \langle \mathbf{r} | \hat{\mathbf{r}} | \mathbf{r}' \rangle \psi^\dagger(\mathbf{r}) \psi(\mathbf{r}') = \int d^3 r \mathbf{r} \psi^\dagger(\mathbf{r}) \psi(\mathbf{r}), \quad (2.146)$$

where we used the property of the position eigenstates  $\langle \mathbf{r} | \hat{\mathbf{r}} | \mathbf{r}' \rangle = \mathbf{r}' \langle \mathbf{r} | \mathbf{r}' \rangle = \mathbf{r}' \delta(\mathbf{r} - \mathbf{r}')$ .

**Examples 3** *Linear momentum operator* In the case of linear momentum  $\mathbf{O}_1 = \mathbf{P}$  and  $\mathbf{O}^{(1)} = \mathbf{p}$  we obtain for arbitrary one-particle states  $\{| 1_i \rangle\}$

$$\mathbf{P} = \sum_{ij} \langle 1_i | \mathbf{p} | 1_j \rangle a_i^\dagger a_j, \quad (2.147)$$

which can be rewritten using the completeness relation for position states  $\int d^3 r | \mathbf{r} \rangle \langle \mathbf{r} | = \mathbb{I}$  as

$$\mathbf{P} = \sum_{ij} \int d^3 r d^3 r' a_i^\dagger \langle 1_i | \mathbf{r} \rangle \langle \mathbf{r} | \mathbf{p} | \mathbf{r}' \rangle \langle \mathbf{r}' | 1_j \rangle a_j = \int d^3 r d^3 r' \psi^\dagger(\mathbf{r}) \langle \mathbf{r} | \mathbf{p} | \mathbf{r}' \rangle \psi(\mathbf{r}'). \quad (2.148)$$

Next, we insert the completeness relation  $\sum_{\mathbf{k}} | \mathbf{k} \rangle \langle \mathbf{k} | = \mathbb{I}$  for the basis of momentum eigenstates  $\mathbf{p}_i | \mathbf{k} \rangle = \mathbf{k} | \mathbf{k} \rangle$ , which yields the final result that the momentum operator is diagonal in this basis (as was to be expected)

$$\mathbf{P} = \sum_{\mathbf{k}\mathbf{k}'} \int d^3 r d^3 r' \psi^\dagger(\mathbf{r}) \langle \mathbf{r} | \mathbf{k} \rangle \langle \mathbf{k} | \mathbf{p} | \mathbf{k}' \rangle \langle \mathbf{k}' | \mathbf{r}' \rangle \psi(\mathbf{r}') = \sum_{\mathbf{k}} \mathbf{k} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}, \quad (2.149)$$

where  $\langle \mathbf{r} | \mathbf{k} \rangle = e^{i\mathbf{k}\cdot\mathbf{r}}$  are plane waves and (2.135) and (2.136) have been used.

We could have obtained this result more directly by choosing as one-particle basis states  $\{| 1_i \rangle\}$  the basis of momentum eigenstates  $\{| \mathbf{k} \rangle\}$  from the outset.

<sup>3</sup> Where, for once, we use the symbol  $\hat{\phantom{x}}$  to distinguish an operator.

However, it is also often useful to stay in the position basis and use the momentum operator in position representation  $\mathbf{p} = -i\nabla$ , so that we can write (2.148) as

$$\mathbf{P} = \int d^3r \psi^\dagger(\mathbf{r}) (-i\nabla) \psi(\mathbf{r}). \quad (2.150)$$

**Examples 4** *Kinetic energy* Similarly the kinetic energy of a particle of mass  $m$

$$\mathbf{O}^{(1)} = \frac{\mathbf{p}^2}{2m} \quad (2.151)$$

yields the kinetic energy of  $N$  identical non-interacting particles

$$\mathcal{H}_0 = \sum_{i=1}^N \frac{\mathbf{p}_i^2}{2m} = \frac{1}{2m} \sum_{ij} \langle u_i | \mathbf{p}^2 | u_j \rangle a_i^\dagger a_j, \quad (2.152)$$

which in the basis of momentum eigenstates becomes again diagonal

$$\mathcal{H}_0 = \sum_{\mathbf{k}} \frac{k^2}{2m} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}. \quad (2.153)$$

In the position basis, we have the useful expression

$$\mathcal{H}_0 = \int d^3r \psi^\dagger(\mathbf{r}) \left( -\frac{1}{2m} \nabla^2 \right) \psi(\mathbf{r}), \quad (2.154)$$

which can be readily generalized to particles in an external potential  $U(\mathbf{r})$

$$\mathcal{H} = \int d^3r \psi^\dagger(\mathbf{r}) \left( -\frac{1}{2m} \nabla^2 + U(\mathbf{r}) \right) \psi(\mathbf{r}). \quad (2.155)$$

**Examples 5** *Particle density* We obtain the particle density from (2.123) together with (2.117) and (2.118), choosing as basis  $\{|\mathbf{k}\rangle\}$  for  $\{|1_\alpha\rangle\}$

$$\rho(\mathbf{r}) = \psi^\dagger(\mathbf{r}) \psi(\mathbf{r}) = \sum_{\mathbf{k}\mathbf{k}'} \langle \mathbf{k} | \mathbf{r} \rangle \langle \mathbf{r} | \mathbf{k}' \rangle a_{\mathbf{k}}^\dagger a_{\mathbf{k}'}, \quad (2.156)$$

whose Fourier transform is

$$\rho(\mathbf{q}) = \int d^3r e^{-i\mathbf{q}\cdot\mathbf{r}} \rho(\mathbf{r}) = \sum_{\mathbf{k}\mathbf{k}'} \left( \int d^3r e^{i(\mathbf{k}' - (\mathbf{k} + \mathbf{q}))\cdot\mathbf{r}} \right) a_{\mathbf{k}}^\dagger a_{\mathbf{k}'}, \quad (2.157)$$

so that

$$\rho(\mathbf{q}) = \sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k} + \mathbf{q}} = \sum_{\mathbf{k}} a_{\mathbf{k} - \mathbf{q}/2}^\dagger a_{\mathbf{k} + \mathbf{q}/2}. \quad (2.158)$$

.....

**EXERCISE 2.9 Current** In the same way it can be shown that the Fourier transform of the particle current

$$\mathbf{j}(\mathbf{r}) = -\frac{i}{2m} \left[ \psi^\dagger(\mathbf{r}) (\nabla \psi(\mathbf{r})) - (\nabla \psi^\dagger(\mathbf{r})) \psi(\mathbf{r}) \right] \quad (2.159)$$

is given by

$$\mathbf{j}(\mathbf{q}) = \frac{1}{m} \sum_{\mathbf{k}} \left( \mathbf{k} + \frac{\mathbf{q}}{2} \right) a_{\mathbf{k}}^\dagger a_{\mathbf{k}+\mathbf{q}}. \quad (2.160)$$

.....

## 2.7 Two-particle operators

A general two-particle operator is

$$\mathbf{O}_2 = \sum_{ij} \mathbf{O}_{ij}^{(2)}, \quad (2.161)$$

where the sum runs over all pairs of particles. The second quantized form in the abstract two-particle basis (2.72) and (2.73) becomes thus

$$\mathbf{O}_2 = \sum_{ijmn} \langle 1_i 1_j | \mathbf{O}^{(2)} | 1_m 1_n \rangle a_i^\dagger a_j^\dagger a_n a_m. \quad (2.162)$$

Note the reversed order of the indices  $n$  and  $m$  of the pair of annihilation operators as compared to their order in the matrix elements. This is a convention we adopt that is useful especially for Fermions where, as we shall see below in sections 2.9 and 2.11, and, especially, 2.12, changing the order of operators produces minus signs.

In the position basis, using (2.117) and (2.118), the two-particle operator becomes

$$\mathbf{O}_2 = \int d^3 r_1 d^3 r'_1 d^3 r_2 d^3 r'_2 \psi^\dagger(\mathbf{r}_1) \psi^\dagger(\mathbf{r}'_1) \langle \mathbf{r}_1, \mathbf{r}'_1 | \mathbf{O}^{(2)} | \mathbf{r}_2, \mathbf{r}'_2 \rangle \psi(\mathbf{r}'_2) \psi(\mathbf{r}_2). \quad (2.163)$$

Note that, as a consequence of the earlier ordering of the creation and annihilation operators in the general two-particle operator (2.162), the sequence of positions in the quantum field operators is  $\mathbf{r}_1, \mathbf{r}'_1, \mathbf{r}'_2, \mathbf{r}_2$ .

If  $\mathbf{O}^{(2)}$  is diagonal in the position space basis, using (2.117) and (2.118), this expression further reduces further to

$$\mathbf{O}_2 = \int d^3 r d^3 r' \psi^\dagger(\mathbf{r}) \psi^\dagger(\mathbf{r}') \mathbf{O}^{(2)}(\mathbf{r}, \mathbf{r}') \psi(\mathbf{r}') \psi(\mathbf{r}). \quad (2.164)$$

An important special case of this last expression is obtained if

$$\mathbf{O}^{(2)}(\mathbf{r}, \mathbf{r}') = \mathbf{O}^{(2)}(\mathbf{r} - \mathbf{r}') \tag{2.165}$$

as is, for instance, the case for many pairwise interaction potentials between particles. In order to exploit it, we start again from the general expression (2.162) for the two-particle operator  $\mathbf{O}_2$  but choose as two-particle basis states  $\{|1_i 1_j\rangle\}$  the momentum eigenstates  $\{|\mathbf{k}_1 \mathbf{k}_2\rangle\}$

$$\mathbf{O}_2 = \sum_{\mathbf{k}_1 \mathbf{k}_2 \mathbf{k}'_1 \mathbf{k}'_2} \langle \mathbf{k}_1 \mathbf{k}_2 | \mathbf{O}^{(2)} | \mathbf{k}'_1 \mathbf{k}'_2 \rangle a_{\mathbf{k}'_1}^\dagger a_{\mathbf{k}'_2}^\dagger a_{\mathbf{k}_2} a_{\mathbf{k}_1}. \tag{2.166}$$

Evaluating the matrix element in this expression in the plane wave representation when (2.165) holds, we finally obtain

$$\mathbf{O}_2 = \sum_{\mathbf{k}_1 \mathbf{k}_2 \mathbf{q}} \mathbf{O}^{(2)}(\mathbf{q}) a_{\mathbf{k}_1}^\dagger a_{\mathbf{k}_2}^\dagger a_{\mathbf{k}_2 + \mathbf{q}} a_{\mathbf{k}_1 - \mathbf{q}} = \sum_{\mathbf{k}_1 \mathbf{k}_2 \mathbf{q}} \mathbf{O}^{(2)}(\mathbf{q}) a_{\mathbf{k}_1 + \mathbf{q}}^\dagger a_{\mathbf{k}_2 - \mathbf{q}}^\dagger a_{\mathbf{k}_2} a_{\mathbf{k}_1}, \tag{2.167}$$

where  $\mathbf{O}^{(2)}(\mathbf{q})$  is the Fourier transform of  $\mathbf{O}^{(2)}(\mathbf{r})$

$$\mathbf{O}^{(2)}(\mathbf{q}) = \int d^3r \mathbf{O}^{(2)}(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}}. \tag{2.168}$$

.....  
**EXERCISE 2.10 Two-particle operator in momentum representation** Complete the steps leading from (2.166) to (2.167).

**EXERCISE 2.11 Fourier transform of the  $1/r$ -interaction in three, two, and one dimension** Calculate the Fourier transform of the interaction potential  $1/r$  for three

$$V(\mathbf{q}) = \int_{-\infty}^{\infty} dz e^{-iq_z z} \int_{-\infty}^{\infty} dy e^{-iq_y y} \int_{-\infty}^{\infty} dx \frac{e^{-iq_x x}}{\sqrt{x^2 + y^2 + z^2}}, \tag{2.169}$$

two

$$V(\mathbf{q}) = \int_{-\infty}^{\infty} dy e^{-iq_y y} \int_{-\infty}^{\infty} dx \frac{e^{-iq_x x}}{\sqrt{x^2 + y^2}}, \tag{2.170}$$

and one dimension

$$V(q) = \int_{-\infty}^{\infty} dx \frac{e^{-iqx}}{x}. \tag{2.171}$$

For the first integral, we can use spherical coordinates instead of Cartesian ones. In this approach we must regularize the integral by introducing a convergence factor which, in the final result, can be set to an appropriate value.

This approach becomes more difficult in two and one dimensions. In two dimensions, the introduction of polar coordinates leads to the appearance of a special function, the Bessel function  $J_0$ , with an appropriate argument.

An interesting approach to calculate the integral in any number of dimensions is to stay with Cartesian coordinates and evaluate the integrals ‘from the inside out’, i.e. start with the integration over  $x$ . A careful perusal of Gradshteyn and Ryzhik (1980) shows that the requisite integrals are all tabulated there, providing, en passant, the result for two dimensions.

However, the one-dimensional case presents a difficulty because the integral diverges. That being said, we can introduce on physical grounds a regularization starting with the innermost integral of the three-dimensional case and setting  $a = \sqrt{y^2 + z^2}$  as the width of the quasi-one-dimensional system. Moreover, it is possible to obtain an expression for the regularized integral in the limit  $q = |q_x| \rightarrow 0$ .

## 2.8 Second quantization of the Schrödinger equation: Bosonic case

In elementary quantum mechanics, the time-dependent Schrödinger equation for a particle in a potential  $V(\mathbf{r})$  is

$$i \frac{\partial \psi}{\partial t} = -\frac{1}{2m} \nabla^2 \psi + V(\mathbf{r})\psi \tag{2.172}$$

where  $\psi(\mathbf{r}, t)$  is the Schrödinger wave function or the Schrödinger field. The stationary eigenvalue equation

$$-\frac{1}{2m} \nabla^2 \psi_n + V(\mathbf{r})\psi_n = E_n \psi_n \tag{2.173}$$

has solutions  $\psi_n(\mathbf{r})$ , which are eigenfunctions with energy eigenvalues  $E_n$ . The general solution of the time-dependent Schrödinger equation is thus

$$\psi(\mathbf{r}, t) = \sum_n a_n(t) \psi_n(\mathbf{r}) \tag{2.174}$$

where the  $a_n(t)$  satisfy

$$\dot{a}_n(t) = -iE_n a_n(t). \tag{2.175}$$

The energy, or, more precisely, the expectation value of the Hamilton operator, can now be written as

$$E = \langle H \rangle = \langle \psi | H | \psi \rangle = \int d^3r \psi^*(\mathbf{r}, t) \left[ -\frac{1}{2m} \nabla^2 + V(\mathbf{r}) \right] \psi(\mathbf{r}, t) \tag{2.176}$$

$$= \sum_n E_n a_n^* a_n = \sum_n \omega_n a_n^* a_n. \quad (2.177)$$

This is the energy of a system of harmonic oscillators with eigenfrequencies  $\omega_n = E_n$ .

Thus, it is consistent to interpret these result in terms of a second quantized Hamiltonian

$$H = \sum_n E_n a_n^\dagger a_n, \quad (2.178)$$

where the creation and annihilation operators satisfy the commutation relations (2.74).

The equation of motion for the creation operators  $a_n$ , its Heisenberg equation of motion, is

$$\frac{da_n}{dt} = i [H, a_n] = -iE_n a_n. \quad (2.179)$$

In section 2.10, we briefly review the second quantization of the Schrödinger for the case of Fermions.

## 2.9 Creation and annihilation operators for Fermions

As shown in section 2.1.3, for Fermions, i.e. particles that obey the Pauli exclusion principle, the wave function is totally antisymmetric, i.e. exchange of particles leads to a change of sign of the wave function. To achieve this, we have introduced an antisymmetrization operator  $\mathcal{A}$ .

Section 2.1.3 also showed that the only possible states in an occupation number representation for Fermions are given by

$$|\phi\rangle = |N_1, N_2, \dots, N_l, \dots\rangle = |\{N\}\rangle, \quad (2.180)$$

with either  $N_l = 1$  or  $N_l = 0$ ,  $l = 1, 2, \dots$ , which expresses the exclusion principle and a fixed number of particles  $\sum_{l=1}^{\infty} N_l = N$ .

The definition of creation and annihilation operators acting on the occupation number states  $|\{N\}\rangle$  is somewhat more delicate than in the Bose case. The Fermionic creation and annihilation operators are more abstract entities than their Bosonic counterparts. They cannot be introduced in any way with recourse to position and momentum operators. This is a consequence of the fact that Fermions are genuinely quantum mechanical objects. Using the notation  $c_i$  and  $c_i^\dagger$  to distinguish from the Bose case, we define

$$c_i |\{N\}\rangle = \Theta_i \sqrt{N_i} |\dots (1 - N_i) \dots\rangle \quad (2.181)$$

$$c_i^\dagger |\{N\}\rangle = \Theta_i \sqrt{1 - N_i} |\dots (1 - N_i) \dots\rangle \quad (2.182)$$

with phase factors  $\Theta_i$ . We could have also introduced phase factors for the definition of the Bose creation and annihilation operators, but choosing them as unity would have been consistently possible. In the Fermi case, however, the phase factors are of crucial importance and cannot be chosen as unity.

A consistent choice is the following. First, order the sequence of occupation number levels  $l$  in  $|\phi\rangle$  in a fixed way that cannot be changed any more. In the definition of the creation and annihilation operators  $c_i$  and  $c_i^\dagger$ , if the number  $\nu_i$  of levels that are occupied by a Fermion is even for the levels which are predecessors of the level  $i$ , then the phase is  $\Theta_i = +1$ , and if it is odd, then put  $\Theta = -1$ . Obviously, we can write

$$\Theta_i = (-1)^{\sum_{j=1}^{i-1} \nu_j} \equiv (-1)^{\nu_i}. \tag{2.183}$$

From the definitions (2.181) and (2.182) of the creation and annihilation operators, we see that

$$(c_i)^2 |\{N\}\rangle = (c_i^\dagger)^2 |\{N\}\rangle = 0, \tag{2.184}$$

which again expresses the Pauli exclusion principle.

For, without limiting generality,  $i < j$ , the definitions (2.181) and (2.182) of the creation and annihilation operators imply the anti-commutation relations

$$\{c_i, c_j\} = c_i c_j + c_j c_i = 0, \tag{2.185}$$

$$\{c_i^\dagger, c_j^\dagger\} = c_i^\dagger c_j^\dagger + c_j^\dagger c_i^\dagger = 0, \tag{2.186}$$

and

$$\{c_i, c_j^\dagger\} = c_i c_j^\dagger + c_j^\dagger c_i = \delta_{ij}. \tag{2.187}$$

.....  
**EXERCISE 2.12 Fermion anti-commutation relations** Derive the Fermion anti-commutation relations using the definitions (2.181) and (2.182) of the creation and annihilation operators.  
 .....

With the help of the creation and annihilation operators for Fermions  $c_i$  and  $c_i^\dagger$  and the definition for vacuum state

$$|vac\rangle = |0, 0, \dots, 0, \dots\rangle, \tag{2.188}$$

a general  $N$ -particle Fermi state can be now be written as

$$|\{N\}\rangle = (c_1^\dagger)^{N_1} (c_2^\dagger)^{N_2} \dots |vac\rangle. \tag{2.189}$$

The creation and annihilation operators for Fermions satisfy

$$c_i^\dagger c_i |\{N\}\rangle = N_i |\{N\}\rangle \tag{2.190}$$

and

$$c_i c_i^\dagger |\{N\}\rangle = (1 - N_i) |\{N\}\rangle, \tag{2.191}$$

which again allows the interpretation of

$$n_i = c_i^\dagger c_i \tag{2.192}$$

as the particle number operator and

$$\mathcal{N} = \sum_{i=1}^{\infty} n_i = \sum_{i=1}^{\infty} c_i^\dagger c_i \tag{2.193}$$

as the operator of total particle number.

If proper care is taken concerning the order of creation and annihilation operators, all results for Bosons remain valid for Fermions.

.....  
**EXERCISE 2.13 Bogoliubov transformation for Fermions** Consider a system consisting of two Fermions,  $c_1$  and  $c_2$ . Which condition must the complex parameters  $u$  and  $v$  satisfy such that the Bogoliubov transformation

$$c_1 = uc_1 + vc_2^\dagger, \tag{2.194}$$

$$c_2^\dagger = -vc_1 + uc_2^\dagger, \tag{2.195}$$

preserves the canonical Fermi anti-commutation relations?

**EXERCISE 2.14 Band splitting** A system of  $N$  electrons in one dimension, disregarding the spin of the electrons, in a periodic potential is described by the Hamilton operator

$$\mathcal{H} = \sum_{j=1}^N \left( -\frac{1}{2m} \frac{d^2}{dx_j^2} + V_0 \cos\left(\frac{2\pi}{a} x_j\right) \right) = \sum_{j=1}^N \mathcal{H}_j = \sum_{j=1}^N \mathcal{H}(x_j). \tag{2.196}$$

Assume  $V_0$  to be a small perturbation to the Hamiltonian of free, i.e. non-interacting, electrons.

- a) Express  $\mathcal{H}$  in the occupation number representation. Which are the appropriate one-particle basis and one-particle wave functions for this problem?
- b) Restrict the Hamiltonian  $\hat{\mathcal{H}}$  in occupation number representation to a small interval

$$I = \left( \frac{K}{2} - \delta, \frac{K}{2} + \delta \right) \tag{2.197}$$

with  $K = \frac{2\pi}{a}$  and  $\delta \ll K$ , i.e.

$$\hat{\mathcal{H}} = \sum_{k \in I} \mathcal{H}_k \tag{2.198}$$

where

$$\mathcal{H}_k = \epsilon_k c_k^\dagger c_k + \epsilon_q c_q^\dagger c_q + \frac{V_0}{2} c_k^\dagger c_q + \frac{V_0}{2} c_q^\dagger c_k \tag{2.199}$$

with  $q = k - K$ .

Diagonalize  $\mathcal{H}_k$  using the appropriate choice of parameters  $\lambda_k$  in the transformation

$$b_k = c_k \cos \lambda_k + c_q \sin \lambda_k, \tag{2.200}$$

$$b_q = -c_k \sin \lambda_k + c_q \cos \lambda_k. \tag{2.201}$$

Which eigenvalues does  $\mathcal{H}_k$  thus have?

- c) The one-particle eigenvalue spectrum  $\epsilon_k$  of free electrons has a parabolic form. The periodic perturbation potential in (2.196) leads to a deviation from this parabolic form, which is called a band splitting. Calculate this band splitting at  $k = \frac{K}{2}$ . In order to do this, expand the eigenvalues of  $\mathcal{H}_k$  up to and including second order in  $\delta$ .

Similar to the case of Bosonic creation and annihilation operators, we now summarize useful formulas for calculations involving Fermionic creation and annihilation operators as exercises. As we shall see, these formulas have a form simpler than their Bosonic counterparts. The reason for this is that for Fermionic creation and annihilation operators, we have

$$c^n = (c^\dagger)^n = 0 \quad \text{for} \quad n \geq 2. \tag{2.202}$$

Using this fact, we can furthermore restrict the functions of Fermionic operators to the two cases

$$f(c) = f(0) + f'(0)c, \tag{2.203}$$

$$f(c^\dagger) = f(0) + f'(0)c^\dagger, \tag{2.204}$$

which yields as immediate consequence the special cases

$$e^{\alpha c} = 1 + \alpha c, \tag{2.205}$$

$$e^{\alpha c^\dagger} = 1 + \alpha c^\dagger \tag{2.206}$$

for any complex number  $\alpha$ .

**EXERCISE 2.15 Functions of Fermionic creation and annihilation operators** As a consequence of (2.203) and (2.204), there are only two non-trivial cases to show

$$e^{-\alpha c^\dagger} c e^{\alpha c^\dagger} = c - \alpha^2 c^\dagger - 2\alpha s, \tag{2.207}$$

$$e^{-\alpha c} c^\dagger e^{\alpha c} = c^\dagger - \alpha^2 c + 2\alpha s \tag{2.208}$$

with the operator

$$s = c^\dagger c - \frac{1}{2}. \tag{2.209}$$

However, the exponential  $e^{\alpha c^\dagger c}$  gives rise to interesting relations that are analogous to the ones in the Bosonic case and can be derived in a completely analogous way. They are

$$e^{\alpha c^\dagger c} c e^{-\alpha c^\dagger c} = e^{-\alpha} c, \tag{2.210}$$

$$e^{\alpha c^\dagger c} c^\dagger e^{-\alpha c^\dagger c} = e^{\alpha} c^\dagger. \tag{2.211}$$

## 2.10 Second quantization of the Schrödinger equation: Fermionic case

The same line of argument as in section 2.8, although via using the anti-commutation relations (2.185–2.187), leads to the formally same results.

In particular, a second quantized Hamiltonian can be identified

$$H = \sum_n E_n c_n^\dagger c_n \tag{2.212}$$

where the creation and annihilation operators satisfy the anti-commutation relations (2.185–2.187).

The equation of motion for the annihilation operators  $c_n$ , its Heisenberg equation of motion, again turns out to be

$$\frac{dc_n}{dt} = i [H, c_n] = -iE_n c_n. \tag{2.213}$$

.....  
**EXERCISE 2.16** Repeat explicitly the steps in section 2.8 for the case of Fermions. Especially ascertain the validity of the Heisenberg equation of motion (2.213) in the Fermionic case.  
 .....

## 2.11 Second quantization formalism and the many-particle wave function

In this penultimate section of part I, we demonstrate that the second quantization formalism is indeed equivalent to the Schrödinger equation of a many-particle system. In order to keep the equations manageable, we restrict this demonstration to the case of two particles. The considerations are valid for both the Bosonic and the Fermionic cases. In order to express this notationally, we use  $b^\dagger$  and  $b$  for creation and annihilation operators. The general two-particle state is created from the vacuum state by applying two creation operators

$$|\phi_2\rangle = \sum_{i,j} c_{ij} b_i^\dagger b_j^\dagger |0\rangle. \tag{2.214}$$

We rewrite this state in terms of quantum field operators

$$b_i^\dagger = \int d^3r \phi_i(\mathbf{r}) \psi^\dagger(\mathbf{r}), \tag{2.215}$$

$$b_i = \int d^3r \phi_i(\mathbf{r}) \psi(\mathbf{r}) \tag{2.216}$$

to obtain

$$|\phi_2\rangle = \sum_{i,j} c_{i,j} \int d^3r \phi_i(\mathbf{r}) \psi^\dagger(\mathbf{r}) \int d^3r' \phi_j(\mathbf{r}') \psi^\dagger(\mathbf{r}') |0\rangle. \quad (2.217)$$

Introducing the function

$$f(\mathbf{r}, \mathbf{r}') = \sum_{i,j} c_{i,j} \phi_i(\mathbf{r}) \phi_j(\mathbf{r}'), \quad (2.218)$$

the two-particle state becomes

$$|\phi_2\rangle = \int d^3r \int d^3r' f(\mathbf{r}, \mathbf{r}') \psi^\dagger(\mathbf{r}) \psi^\dagger(\mathbf{r}') |0\rangle \quad (2.219)$$

$$= \int d^3r \int d^3r' f(\mathbf{r}', \mathbf{r}) \psi^\dagger(\mathbf{r}') \psi^\dagger(\mathbf{r}) |0\rangle \quad (2.220)$$

$$= \int d^3r \int d^3r' f(\mathbf{r}', \mathbf{r}) \left( \pm \psi^\dagger(\mathbf{r}) \psi^\dagger(\mathbf{r}') \right) |0\rangle, \quad (2.221)$$

where, going from the first line to the second, we have exchanged the variables  $\mathbf{r}$  and  $\mathbf{r}'$ , and then, going from the second line to the third, we used the Bose (upper sign) and Fermi (lower sign) commutation and anti-commutation relations, respectively. Comparing the first and last lines, we find

$$f(\mathbf{r}, \mathbf{r}') = \pm f(\mathbf{r}', \mathbf{r}) \quad (2.222)$$

for Bosons (upper sign) and Fermions (lower sign), respectively.

As we have seen, in sections 2.6 and 2.7 respectively, the second quantized Hamiltonian in the position basis of a many-particle system in an external potential  $U(\mathbf{r})$  and with two-particle interactions  $V(\mathbf{r}, \mathbf{r}')$  can be written as

$$\begin{aligned} \mathcal{H} &= \int d^3r \psi^\dagger(\mathbf{r}) \left( -\frac{1}{2m} \nabla^2 + U(\mathbf{r}) \right) \psi(\mathbf{r}) \\ &+ \frac{1}{2} \int d^3r \int d^3r' \psi^\dagger(\mathbf{r}) \psi^\dagger(\mathbf{r}') V(\mathbf{r}, \mathbf{r}') \psi(\mathbf{r}') \psi(\mathbf{r}) \end{aligned} \quad (2.223)$$

$$= \mathcal{H}_1 + \mathcal{H}_2 \equiv \mathcal{H}_1 + \mathcal{V} \quad (2.224)$$

where the factor 1/2 avoids double counting of the interactions and the two-particle interaction potential could, e.g. be the Coulomb potential

$$V(\mathbf{r}, \mathbf{r}') = V(\mathbf{r} - \mathbf{r}') = \frac{e^2}{|\mathbf{r} - \mathbf{r}'|}. \quad (2.225)$$

The Schrödinger equation

$$\mathcal{H}|\phi_2\rangle = E|\phi_2\rangle \quad (2.226)$$

for the two-particle state can now be rewritten as the Schrödinger equation for the two-particle wave function  $f(\mathbf{r}_1, \mathbf{r}_2)$

$$\left( -\frac{1}{2m}\nabla_1^2 + U(\mathbf{r}_1) - \frac{1}{2m}\nabla_2^2 + U(\mathbf{r}_2) + V(\mathbf{r}_1, \mathbf{r}_2) \right) f(\mathbf{r}_1, \mathbf{r}_2) = Ef(\mathbf{r}_1, \mathbf{r}_2). \quad (2.227)$$

In order to verify this result, we have to use the commutation or anti-commutation relations for quantum field operators of Bosons and Fermions, respectively. Moreover, we need a twofold partial integration in the integrals containing the single-particle Hamiltonian  $\mathcal{H}_1$ .

## 2.12 Normal ordering

In section 2.11 and in section 2.7 on two-particle operators, we have always written the field and particle creation and annihilation operators in such a way that all creation operators appeared to the left of the annihilation operators. This convention is called normal ordering. Adopting this convention ensures that the vacuum expectation value vanishes

$$\langle 0|\mathcal{V}|0\rangle = 0 \quad (2.228)$$

with  $\mathcal{V}$  given in (2.224) and (2.223) where we have also observed the convention  $\mathbf{r}, \mathbf{r}', \mathbf{r}', \mathbf{r}$  for the order of arguments of the quantum field creation and annihilation operators.

.....  
**EXERCISE 2.17 Normal ordering of two-particle potential operator: wrong choice** Show that the apparently obvious choice for the second quantized form of a two-particle potential operator

$$\mathcal{V} = \frac{1}{2} \int d^3r d^3r' V(\mathbf{r}, \mathbf{r}') \rho(\mathbf{r}) \rho(\mathbf{r}') \quad (2.229)$$

where

$$\rho(\mathbf{r}) = \psi^\dagger(\mathbf{r})\psi(\mathbf{r}) \quad (2.230)$$

leads to an unwanted self-energy term

$$\frac{1}{2} \int d^3r V(\mathbf{r}, \mathbf{r}) \psi^\dagger(\mathbf{r}) \psi(\mathbf{r}). \quad (2.231)$$

Therefore, observing normal ordering of the creation and annihilation operators from the start avoids unnecessary arguments about why certain terms are to be disregarded later on.

The following exercise confirms this lesson from the positive side.

**EXERCISE 2.18 Correct normal ordering** Show that the normal ordered two-particle potential operator

$$\mathcal{V} = \frac{1}{2} \int d^3r d^3r' \psi^\dagger(\mathbf{r}) \psi^\dagger(\mathbf{r}') V(\mathbf{r}, \mathbf{r}') \psi(\mathbf{r}') \psi(\mathbf{r}) \quad (2.232)$$

for a symmetric two-particle potential  $V(\mathbf{r}, \mathbf{r}') = V(\mathbf{r}', \mathbf{r})$  applied to a many-particle state

$$|\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N\rangle = \psi^\dagger(\mathbf{r}_1) \psi^\dagger(\mathbf{r}_2) \dots \psi^\dagger(\mathbf{r}_N) |0\rangle \quad (2.233)$$

reproduces the correct (first quantized) expression

$$\mathcal{V} |\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N\rangle = \frac{1}{2} \sum_{n \neq m} V(\mathbf{r}_n, \mathbf{r}_m) |\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N\rangle. \quad (2.234)$$

Furthermore, show that the two-particle potential operator of the previous exercise does not reproduce this result.

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This chapter has introduced and reviewed the basics of the theory of quantum many-particle systems, especially the method of second quantization. We will use these concepts and results throughout the book.

Of course, the theory of quantum many-particle systems contains much more than the method of second quantization. The books mentioned at the beginning of this chapter provide more comprehensive expositions of this theory.

# 3

## Angular Momentum

---

*No, it's quite impossible for the electron to have a spin. I have thought of that myself, and if the electron did have a spin, the speed of the surface of the electron would be greater than the velocity of light. So, it's quite impossible.*

Hendrik Antoon Lorentz (1853–1928) to Uhlenbeck and Goudsmit (fortunately Ehrenfest had already submitted their paper)

The first model solved by Bethe ansatz, by Hans Bethe himself in 1931, is a model of atoms arranged in a one-dimensional lattice whose magnetic moments or, for short, quantum spins, interact—the so-called Heisenberg model for magnetism.

Therefore, this chapter briefly reviews the concept of angular momentum in quantum mechanics, especially the coupling of spin- $\frac{1}{2}$  operators for several quantum spins. We shall be needing this when we discuss the properties of quantum many-particle Hamiltonians, for example, the Heisenberg quantum spin chain Hamiltonian in parts II and III.

Section 3.1 briefly develops the theory of angular momentum for a single quantum particle, first discussing its general theory, then specialized to case of spin- $\frac{1}{2}$ , which has no classical counterpart but is a special case of an internal property of quantum particles. Section 3.2 is devoted to a discussion of the angular momentum of several quantum particles.

### 3.1 Angular momentum of a single quantum particle

#### 3.1.1 General theory

The operator<sup>1</sup>  $\mathbf{L}$  for angular momentum in quantum mechanics is defined in analogy to the corresponding relation of classical mechanics

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} \tag{3.1}$$

<sup>1</sup> Again we shall not distinguish, for instance by using hats ( $\hat{\ }$ ), between quantum mechanical operators and classical dynamical variables except in cases where such a distinction reduces the chances of possible confusion.

where position<sup>2</sup> and (linear) momentum

$$\mathbf{r} = (x, y, z)^T = (r_1, r_2, r_3)^T, \quad \mathbf{p} = (p_x, p_y, p_z)^T = (p_1, p_2, p_3)^T \quad (3.2)$$

are now identified with operators  $\mathbf{r}$  and  $\mathbf{p}$  with non-vanishing commutators which, in components, are given by

$$[r_j, p_k] = i\delta_{jk}. \quad (3.3)$$

From these commutators follow the commutators for the components  $L_1, L_2,$  and  $L_3$  of the angular momentum operator  $\mathbf{L}$

$$[L_j, L_k] = i\epsilon_{jkl}L_l, \quad (3.4)$$

where  $\epsilon_{jkl}$  are the components of the totally antisymmetric Levi–Civita tensor

$$\epsilon_{123} = 1, \quad \epsilon_{jkl} = -\epsilon_{kjl} = -\epsilon_{ilk} = -\epsilon_{lkj}. \quad (3.5)$$

.....  
**EXERCISE 3.1 Angular momentum commutator** It is a good exercise to verify (3.4) with the help of the commutation relations (3.3).  
 .....

It follows from (3.4) and the corresponding Heisenberg uncertainty relation that the components  $L_j$  of the angular momentum operator  $\mathbf{L}$  cannot be sharply measured simultaneously. However, for the square of the angular momentum

$$\mathbf{L} \cdot \mathbf{L} = L^2 = L_1^2 + L_2^2 + L_3^2 \quad (3.6)$$

we find that all its commutators with the components of  $\mathbf{L}$  vanish

$$[L^2, L_j] = 0, \quad j = 1, 2, 3, \quad (3.7)$$

which means that the square  $L^2$ , and *one* component  $L_j$  of the angular momentum  $\mathbf{L}$ , can be measured simultaneously with arbitrary precision. This component is conventionally chosen to be  $L_3$ . Moreover, we can always find simultaneous eigenstates of  $L^2$  and  $L_3$ . In order to show (3.7), it is helpful to use the general relation for commutators involving three operators  $A, B,$  and  $C$

<sup>2</sup> In this chapter, we use several conventions since all of them are appropriate in certain situations. We label quantities at times by their Cartesian component, e.g.  $p_x$  for the  $x$ -component of momentum, at other times by a numerical label  $i$  with  $i = 1, 2, 3$ , e.g.  $\sigma_3$  for the 3-component instead of  $\sigma_z$  for the  $z$ -component of the vector of Pauli matrices. Moreover, it will sometimes be convenient to resort to upper indices, like in  $\sigma_i^z$  where there is also a lower index  $i$  to distinguish between the spin of different particles.

$$[AB, C] = A[B, C] + [A, C]B. \quad (3.8)$$

In order to investigate the eigenvalues and eigenfunctions of the angular momentum operators further, it will prove useful to introduce two operators with the help of the components of the angular momentum operator  $\mathbf{L}$

$$L^+ = L_1 + iL_2, \quad (3.9)$$

and

$$L^- = L_1 - iL_2, \quad (3.10)$$

which, together with  $L_3$ , satisfy the commutation relations

$$[L_3, L^+] = L^+, \quad (3.11)$$

$$[L_3, L^-] = -L^-, \quad (3.12)$$

and

$$[L^+, L^-] = 2L_3. \quad (3.13)$$

The operators  $L^\pm$  are constructed in analogy to the harmonic oscillator creation and annihilation operators. It is instructive to demonstrate how the operators  $L^\pm$  can be motivated by the following consideration. Assume we have an eigenstate  $|m\rangle$  of the operator  $L_3$

$$L_3|m\rangle = m|m\rangle. \quad (3.14)$$

We now want to find an operator  $L_S$  which produces a state  $|\lambda\rangle = L_S|m\rangle$  with a shifted eigenvalue, i.e.

$$L_3|\lambda\rangle = L_3(L_S|m\rangle) = (m + \lambda)(L_S|m\rangle). \quad (3.15)$$

Multiplying (3.14) by  $L_S$  and subtracting it from (3.15) gives

$$[L_3, L_S]|m\rangle = \lambda L_S|m\rangle \quad (3.16)$$

or, as an operator equation

$$[L_3, L_S] = \lambda L_S. \quad (3.17)$$

In order to satisfy (3.17), it suffices to construct the shift operator  $L_S$  as a linear combination of the operators  $L_1$  and  $L_2$

$$L_S = L_1 + aL_2. \quad (3.18)$$

so that from (3.17)

$$[L_3, L_1] + a[L_3, L_2] = iL_2 - iaL_1 = \lambda L_1 + \lambda aL_2 \quad (3.19)$$

or

$$i = a\lambda \quad \text{and} \quad -ia = \lambda \quad (3.20)$$

must hold. The latter two equations are only compatible if  $\lambda = \pm 1$ . The shift operator can thus be identified with the operators  $L^+$  and  $L^-$  of (3.9) and (3.10), creating states where the eigenvalue  $m$  of an eigenstate  $|m\rangle$  of  $L_3$  is shifted by  $\pm 1$ .

In terms of the operators  $L^+$ ,  $L^-$ , and  $L_3$ , the square of the angular momentum operator can be expressed in three ways, which will prove useful for the following considerations

$$L^2 = \left( L_3^2 + \frac{1}{2}(L_+L_- + L_-L_+) \right) \quad (3.21)$$

$$= \left( L_3^2 + L_3 + L_-L_+ \right) \quad (3.22)$$

$$= \left( L_3^2 - L_3 + L_+L_- \right). \quad (3.23)$$

We consider a simultaneous eigenstate  $|\Psi\rangle$  of  $L^2$  and  $L_3$  with eigenvalues  $C^2$  and  $m$ , respectively, i.e.

$$L^2|\Psi\rangle = C^2|\Psi\rangle, \quad (3.24)$$

and

$$L_3|\Psi\rangle = m|\Psi\rangle, \quad (3.25)$$

which, as we have seen, is always possible. But what happens if we act with  $L^\pm$  on this state? Let us thus consider the states

$$|\Phi^\pm\rangle = L^\pm|\Psi\rangle. \quad (3.26)$$

We already know that the eigenvalue of  $L_3$  gets shifted

$$L_3|\Phi^\pm\rangle = (m \pm 1)|\Phi^\pm\rangle. \quad (3.27)$$

Furthermore, since  $L^2$  commutes with all component of  $\mathbf{L}$ , we obtain

$$L^2|\Phi^\pm\rangle = L^2L^\pm|\Psi\rangle = L^\pm L^2|\Psi\rangle = C^2(L^\pm|\Psi\rangle) = C^2|\Phi^\pm\rangle. \quad (3.28)$$

In summary, the operator  $L^+$  thus increases and the operator  $L^-$  decreases the eigenvalue of the third component  $L_3$  of the angular momentum by one, while leaving the eigenvalue of the square of the angular momentum  $L^2$  unchanged. Because of the properties just discussed, the angular momentum operators  $L^+$  and  $L^-$  are also called ladder operators, with  $L^+$  being the raising, and  $L^-$  the lowering, operator.

More generally, we have, by iteration,

$$L_3((L^\pm)^n|\Psi\rangle) = (m \pm n)((L^\pm)^n|\Psi\rangle). \quad (3.29)$$

The square of the third component of the angular momentum cannot exceed the square of the angular momentum, i.e.

$$(m + n)^2 \leq C^2, \quad (3.30)$$

which can also be seen from the expectation values in the state  $|\Psi\rangle$

$$\langle L^2 \rangle \equiv \langle \Psi | L^2 | \Psi \rangle = \langle L_1^2 \rangle + \langle L_2^2 \rangle + \langle L_3^2 \rangle, \quad (3.31)$$

i.e.

$$C^2 = \langle L_1^2 \rangle + \langle L_2^2 \rangle + m^2 \geq m^2. \quad (3.32)$$

Thus,  $m$  must be bounded from above and below, i.e. there must be a largest value  $m_{\max}$  and a smallest value  $m_{\min}$  with

$$m_{\max} \leq m \leq m_{\min} \quad (3.33)$$

such that

$$L_3|m_{\max}\rangle = m_{\max}|m_{\max}\rangle \quad \text{and} \quad L^+|m_{\max}\rangle = 0, \quad (3.34)$$

$$L_3|m_{\min}\rangle = m_{\min}|m_{\min}\rangle \quad \text{and} \quad L^-|m_{\min}\rangle = 0. \quad (3.35)$$

Choosing  $|m_{\max}\rangle$  and  $|m_{\min}\rangle$  as simultaneous eigenstates of  $L^2$ , we find with the help of (3.22) and (3.23)

$$L^2|m_{\max}\rangle = C^2|m_{\max}\rangle = (L^-L^+ + L_3^2 + L_3)|m_{\max}\rangle \quad (3.36)$$

$$= m_{\max}(m_{\max} + 1)|m_{\max}\rangle \quad (3.37)$$

and

$$L^2|m_{\min}\rangle = C^2|m_{\min}\rangle = (L^+L^- + L_3^2 - L_3)|m_{\min}\rangle \quad (3.38)$$

$$= m_{\min}(m_{\min} - 1)|m_{\min}\rangle, \quad (3.39)$$

which are only compatible if  $m_{\min} = -m_{\max}$ .

It is conventional to denote  $m_{\max}$  by the letter  $l$  and the corresponding simultaneous eigenstate of the square  $L^2$  and the third component  $L_3$  of the angular momentum operator by  $|l, l\rangle$ .

This state thus satisfies

$$L^+|l, l\rangle = 0, \quad (3.40)$$

$$L_3|l, l\rangle = l|l, l\rangle. \quad (3.41)$$

and

$$L^2|l, l\rangle = C^2|l, l\rangle = l(l+1)|l, l\rangle, \quad (3.42)$$

i.e. the eigenvalue of the square  $L^2$  of the angular momentum is  $C^2 = l(l+1)$ . Moreover, we can conclude from the action of  $L^\pm$  (cf. (3.29)) that the possible values of  $m$  extend from  $-l$  to  $l$  in integer steps and that  $l$  can only take integer or half-odd integer values.

We conclude that the states of the system are labelled, for any fixed value of  $l$ , by

$$|l, m\rangle, \quad 2l = 0, 1, 2, \dots, \quad -l \leq m \leq l. \quad (3.43)$$

The corresponding state space, denoted by  $\mathcal{V}_l$ , has dimension  $\dim \mathcal{V}_l = 2l + 1$ . Another name for the eigenvalue of  $L_3$  of a state  $|\Phi\rangle$ , often used in connection with quantum groups, is the *weight* of  $|\Phi\rangle$ . We call any state  $|\Phi\rangle$  satisfying

$$L^-|\Phi\rangle = 0 \quad (3.44)$$

a *lowest weight state*.

For the states  $|l, m\rangle$  we have just constructed, the weight is given by  $m$ , also called the azimuthal quantum number, and the lowest weight state is  $|l, -l\rangle$ .

So far, the states  $|l, m\rangle$  have not been normalized. Normalizing them, we find the eigenvalues of the operators  $L^+$  and  $L^-$  as well. If we write

$$L^\pm|l, m\rangle = N_{l,m}^\pm|l, m \pm 1\rangle, \quad (3.45)$$

now assuming that both states  $|l, m\rangle$  and  $|l, m \pm 1\rangle$  are normalized, we find with the help of the relations (3.21–3.23) that

$$N_{l,m}^{\pm} = [l(l+1) - m(m \pm 1)]^{\frac{1}{2}}. \quad (3.46)$$

Our results can be interpreted in terms the Heisenberg uncertainty relation. The maximally possible eigenvalue of  $L_3$  is  $l$  and, hence, the maximally possible value of  $L_3^2$  is  $l^2$ . However, the eigenvalue of  $L^2$  is  $l(l+1)$ , larger than  $l^2$ . This implies that the angular momentum operator  $\mathbf{L}$  can never align with certainty with  $L_3$  and the uncertainty principle is satisfied. If  $\mathbf{L}$  could be aligned with  $L_3$ , then  $L_1 = L_2 = 0$  and we would have simultaneously sharp values of all three components of the angular momentum operator, in contradiction to Heisenberg's uncertainty relations, which follow from (3.4).

### 3.1.2 Spin

The half-odd integer values of angular momentum of the form  $l = \frac{2n+1}{2}$ , with  $n$  a non-negative integer, which we have found as a possibility in quantum mechanics in the previous section, have no correspondence in terms of classical angular momentum of the orbital form (3.1) given at the beginning of the previous section. However, they are realized in nature and correspond to the internal structure of the quantum particle and are referred to as *spin*. In this connection, the symbol  $\mathbf{S}$  is used instead of  $\mathbf{L}$ .

As also discussed extensively in chapter 2, there is a fundamental distinction between particles with half-odd integer spin, called *Fermions*, which obey the Pauli exclusion principle, and those with integer spin,<sup>3</sup> called *Bosons*, which do not obey the Pauli exclusion principle. This distinction is rather deep and manifests itself also in different thermodynamic behaviour of Bosons and Fermions. Where the former have a many-particle wave function that is symmetric with respect to the exchange of particles, and they obey Bose–Einstein statistics, the latter have an antisymmetric many-particle wave function with respect to particle exchange and they obey Fermi–Dirac statistics. Some of the many-particle aspects of this distinction have been discussed in chapter 2, and the corresponding aspects of statistical mechanics and thermodynamics will be discussed in chapter 4. This chapter, focuses on the angular momentum, especially of Fermions with spin- $\frac{1}{2}$ .

For the special case  $l \equiv s = \frac{1}{2}$ , on which we focus from now on, we introduce the operator  $\mathbf{S}$  whose components satisfy (3.4), i.e.

$$[S_x, S_y] = iS_z, \quad [S_y, S_z] = iS_x, \quad [S_z, S_x] = iS_y. \quad (3.47)$$

The weight of a state  $|\chi\rangle$ , as previously introduced, measures the eigenvalue of the spin operator of the state, e.g. in the 3- or  $z$ -direction, of the quantum particle

$$S_3|\chi\rangle = m_S|\chi\rangle = \pm\frac{1}{2}|\chi\rangle \quad (3.48)$$

<sup>3</sup> Nevertheless, there is no interpretation of quantum particles with integer spin in terms of  $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ !

and

$$\mathbf{S}^2|\chi\rangle = s(s+1)|\chi\rangle = \frac{3}{4}|\chi\rangle \quad (3.49)$$

with

$$-s \leq m_s \leq s, \quad \text{i.e.} \quad m_S = \pm \frac{1}{2}, \quad (3.50)$$

where  $s$  (which is  $s = \frac{1}{2}$  in this case) is often simply denoted as the spin of the quantum particle.

Corresponding to  $m_S = \pm \frac{1}{2}$ , we introduce a two-dimensional basis for a spin- $\frac{1}{2}$  particle. The general element of the space spanned by this basis is called a spinor and can be formally written as

$$|\chi\rangle = \begin{pmatrix} |\chi_+\rangle \\ |\chi_-\rangle \end{pmatrix}, \quad (3.51)$$

and whose components are in general complex numbers and which is in general a function of position and time  $|\chi\rangle = |\chi(\mathbf{r}, t)\rangle$ . Moreover,  $||\chi_{\pm}\rangle|^2$  is interpreted as the probability to find that the particle in the state  $|\chi\rangle$  has  $m_S = \pm \frac{1}{2}$ .

Fixing the coordinate system, we have two possible states: the spin state with  $m_S = \frac{1}{2}$

$$\left| \frac{1}{2}, \frac{1}{2} \right\rangle = |\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad (3.52)$$

and the spin state with  $m_S = -\frac{1}{2}$

$$\left| \frac{1}{2}, -\frac{1}{2} \right\rangle = |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad (3.53)$$

which we can choose as basis states. The different notations depend on the context we want to emphasize.

In order to find realizations for the spin operators  $S_i$ , we introduce first an operator

$$S^+ \equiv S_1 + iS_2, \quad (3.54)$$

a special case of (3.9), which increases  $m_S$  by one. In analogy to the general case, this operator satisfies

$$S^+|\uparrow\rangle = 0 \quad \text{and} \quad S^+|\downarrow\rangle = S^+ \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \quad (3.55)$$

In the same way, the operator  $S^-$ , a special case of (3.10), decreases  $m_S$  by one

$$S^- = S_1 - iS_2 \quad (3.56)$$

i.e.

$$S^-|\uparrow\rangle = S^- \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \text{and} \quad S^-|\downarrow\rangle = 0. \quad (3.57)$$

In the expressions above, we have used that (3.46) in these cases gives

$$N_{\frac{1}{2},\frac{1}{2}}^+ = N_{\frac{1}{2},-\frac{1}{2}}^- = 0 \quad \text{and} \quad N_{\frac{1}{2},-\frac{1}{2}}^+ = N_{\frac{1}{2},\frac{1}{2}}^- = 1. \quad (3.58)$$

From these results, we deduce that

$$(S^+ + S^-) \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 2S_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (3.59)$$

and

$$(S^+ + S^-) \begin{pmatrix} 0 \\ 1 \end{pmatrix} = 2S_1 \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \quad (3.60)$$

Both of these equations can be realized by  $S_1$  in the form of the  $2 \times 2$  matrix

$$S_1 = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \quad (3.61)$$

Repeating the arguments above for  $S^+ - S^- = 2iS_2$ , we find

$$S_2 = \frac{1}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \quad (3.62)$$

Finally, the matrix for  $S_3$  produces the eigenvalues  $m_S = \pm \frac{1}{2}$

$$S_3 = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad S_3 \left| \frac{1}{2}, \pm \frac{1}{2} \right\rangle = \pm \frac{1}{2} \left| \frac{1}{2}, \pm \frac{1}{2} \right\rangle. \quad (3.63)$$

Here are some elementary exercises to get acquainted with spin matrices and spinors.

**EXERCISE 3.2 Spin operators in matrix form** Verify that the spin operators in matrix form that we just derived satisfy the commutation relations (3.47).

Show that they also satisfy the relations

$$S_1 S_2 = -S_2 S_1 = \frac{i}{2} S_3, \quad S_3 S_1 = -S_1 S_3 = \frac{i}{2} S_2, \quad S_2 S_3 = -S_3 S_2 = \frac{i}{2} S_1 \quad (3.64)$$

and that hence the anti-commutators of the spin matrices vanish.

Moreover, show that the squares of the spin matrices are proportional to the  $2 \times 2$  unit matrix.

Summarizing the matrix realizations of the spin operator  $\mathbf{S}$  we introduce the vector of the Pauli spin matrices  $\sigma$

$$\mathbf{S} = \frac{1}{2} \boldsymbol{\sigma} \quad (3.65)$$

or, in components

$$S_1 = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{1}{2} \sigma_1, \quad S_2 = \frac{1}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \frac{1}{2} \sigma_2, \quad S_3 = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{1}{2} \sigma_3, \quad (3.66)$$

which satisfy the relations (3.4) and (3.47), respectively.

**EXERCISE 3.3 A useful relation** Prove that for two vectors  $\mathbf{a}$  and  $\mathbf{b}$

$$(\mathbf{a} \cdot \boldsymbol{\sigma})(\mathbf{b} \cdot \boldsymbol{\sigma}) = \mathbf{a} \cdot \mathbf{b} + i(\mathbf{a} \times \mathbf{b}) \cdot \boldsymbol{\sigma} \quad (3.67)$$

**EXERCISE 3.4 Unit vector corresponding to a spinor** We define a unit vector  $\mathbf{e}$  in the spinor state  $|\chi\rangle$  by

$$\mathbf{e} = \langle \boldsymbol{\sigma} \rangle_\chi = \langle \chi | \boldsymbol{\sigma} | \chi \rangle. \quad (3.68)$$

Calculate  $\mathbf{e}$  for the spinor

$$|\zeta\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad (3.69)$$

and show how, once you have the unit vector  $\mathbf{e}$ , you can recover the spinor  $|\zeta\rangle$ .

**EXERCISE 3.5 A simple spin Hamiltonian** Calculate the energy eigenvalues and the eigenstates of the Hamiltonian

$$\mathcal{H} = B \cos \theta \cdot \sigma_x + B \sin \theta \cdot \sigma_y. \quad (3.70)$$

**EXERCISE 3.6 Two-level system** A two-level system can be described by the Hamiltonian

$$\mathcal{H}_0 = \sigma_x. \quad (3.71)$$

Add a term

$$\mathcal{V} = B\sigma_z \quad (3.72)$$

and calculate the energy eigenvalues of  $\mathcal{H} = \mathcal{H}_0 + \mathcal{V}$  by direct diagonalization.

For small field  $B \ll 1$  you may consider  $\mathcal{V}$  as a perturbation. Calculate the corrections to the energy eigenvalues of  $\mathcal{H}_0$  up to second order in perturbation theory and compare with the exact result.

**EXERCISE 3.7 Useful relations for spin- $\frac{1}{2}$  operators** The spin-1/2 raising and lowering operators in terms of Pauli matrices are

$$\sigma^\pm = \frac{1}{2} (\sigma^x \pm i\sigma^y) \quad (3.73)$$

Calculate all products between pairs of these two operators and their commutation and anti-commutation relations. Furthermore, calculate the commutation and anti-commutation relations between the raising and lowering operators and the Pauli operators  $\sigma^x$ ,  $\sigma^y$ , and  $\sigma^z$ .

Show that a function  $f$  that can be expanded into a power series can, as an operator function of the product of the spin- $\frac{1}{2}$  raising and lowering operators, only have the form

$$f(\sigma^+ \sigma^-) = f(0) + [f(1) - f(0)] \sigma^+ \sigma^-, \quad (3.74)$$

$$f(\sigma^- \sigma^+) = f(0) + [f(1) - f(0)] \sigma^- \sigma^+. \quad (3.75)$$

Moreover, show that the following relations hold

$$e^{\frac{\alpha\sigma_z}{2}} \sigma^+ e^{\frac{\alpha\sigma_z}{2}} = e^\alpha \sigma^+, \quad (3.76)$$

$$e^{\frac{\alpha\sigma_z}{2}} \sigma^- e^{\frac{\alpha\sigma_z}{2}} = e^\alpha \sigma^-. \quad (3.77)$$

In order to conclude this section on the spin of one particle, we now demonstrate that the spin- $\frac{1}{2}$  degree of freedom has a most remarkable property. Consider a new coordinate system where spin space has been rotated by an angle  $\theta$  about the 2-axis. This rotation transforms  $S_3$  into

$$S'_3 = S_3 \cos \theta + S_1 \sin \theta = \frac{1}{2} \cos \theta \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + \frac{1}{2} \sin \theta \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (3.78)$$

$$= \frac{1}{2} \begin{pmatrix} \cos \theta & \sin \theta \\ \sin \theta & -\cos \theta \end{pmatrix}. \quad (3.79)$$

The transformed spin operator  $S'_3$  must have the same eigenvalues  $m_S = \pm \frac{1}{2}$  in the rotated system as the original spin operator  $S_3$  had in the unrotated system. In the rotated coordinate system the eigenvector  $|\uparrow'\rangle$  for eigenvalue  $(+\frac{1}{2})$ , i.e.

$$S'_3 |\uparrow'\rangle = +\frac{1}{2} |\uparrow'\rangle \quad (3.80)$$

is

$$|\uparrow'\rangle = \begin{pmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} \end{pmatrix} = \cos \frac{\theta}{2} |\uparrow\rangle + \sin \frac{\theta}{2} |\downarrow\rangle \quad (3.81)$$

and for eigenvalue  $(-\frac{1}{2})$ , i.e.

$$S'_3 |\downarrow'\rangle = -\frac{1}{2} |\downarrow'\rangle \quad (3.82)$$

we have

$$|\downarrow'\rangle = \begin{pmatrix} -\sin \frac{\theta}{2} \\ \cos \frac{\theta}{2} \end{pmatrix} = -\sin \frac{\theta}{2} |\uparrow\rangle + \cos \frac{\theta}{2} |\downarrow\rangle. \quad (3.83)$$

Therefore, if we measure the spin to be in the spin up state in the rotated coordinate system, we shall, upon measuring, find it in the original coordinate system in the spin up state with probability  $\cos^2 \frac{\theta}{2}$  and in the spin down state with probability  $\sin^2 \frac{\theta}{2}$ .

Now, if we rotate through an angle of  $2\pi$ , a remarkable situation arises. A particle we measure to be in the spin up state in the rotated coordinate system will be with probability 1 in the down state with respect to the original coordinate system. In other words, a rotation of the universe by  $2\pi$  causes all spin- $\frac{1}{2}$  particles to assume unitarily transformed eigenstates, a distinguishing feature between intrinsic spin and the usual notion of angular momentum.

## 3.2 Angular momentum of several quantum particles

We begin our discussion of the coupling of the angular momentum of several quantum particles by first considering the case of spin  $s = l$  before we specialize to  $s = \frac{1}{2}$ , which is the case most important for us. In order to gain a clear understanding, in this section

we shall use a slightly cumbersome but precise notation that we will later abandon again (in most cases), except when it may be rendered necessary by the demands of a special situation.

The total spin vector of a system of  $N$  identical particles each of spin  $s = l$  is

$$\mathbf{S}(N) = \sum_{i=1}^N \mathbf{S}_i \quad (3.84)$$

where

$$\mathbf{S}_i = I \otimes I \otimes \dots \otimes \underbrace{\mathbf{S}}_i \otimes \dots \otimes I \quad (3.85)$$

acts non-trivially only on the spin state of particle  $i$ . The unit operators  $I$  in the tensor product act on the spins of all particles except the spin of particle  $i$ . The total state space is written as the  $N$ -fold tensor product<sup>4</sup> of the state space  $\mathcal{V}_i$  of a single particle's spin state space

$$\mathcal{V} = \underbrace{\mathcal{V}_1 \otimes \mathcal{V}_1 \otimes \dots \otimes \mathcal{V}_1}_N, \quad (3.86)$$

which is the vector space whose basis states are  $N$ -fold product states of the single-particle basis states  $|l, m_i\rangle$

$$|l, \mathbf{m}\rangle = |l, m_1\rangle \otimes |l, m_2\rangle \otimes \dots \otimes |l, m_N\rangle. \quad (3.87)$$

The components of the total spin operators  $S^\alpha$ ,  $\alpha = 1, 2, 3$  acting on the spin of particle  $i$ <sup>5</sup> are given by

$$S^\alpha(N) = \sum_{i=1}^N \left( I \otimes I \otimes \dots \otimes \underbrace{S^\alpha}_i \otimes \dots \otimes I \right). \quad (3.88)$$

Hence,  $S^\alpha(N)$  can be realized by a  $(2l+1)^N \times (2l+1)^N$  matrix. The many-particle spin operators  $S^\alpha(N)$  also obey the commutation relations (3.4).

<sup>4</sup> For more on tensor products, see section 10.7.1.

<sup>5</sup> Cf. footnote 2.