Algebraic Approach towards Conductivity in Ergodic Media

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Zusammenfassung

Die vorliegende Arbeit enthält einen operatoralgebraischen Zugang zur Berechnung der elektrischen Leitfähigkeit von ungeordneten Festkörpern auf Grundlage der Betrachtung von Viel-Teilchen Quantensystemen. Dieser Zugang ist von besonderem Interesse, da er die Beschreibung wechselwirkender Elektronengase ermöglicht, welche bisherige Zugänge verwehrten.
Zur Beschreibung von Elektronengasen in ergodisch ungeordneten Festkörpern werden die in diesem Zusammenhang neuen Konzepte des kovarianten Zustands sowie des kovarianten Morphismus entwickelt. Kombiniert wird weiterhin das Konzept des kovarianten Zustands mit dem des KMS Zustands.
Die der Beschreibung von sich im thermischen Gleichgewicht befindlichen Systemen dienenden KMS Zustände stellen in ihrer kovarianten Form die Ausgangszustände der betrachteten Elektronengase dar, bevor das System von außen durch ein elektrisches Feld beeinflusst wird. Das elektrische Feld induziert Ströme, bringt das Elektronengas somit aus dem thermischen Gleichgewicht und führt zu einer zeitlichen Evolution des kovarianten Zustands des Systems, welche wiederum durch kovariante Automorphismen beschrieben wird. Letztlich führt dies zu einem zeitlich abhängigen, kovarianten Zustand des Systems welcher auf der Algebra der beschränkten lokalen Operatoren des fermionischen Fockraums eines zugehörigen Ein-Teilchen Hilbertraums definiert ist. Für diskrete, ausgedehnte Elektronengase in einer Raumdimension versehen mit einer Paarwechselwirkung endlicher Reichweite werden explizit Methoden zur Konstruktion eines solchen Zustands vorgestellt. Für wechselwirkungsfreie Elektronengase wird eine entsprechende Konstruktion sogar in beliebiger Raumdimension durchgeführt.
Da Messungen am Elektronengas im ergodisch ungeordneten Festkörper durch die Wirkung des zuvor konstruierten zeitlich abhängigen kovarianten Zustands auf lokale, beschränkte und selbstadjungierte Operatoren beschrieben werden, wird zur Definition der Stromdichte, als Ergebnis einer Messung, das neue Konzept des sogenannten Stromdichte Operators eingeführt. Das Transformationsverhalten des Stromdichte Operators kombiniert mit dem Transformationsverhalten kovarianter Zustände führt unter Anwendung des Birkhoffschen Ergodensatzes zu dem Resultat, dass die Stromdichte im räumlichen Mittel unabhängig von der Realisierung des Systems ist.
Die elektrische Leitfähigkeit beschreibt die lineare Abhängigkeit der räumlich gemittelten Stromdichte vom äußeren elektrischen Feld bei kleinen Feldstärken. Für das bereits zuvor erwähnte Modell des wechelwirkungsfreien Elektronengases wird schließlich mittels sogenannter Linearer Antwort Theorie ein expliziter Ausdruck für die elektrische Leitfähigkeit in Form einer Kubo Formel hergeleitet. Die Herleitung der Kubo Formel erfordert die Erfüllung einer Lokalisierungsbedingung durch das System, wobei die Formulierung der Bedingung spezifisch für den Fall wechselwirkungsfreier Elektronengase ist. In Hinblick auf eine Lineare Antwort Theorie wechselwirkender Elektronengase werden deshalb mögliche Verallgemeinerungen der Lokalisierungsbedingung diskutiert.

Abstract

This thesis is about an operator algebraic approach towards the derivation of the electrical conductivity in disordered solid states based on the theory of quantum many-particle systems. Such an approach is of interest since it allows for the description of interacting electron gases, which is a feature not present in previous work.

In the context of the description of ergodic media, new concepts are introduced, such as covariant states and covariant morphisms. Moreover, the concept of covariant states is combined with the well-known concept of KMS states.

In its covariant form, KMS states describe electron gases in ergodic media at thermal equilibrium. Such states are the starting point of the electron gases considered here. An external electric field is applied to the system, influences the electron gas and causes internal electric currents. Thus, the equilibrium position of the system is disturbed, leading to a time evolution of the system, which is described by covariant automorphisms. Summing up, the system is given in a time dependent, covariant state that acts on the algebra of bounded and local operators on the fermionic Fock space defined over some given one-particle Hilbert space. For a discrete model of an extended electron gas in one space dimension with a pair interaction of finite range, explicit constructions of the above states are presented. In addition, for the special case of non-interacting electron gases, the construction of the time dependent covariant state is carried out in arbitrary space dimension.

Since measurements in a quantum system are implemented by the action of its state on bounded, local and self-adjoint operators, the concept of a current density operator is introduced. The current density is then defined as the result of the measurement of the current density operator. By an application of Birkhoff's ergodic theorem, the transformation law of the current density operator together with the covariant transformation law of the state of the electron gas implies the almost sure existence of the spatial mean of the current density. Moreover, the spatial mean current density is almost surely independent of the concrete realisation given.

The electric current density describes the linear dependence of the spatial mean current density on the external electric field, for small strengths. Via linear response theory for the non-interacting model of an electron gas, an explicit expression for the current density is derived in terms of a so called Kubo formula. For the derivation the system needs to satisfy a localisation condition, which is specifically designed for non-interacting electron gases. In view of a linear response theory of interacting electron gases, candidates for a generalisation of this localisation criterion that also apply to interacting systems are introduced.

Contents

1 Introduction

Das Streben dieser Abhandlung geht dahin, aus einigen wenigen, größtentheils durch die Erfahrung gegebenen Prinzipien den Inbegriff derjenigen elektrischen Erscheinungen in geschlossenem Zusammenhange abzuleiten, welche durch die Berührung zweier oder mehrerer Körper unter einander hervorgebracht und unter dem Namen der galvanischen begriffen werden; ihre Absicht ist erreicht, wenn auf solche Weise die Mannigfaltigkeit der Thatsachen unter die Einheit des Gedankens gestellt wird.

(Georg Simon Ohm)

It seems to be a desirable characteristic of a thesis in mathematical physics to rely on physics that is common not only to physicists but also to people who have a general interest in that field. In order to fulfill this criterion, one could say that this thesis is based on Ohm's law. Considering this, the question immediately arises about the necessity, or at least the importance, in publishing a thesis in 2013 which is related to something that seems to be as easy and well understood as Ohm's law, a physical law that was discovered 200 years ago. Although it is much more difficult to answer this question satisfactorily, we want to face this challenge. Our answer is deeply connected to a natural evolution of knowledge in physics.

The elegance of a physical theory is given by the simplicity of its fundamental laws as well as by the amount of phenomena observed in nature the theory describes. Thus, it may not seem worth mentioning that all theories that survived decades or even centuries, share the attributes of an intuitive mathematical language as well as a huge extent of validity. Examples of such theories are classical mechanics, thermodynamics, electrodynamics, quantum mechanics and the theories of special and general relativity. Each of these theories either succeeded in the efficient description of phenomena in nature to which a reasonable explanation was missing or managed to unify different theories, i.e. showed that different pre-existing theories could be seen as special cases of one new, more general and more powerful theory.

The latter situation might lead to the conclusion that once such a new theory is found, one could forget about the old ones that are special cases of the new. However, this would be the wrong way to proceed, since more general theories also appear to have more abstract formalisms. For example, quantum mechanics is a more general theory than classical mechanics, since it is valid not only on macroscopic scales, where classical mechanics applies, but also on microscopic scales, where classical mechanics fails to explain certain results of measurements. Nevertheless, it would be unnecessary to analyse the dynamics of a football being shot by Lionel Messi by considering the football and Lionel Messi as a quantum mechanical system, since, however short Lionel Messi might be, the behaviour one is interested in takes place on macroscopic scales, i.e. quantum effects are negligible, so that the less abstract and more intuitive formalisms of classical mechanics apply.

Nevertheless, once a new theory is established, already existing theories may appear in a new

context. In this case, it is of interest to review central and well-known results in light of the new theory, at the very least in order to check for consistency. So, to refine the statement above, this thesis is about Ohm's law in the context of the quantum mechanics of many-particle systems.
We will state two examples that illustrate the evolution of knowledge in physics that we tried to characterise in general terms above. The first example sketches the history of the evolution from Kepler's laws to the theory of general relativity. It is part of physics folklore and was often treated in popular scientific literature. The second example is the evolution of Ohm's law to the theory of quantum statistical mechanics. It motivated this thesis but is less folkloric than the first one. Concerning this, the author of the present thesis hopes to illustrate that there is a strong analogy between the two evolutions in order to emphasise the fact that this work answers questions that appear naturally within our current understanding of physics.

1.1. From Kepler to General Relativity

In 1619, Johannes Kepler proclaimed three laws on the motion of planets. He obtained these laws from observations, but they remained phenomenological in the sense that they were standing on their own until Isaac Newton formulated the theory of vector mechanics. Newton's theory was able to reproduce Kepler's laws in the context of a theory that applied to many other phenomena in nature, such as to the motion of spinning tops. At the same time it is elegant and intuitive. In addition, Newtonian mechanics was able to bring new insight to Kepler's laws, since it turned out that Kepler's second law was the statement of preservation of angular momentum, a quantity that is of general interest in mechanics, especially for spinning tops.
However, physics did not end with the breakthrough of Newtonian mechanics. Even within classical mechanics, an evolution took place during which more powerful formalisms first of Joseph-Louis Lagrange and later of William Rowan Hamilton and Carl Gustav Jacob Jacobi were found. These formalisms are nowadays known as analytical mechanics. They are less intuitive than Newtonian mechanics, yet very elegant. Furthermore, they added new insight to known results. For example, it turned out that preservation of certain quantities of a system such as energy, momentum and angular momentum are deeply connected to homogeneity in time, homogeneity in space and isotropy in space, respectively. The latter are properties that can be read from the Lagrange or the Hamilton functions which inherit the basic information of a system. These correspondences were found by Emmy Noether in 1918.
The modern approaches to classical mechanics basically share the playground with Newtonian mechanics but in certain situations, such as the implementation of constraints, the former theories are easier to control than the latter theory. Moreover, they were also the reference for the mathematical physicists of the 20^{th} century for the formulation of the theories of quantum mechanics and general relativity.
In contrast to the earlier theories, quantum mechanics and the theories of special and general relativity do not share the playground with Newtonian mechanics. They are able to describe physical phenomena, where classical mechanics fails. Quantum mechanics became the theory that describes physical systems on microscopic scales. The theories of special and general relativity changed the understanding of time and space. Furthermore, they treat the corresponding variables in a very systematic way, at least more so than classical mechanics. This is, for example, reflected by the fact that on an abstract level Poincaré symmetry in special relativity can be stated more concisely than the Galilean symmetry in classical mechanics. Moreover, the theory of general relativity contributed a new understanding of gravitation and was able to explain, for example, the apsidal precession of planet Mercury, a phenomenon that up to the breakthrough of general relativity remained to be difficult to describe. So again a new theory added insight to

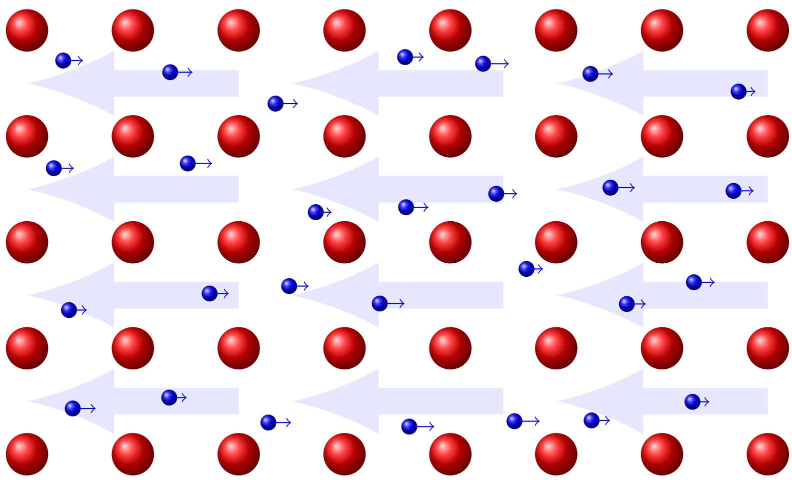
something that seemed well understood for hundreds of years, such as the motion of the planets of our solar system.

1.2. From Ohm to Quantum Statistical Mechanics

In 1827, Georg Simon Ohm published a thesis on chains of galvanic batteries (Ohm27). From this work, a law originated that even many non-physicists will remember from their physics classes at school as Ohm's law. For many objects, such as a copper wire, this law states that the total electric current I through the object caused by a difference U of an external electric potential is proportional to U by the inverse of a positive constant R which is called the electrical resistance of the object, i.e.

$$I = \frac{U}{R} \,. \tag{1.1}$$

Given a sample, its electrical resistance will depend on the material it is made of, as well as on its temperature, dimensions and geometry. For example, for fixed values of temperature, length and potential difference between its ends the total electric current I through a copper wire will be the higher the bigger the diameter of the wire is. In this case, the electrical resistance R is a monotonously decreasing function of the diameter of the wire.
As the electrical resistance R of any kind of sample could also be defined by Equation (1.1), the basic statement of Ohms law is that R is independent of I and U at least within a certain range of values of the latter variables, the range of ohmic behaviour.
Given any sample with ohmic behaviour, its electrical resistance can be determined by measuring the total electric currents I while applying various differences U of electric potential between its ends. On this level Ohm's law, like Kepler's laws, would be phenomenological, since these procedures do not indicate that one is trying to calculate the value of the electrical resistance of a sample from other data one has about it, such as the knowledge about its material, geometry, dimensions and temperature.
On a microscopic scale, the total electric current I through a given solid sample stems from electrons moving through the solid forced by an electric field E which is applied from outside the solid causing a difference U of electric potential between the ends of the sample. This is illustrated by the following figure.



The ensemble of moving electrons then defines a density j of electric current. Intuitively, it seems clear that an analogous result to Ohm's law should hold on this microscopic level, i.e.

the electric current density j is higher the stronger the external electric field E is. The former quantity should depend linearly on the latter. The first to find such a reformulation was Gustav Robert Kirchhoff. His law states

$$j = \sigma E \tag{1.2}$$

with a quantity σ called *electrical conductivity* depending only on the material of the solid and its temperature. In contrast to Ohm's law, there is no dependence on dimensions of the sample. It is a vectorial equation so that σ, being the analogon to the electrical resistance R, is not a scalar but a tensorial quantity. Integration over the volume of the sample then leads from Kirchhoff's microscopical law (1.2) back to Ohm's macroscopical law (1.1).
The dependence of the electrical conductivity tensor σ on the material of the solid is given by the interaction of the moving electrons in the solid with the ions that the solid consists of which have fixed positions. So, for a given temperature it should be possible to determine σ from the atomic data of the solid, i.e. the knowledge of the position of the ions of the solid and the knowledge of their interaction with electrons.
In 1900, Paul Drude was the first to face the problem of determining the electrical conductivity σ for metals from their atomic data (Dru00). His model treats electrons like pinballs, bouncing between the ions of a given solid. The electrons are accelerated by the external electric field, but due to collisions with the ions of the solid, which lead to reflections in arbitrary directions, an electron will take a complicated path through the solid having a finite drift velocity v_D towards the direction of the electric field, depending on the atomic structure of the solid.
Because Drude's model is the most simple to understand Ohm's law on a microscopic scale, it will be explained in further detail. Drude introduced a relaxation time τ implementing the mean time between two consecutive collisions which inherits the atomic data of the solid. In addition, it is the parameter with which a dependence on the temperature enters the model. According to Drude's model, the equation of motion for a single electron is given by

$$m\dot{v} = -eE - \frac{m}{\tau} v_D \; ,$$

where m is the mass of the electron, e its charge and v its velocity. Drude supposed the system would end up in a dynamical equilibrium which is characterised by the fact that there is no change in the electrons velocity, i.e. $\dot{v} = 0$, implying

$$v_D = -\frac{e\tau}{m} E \; .$$

Multiplying both sides of this equation with the number density n of the electrons, one obtains the expression

$$j = -env_D = \frac{e^2 n\tau}{m} E$$

for the electric current density. In view of Equation (1.2) this leads to the formula

$$\sigma = \frac{e^2 n\tau}{m} \tag{1.3}$$

for the electrical conductivity. Drude's theory treats the system on microscopic scales in a classical way. But the current understanding of microscopic systems is given by quantum theories, i.e. Drude's approach relies on a theory that is known to be invalid on microscopic scales. Furthermore, the electrons are considered to have no interaction between each other.

But as a result of the Pauli exclusion principle in quantum mechanics, electrons underlie Fermi statistics. In its role the Pauli principle can be seen as a certain type of interaction making indistinguishable particles of an ideal quantum gas aware of each others existence by forbidding any pair of such particles to occupy the same quantum numbers. The resulting Fermi statistics differs decisively from Boltzmann statistics that corresponds to the classical description of electrons in Drude's model. Clearly, this causes the conductivities calculated using Drude's model to differ from the ones measured in experiment by an approximate factor of six. For similar reasons, Drude's model is in contradiction with the so called Dulong-Petit law, which was obtained from experimental data.

In order to make the description more precise and to determine the conductivity of a given sample from its atomic data, one has to use the formalism of quantum mechanics of many-particle systems, also known as quantum statistical mechanics. Physical as well as mathematical works were published on that problem.

In 1933, Arnold Sommerfeld and Hans Bethe improved Drude's theory by the use of quantum mechanics (BS67). Their model includes Fermi statistics but excludes any other kind of interaction between the electrons. Nevertheless, it is a very successful model, for example, since it calculates conductivity in agreement with measured values for many metals and since it explains the Wiedemann-Franz law, which relates the electronic contribution to the thermal conductivity of metals to their electrical conductivity.

In 1957, Ryogo Kubo published a work presenting the statistical-mechanical theory of irreversible processes (Kub57), improving the theory of Sommerfeld and Bethe. Using a very general approach including so called linear response theory, Kubo was able to give expressions for quantities, such as the electrical conductivity. In contrast to the earlier work by Drude, Sommerfeld and Bethe, electrons are allowed to interact in Kubo's formalism, for example, via a repulsive potential.

This quantum statistical point of view on conductivity not only inspired the title of the present section but also is a guideline for this thesis. However, in order to understand the playground of this thesis, another aspect, namely disordered media, has to be introduced. This aspect is motivated and explained in the following section.

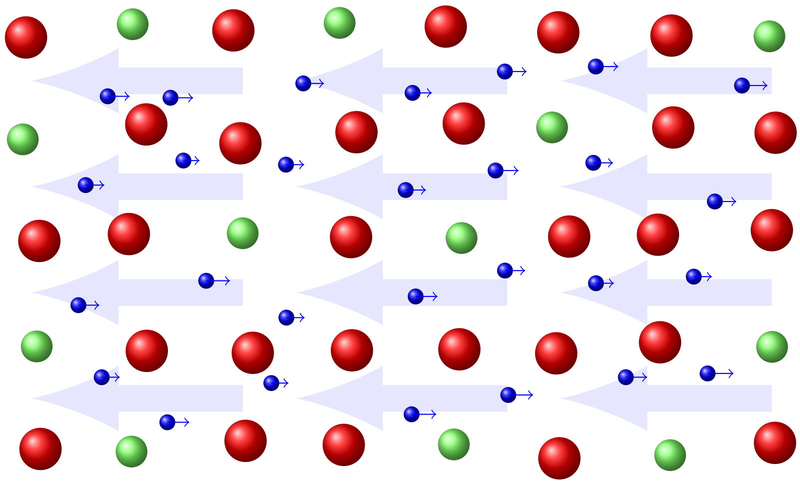
1.3. Conductivity of Ergodic Media

Considering solids on atomic scales, one typically likes to think of perfect materials, i.e. crystals with an absolute periodic structure only containing a few different species of ions. An example would be an ideal crystal of pure polonium, which shows a cubic structure. However, the solids that appear most frequently in nature do not feature such a perfect structure, but are affected by types of disorder.

For example, to describe solids, such as glasses, one at least has to consider models not having every ion centred at a site of a periodic lattice but instead dislocated from these positions, where the deflection of an ion is given by a random vector.

Another interesting type of disordered media are alloys. As an example, one may think of a sample of brass, a mixture of copper and zinc. Even if the ions of such a sample are centred at the sites of a perfect lattice, disorder appears, since the lattice sites are occupied by the different types of ions in a random way.

The general picture of disordered media, that the author of this thesis has in mind, is given by the following figure.



The figure shows an alloy of two different species of ions R and G sitting approximately at the sites of a cubic lattice. At each site, one finds either an ion of species R or of species G, deflected from its ideal lattice position by an individual displacement vector. Moreover, a homogeneous atomic structure is indicated, meaning, for example, that the concentration of ions of species G does not vary within the volume of the solid. This type of disorder characterises solids that we refer to as ergodic media. The formalism to describe such media uses probability theory. Different realisations of ergodic media are identified with different elements of a probability space. Fundamental mathematical works on transport phenomena in disordered solid states are for example (FS83, AG98, BSB98a, BSB98b, Nak02, BGKS05).

It seems plausible that the electrical conductivity σ as well as other quantities of ergodic media should not depend on the concrete realisation of the sample in the sense that one would need the complete atomic data of the sample in order to calculate σ. The electrical conductivity of a homogeneous alloy should depend only on the concentrations of the atomic components, and not on the exact position of every ion, i.e. in a huge sample the electrical conductivity σ should not change if the positions of two different ions are interchanged. Anyway, it would be impossible to know the position and the species of each ion in a given macroscopic solid sample of about 10^{23} ions. Having this practical reason in view, the above suggestion that knowledge of the average microscopic structure of the solid sample is sufficient to calculate its electrical conductivity σ would be a very motivating feature.

Indeed, this statement holds true for ergodic media, as it was shown in (BSB98b, BGKS05). In particular, like Kubo, the authors of (BGKS05) used linear response theory to give an expression for the electrical conductivity tensor σ of an ergodic solid. The special feature of the media to be ergodic leads to the result that the electrical conductivity tensor does not depend on the concrete realisation of the sample but on its average atomic structure. In contrast to Kubo, the authors of (BGKS05) considered electrons having no other type of interaction than that given by the Pauli exclusion principle, making the electrons obey Fermi statistics. The advantage of this idealisation is that the analysis in (BGKS05) takes place on an effective one-particle level, which is easier to control than a more involved many-particle formulation one would have to use in order to admit more general types of interactions between the electrons.

But since electrons interact via a repulsive potential, it is natural to look for a generalisation of the results of (BGKS05) towards interacting systems. The goal of this thesis is to present a mathematically rigorous way to define the concept of a conductivity tensor, resulting in methods that in principle also apply to interacting electron gases.

2 Results

Les questions les plus importantes de la vie ne sont en effet, pour la plupart, que des problèmes de probabilité.

(Pierre Simon Marquis de Laplace)

We would like to start by stating the results of this thesis in order to motivate its structure to the reader. As it turned out, a generalisation of the analysis presented in the fundamental work (BGKS05) towards interacting quantum gases necessarily has to undergo strong modifications. In this thesis, these modifications culminate in an operator algebraic approach towards the problem, also featuring new concepts, such as covariant states, covariant automorphisms and a current density operator. We will explain this in more detail.

As already mentioned in the previous chapter, the analysis in (BGKS05) benefits from the fact that only non-interacting electron gases are considered. One advantage is the possibility of an effective one-particle formulation of the problem. Many-particle spaces and many-particle operators can be avoided. But clearly, in order to describe interacting electrons, at least a two-electron level has to appear in a generalising formalism, since this is the lowest level in which interaction between electrons can enter the stage of the theory.

In fact, as it will turn out, the Fermi distribution appearing in (BGKS05) is a relict of the equilibrium state of the corresponding free electron gas on Fock space. Here, the term state is meant in the sense of a normalised and positive linear functional on an algebra of operators, more precisely, the Fermi algebra over a Hilbert space corresponding to one single electron.

Only by focusing on non-interacting electron gases and only if the state of the system is applied to a certain type of operator, namely the operators which are quadratic in creation and annihilation operators, the expectation value of a measurement, as the result of the state being applied to the operator implementing the measurement, can be expressed explicitly via the Fermi distribution and the trace over the Hilbert space of a single electron.

In more general situations, where interaction between electrons is present, one cannot dispose of many-particle spaces in the formulation of the theory. Accordingly, considering quantum statistical mechanics, an operator algebraic approach proved to be an adequate framework for a theory of conductivity in random ergodic media. At least, apart from being the approach chosen in this thesis, operator algebras are also used in (BSPK13a) and a series of papers to be published by the same authors.

The first part of the thesis is spanned by the Chapters 3-5 and presents the general operator algebraic framework needed to describe random ergodic quantum many-particle systems.

In the second part, covering Chapters 6-7, a concrete model is presented, creating examples for the algebraic objects only defined abstractly in the first part. The model constructed is a discrete interacting electron gas trapped in a random ergodic solid state.

This specific model allows the definition of electric current densities and conductivities. The formal definitions of these objects are given in Chapter 8.

Subject to Chapter 9 is the construction of these objects for the special case of a non-interacting electron gas.
The analysis of this chapter uses a localisation assumption specifically designed for non-interacting systems. Attempts for a generalisation of the latter localisation property towards interacting systems are presented in Chapter 10.
Appendix A ties to Chapters 6 and 7 and demonstrates that apart from current densities and conductivities, there are other interesting quantities to focus on. As an example we consider the particle density of a system.
A central part of our analysis is done on Fock space. The mathematical language we use in this context is established in Appendix B.
We like to sketch the general structure as well as the central aspects and results of this thesis in the following sections.

2.1. General Algebraic Framework

As mentioned above, the first part of this thesis establishes an operator algebraic framework for the description of random ergodic quantum many-particle systems. The basic notions of the fertile field of operator algebras, especially C^*-algebras, are presented in Chapter 3. Due to our understanding of quantum statistical mechanics, one can think of a C^*-algebra $\mathfrak{A}$ as the algebra of operators on a Hilbert space implementing measurements on a physical system corresponding to that Hilbert space. The state of a physical system at time $t \in \mathbb{R}$ is then given by a normalised and positive linear functional $\rho_t : \mathfrak{A} \to \mathbb{C}$. In this context, another important class of objects are the morphisms between operator algebras, i.e. maps that preserve algebraic structure. For instance, automorphisms $\tau_{s,t} : \mathfrak{A} \to \mathfrak{A}$ describe the time evolution of physical systems between the times $s, t \in \mathbb{R}$ in the sense that $\rho_t = \rho_s \circ \tau_{s,t}$ holds.
In order to define a conductivity tensor, we will be interested in disturbing a many-electron system in some thermal equilibrium state via an external electric field. Therefore, we first have to specify the meaning of thermal equilibrium. In the context of C^*-dynamical systems $(\mathfrak{A}, \tau)$, where the algebra is equipped with a one parameter group of time evolution automorphisms $\{\tau_t : \mathfrak{A} \to \mathfrak{A} : t \in \mathbb{R}\}$, this is achieved by the concept of KMS states. The latter first appeared in (Kub57, MS59). Fundamentals of this field are subject to Chapter 4.
Finally, since we are interested in the description of random ergodic systems, it is necessary to introduce new concepts, which implement the property of a physical system to be random ergodic within the language of operator algebras. This is achieved in Chapter 5 via Definitions 5.1 - 5.4. The main concepts are those of covariant states and covariant automorphisms. Covariant states and covariant automorphisms are mappings $\rho : \Omega \to \mathrm{Sta}(\mathfrak{A})$, $\omega \mapsto \rho_\omega$ and $\pi : \Omega \to \mathrm{Aut}(\mathfrak{A})$, $\omega \mapsto \pi_\omega$ from a probability space Ω to the spaces $\mathrm{Sta}(\mathfrak{A})$ and $\mathrm{Aut}(\mathfrak{A})$ of states and automorphisms on the algebra $\mathfrak{A}$, respectively, which in addition satisfy a certain transformation law. In more detail, the probability space is equipped with an ergodic group of measure preserving transformations $\{\phi_a : \Omega \to \Omega : a \in \mathbb{Z}^d\}$, whereas for the operator algebra $\mathfrak{A}$ one is given a representation of $\mathbb{Z}^d$ via a group of automorphisms $\{\varphi_a : \mathfrak{A} \to \mathfrak{A} : a \in \mathbb{Z}^d\}$. The defining property of covariant states and automorphisms are the transformation laws

$$\rho_\omega = \rho_{\phi_a(\omega)} \circ \varphi_a \, , \tag{2.1}$$

$$\varphi_a \circ \pi_\omega = \pi_{\phi_a(\omega)} \circ \varphi_a \, , \tag{2.2}$$

which are satisfied for almost every $\omega \in \Omega$ and all $a \in \mathbb{Z}^d$, respectively. Clearly, it is interesting to combine these two concepts with the concept of KMS states. Then, for each realisation

$\omega \in \Omega$ of a random system one is given a C^*-dynamical system $(\mathfrak{A}, \tau_\omega)$ as defined in Definition 3.4 and those mappings $\varrho : \Omega \to \mathrm{Sta}(\mathfrak{A}),\ \omega \mapsto \varrho_\omega$ are of special interest, where in addition ϱ_ω is a (τ_ω,β)-KMS state for each $\omega \in \Omega$. Assuming uniqueness of the KMS state in each realisation $\omega \in \Omega$ of the system as well as a covariant transformation law of the time evolutions, in Theorem 5.6 we prove that ϱ is a covariant state.

2.2. Concrete Model Systems

We apply the operator algebraic approach to discrete interacting many-electron models on $\mathbb{Z}^d$. The construction of the model starts in Section 6.1, where we first construct the model on the one-electron Hilbert space $\mathfrak{h} = \ell^2(\mathbb{Z}^d)$. Randomness enters via a probability space Ω, which is equipped with an ergodic family of measure preserving transformations $\{\phi_a : a \in \mathbb{Z}^d\}$. In this situation, there are unitary shift operators $T(a)$ on $\mathfrak{h}$ defined by

$$(T(a)\psi)(x) := \mathrm{e}^{\mathrm{i}\langle a,S\,x\rangle}\psi(x-a) \tag{2.3}$$

for any $x, a \in \mathbb{Z}^d$ and $\psi \in \mathfrak{h}$, where S is some given real $d\times d$-matrix. Without any electric field being applied from outside, the random Schrödinger operator of a single electron is given by

$$H_\omega^{(\mu)} := -\Delta(\vartheta_\omega) - \mu + V_\omega\ , \tag{2.4}$$

for each $\omega \in \Omega$. The multiplication operator V_ω implements the electric interaction of the random solid state background with the electron, $\mu \in \mathbb{R}$ is the so called *chemical potential*. The magnetic Laplacian $\Delta(\vartheta_\omega)$ describes the kinetic energy of the electron as well as the influence of a random magnetic background on it. It is given by

$$(\Delta(\vartheta_\omega)\psi)(x) := -\sum_{\substack{y\in\mathbb{Z}^d,\\ |x-y|=1}} \mathrm{e}^{-\mathrm{i}\vartheta_\omega(x,y)}\ \psi(y) \tag{2.5}$$

for any $\omega \in \Omega$, $\psi \in \mathfrak{h}$ and $x \in \mathbb{Z}^d$. The random potentials V_ω and ϑ_ω are such that the Schrödinger operator becomes bounded, self-adjoint and transforms covariantly, in the sense that for any $a \in \mathbb{Z}^d$ and almost every $\omega \in \Omega$ the relation

$$T(a)H_\omega^{(\mu)}T(a)^* = H_{\phi_a(\omega)}^{(\mu)} \tag{2.6}$$

holds. A homogeneous and time dependent electric field $E : \mathbb{R} \to \mathbb{R}^d$ is applied from outside the solid state, causing a time dependence of the random Schrödinger operator itself via

$$F^{(E)}(t) := \int_{-\infty}^{t} E(r)\,\mathrm{d}r\ , \tag{2.7}$$

$$G^{(E)}(t) := \mathrm{e}^{\mathrm{i}\langle F^{(E)}(t),X\rangle}\ , \tag{2.8}$$

$$H_\omega^{(E,\mu)}(t) := G^{(E)}(t)H_\omega^{(\mu)}G^{(E)}(t)^* \tag{2.9}$$

for any $t \in \mathbb{R}$ and $\omega \in \Omega$, where X is the position operator on $\mathfrak{h}$. Furthermore, the velocity operator and, as a new concept, the current density operator of a single electron are defined as

$$D_{\omega,k}^{(E)}(t) := \frac{\mathrm{i}}{2}[H_\omega^{(E,\mu)}(t), X_k]\ , \tag{2.10}$$

$$J_{\omega,k}^{(E)}(t,y) := \{D_{\omega,k}^{(E)}(t), \chi_y\}\ , \tag{2.11}$$

respectively, for any $t \in \mathbb{R}$, $y \in \mathbb{Z}^d$, $\omega \in \Omega$ and each component $k \in \{1, ..., d\}$. Here, on the right hand side of Equation (2.10) for $k \in \{1, ..., d\}$ the k-th component of the position operator X_k appears. The right hand side of Equation (2.11) is an anti-commutator containing the characteristic function χ_y of $\{y\}$. The current density operator measures the probability of the single electron to appear at position $y \in \mathbb{Z}^d$ as well as the velocity of the electron. Note that because of the characteristic function in its definition, the current density operator does not transform covariantly.

In Section 6.2 we construct a many-particle model allowing two-electron interactions. The corresponding Hilbert spaces are the N-electron spaces $\mathfrak{F}_{N,-}(\mathfrak{h})$ and Fock space $\mathfrak{F}_{-}(\mathfrak{h})$. The interaction of the electrons is given via a mapping $\Phi : \mathbb{Z}^d \to \mathbb{R}$ which describes the pairwise interaction of two electrons. We make several assumptions on the electron pair repulsion Φ.

Assumption

(S) Φ is symmetric, i.e. $\Phi(x) = \Phi(-x)$ for all $x \in \mathbb{Z}^d$.

(C) Φ has finite support, i.e. there is an $R \geq 0$ such that $\Phi(x) = 0$ for $|x| \geq R$.

On $\mathfrak{F}_{N,-}(\mathfrak{h})$ the interaction and the total energy of N-electrons is described by the operators

$$W_{N,-} := \frac{1}{2} \sum_{\substack{m,n=1,\\ k\neq l}}^{N} \Phi(X_{N,m} - X_{N,n}) , \tag{2.12}$$

$$H^{(E,\mu)}_{\omega,N,-}(t) := \mathrm{d}\Gamma_{N,-}(H^{(E,\mu)}_{\omega}(t)) + W_{N,-} , \tag{2.13}$$

respectively, for any $\omega \in \Omega$, $N \in \mathbb{N}_0$ and $t \in \mathbb{R}$. Here, the Γ-notation as well as $X_{N,n}$ for any $N \in \mathbb{N}_0$ and $n \in \{1, ..., N\}$ express the constructions presented in the context of second quantisation in Appendix B. For each N-electron space the Schrödinger operator (2.13) has a unitary propagator $U^{(E,\mu)}_{\omega,N,-}(t, s)$, describing the time evolution of the system between the times $t, s \in \mathbb{R}$. The corresponding operators on Fock space are

$$H^{(E,\mu)}_{\omega,-}(t) := \bigoplus_{N\in\mathbb{N}_0} H^{(E,\mu)}_{\omega,N,-}(t) , \tag{2.14}$$

$$U^{(E,\mu)}_{\omega,-}(t, s) := \bigoplus_{N\in\mathbb{N}_0} U^{(E,\mu)}_{\omega,N,-}(t, s) , \tag{2.15}$$

with (2.15) being the unitary propagator induced by the Schrödinger operator (2.14). In this context, the important C^*-algebra is the Fermi algebra $\mathfrak{B}_-$ on $\mathfrak{h}$, its element of interest is the current density operator on Fock space, which is defined as

$$J^{(E)}_{\omega,k,-}(t, y) := \mathrm{d}\Gamma_{-}(J^{(E)}_{\omega,k}(t, y)) \tag{2.16}$$

for any $\omega \in \Omega$, $t \in \mathbb{R}$, $y \in \mathbb{Z}^d$ and $k \in \{1, ..., d\}$. The unitary operators in Equations (2.3), (2.8) and (2.15) induce shift automorphisms $\varphi_{a,-}$, gauge automorphisms $\gamma^{(E)}_{t,-}$ and time evolution automorphisms $\tau^{(E,\mu)}_{\omega,t,s,-}$ on $\mathfrak{B}_-$ for any $a \in \mathbb{Z}^d$, $t, s \in \mathbb{R}$ and $\omega \in \Omega$ via

$$\varphi_{a,-}(B_-) := \Gamma_-(T(a))B_-\Gamma_-(T(a))^* , \tag{2.17}$$

$$\gamma^{(E)}_{t,-}(B_-) := \Gamma_-(G^{(E)}(t))B_-\Gamma_-(G^{(E)}(t))^* , \tag{2.18}$$

$$\tau^{(E,\mu)}_{\omega,t,s,-}(B_-) := U^{(E,\mu)}_{\omega,-}(t, s)B_-U^{(E,\mu)}_{\omega,-}(s, t) \tag{2.19}$$

for any $B_- \in \mathfrak{B}_-$. The mappings $\Omega \to \mathrm{Aut}(\mathfrak{B}_-),\ \omega \mapsto \gamma^{(E)}_{t,-}$ and $\Omega \to \mathrm{Aut}(\mathfrak{B}_-),\ \omega \mapsto \tau^{(E,\mu)}_{\omega,t,s,-}$ form covariant automorphisms in the sense of Equations (2.1) and (2.2). So,

$$\varphi_{a,-} \circ \gamma^{(E)}_{t,-} = \gamma^{(E)}_{t,-} \circ \varphi_{a,-}\ , \tag{2.20}$$

$$\varphi_{a,-} \circ \tau^{(E,\mu)}_{\omega,t,s,-} = \tau^{(E,\mu)}_{\phi_a(\omega),t,s,-} \circ \varphi_{a,-} \tag{2.21}$$

holds for any $a \in \mathbb{Z}^d$ and almost every $\omega \in \Omega$. For the case of a vanishing electric field, the time evolution just depends on the difference of the times, so we write $\tau^{(\mu)}_{\omega,t-s,-}$ instead. Analogously, if there is no time dependence, we drop the electric field as well as the time as arguments in the definitions of velocity operator and current density operator. Note that the current density operator in Equation (2.16) does not transform covariantly, but in Theorems 6.12 and 6.20 we prove a similar transformation law for it. Moreover, in Theorem 6.19 we express the current density in terms of creation and annihilation operators.

Subject to Chapter 7 is the construction of the covariant state on $\mathfrak{B}_-$, which describes the electron gas. Without any external electric field present, we consider the electron gas in thermal equilibrium, i.e. in a covariant state $\varrho^{(\beta,\mu)}_- : \Omega \to \mathrm{Sta}(\mathfrak{B}_-),\ \omega \mapsto \varrho^{(\beta,\mu)}_{\omega,-}$, such that for each realisation $\omega \in \Omega$ the state $\varrho^{(\beta,\mu)}_{\omega,-}$ is a KMS state for the time evolution $\tau^{(\mu)}_{\omega,t,-}$ at inverse temperature β. Assuming uniqueness of phase and using the Banach-Alaoglu theorem, we construct such covariant KMS states in Section 7.1.

First, for each realisation $\omega \in \Omega$ separately, the existence of a $(\tau^{(\mu)}_{\omega,-},\beta)$-KMS state $\varrho^{(\beta,\mu)}_{\omega,-}$ is achieved in Theorem 7.1 concerning the special case of the interacting discrete electron model in one space dimension. Then, covariance of the mapping $\varrho^{(\beta,\mu)}_- : \Omega \to \mathrm{Sta}(\mathfrak{B}_-),\ \omega \mapsto \varrho^{(\beta,\mu)}_{\omega,-}$ is achieved in Theorem 7.5.

In addition, for the special case of a non-interacting electron gas but in arbitrary space dimension, we construct the covariant $(\tau^{(\mu)}_{\omega,-},\beta)$-KMS state piecewise in Theorems 7.2, 7.3 and 7.4. In this case, not only one obtains existence of the state, but also one may derive a concrete form of it. Namely, the state is completely determined in terms of the two-point function, which is

$$\varrho^{(\beta,\mu)}_{\omega,-}(a^*_-(\psi)a_-(\phi)) = \langle \phi, F^{(\beta)}(H^{(\mu)}_\omega)\psi \rangle\ , \tag{2.22}$$

for any $\phi, \psi \in \mathfrak{h}$, where on the left hand side fermionic creation and annihilation operators appear and on the right hand side the Fermi distribution given by

$$F^{(\beta)}(\varepsilon) = \begin{cases} (\mathrm{e}^{\beta\varepsilon}+1)^{-1} & \text{for } 0 < \beta < \infty \\ \chi_{]-\infty,0]}(\varepsilon) & \text{for } \beta = \infty \\ \quad 1 & \text{for } \beta = 0 \end{cases} \tag{2.23}$$

occurs. In any case, the time dependent covariant state of the system disturbed by a homogeneous external electric field is $\rho^{(E,\beta,\mu)}_{t,r,-} : \Omega \to \mathrm{Sta}(\mathfrak{B}_-),\ \omega \mapsto \rho^{(E,\beta,\mu)}_{\omega,t,r,-}$ given by

$$\rho^{(E,\beta,\mu)}_{\omega,t,r,-} := \varrho^{(\beta,\mu)}_{\omega,-} \circ (\tau^{(E,\mu)}_{\omega,t,r,-} \circ \gamma^{(E)}_{r,-})^{-1}\ . \tag{2.24}$$

Summing up, the idea of the operator algebraic approach is to describe the system in terms of $\varrho^{(\beta,\mu)}_{\omega,-}$, $\tau^{(E,\mu)}_{\omega,t,r,-}$ and $\gamma^{(E)}_{r,-}$ instead of $F^{(\beta)}(H^{(\mu)}_\omega)$, $U^{(E,\mu)}_{\omega,-}(t,r)$ and $G^{(E)}_-(r) := \Gamma_-(G^{(E)}(r))$.

In Chapter 8 we formally define the meaning of current density, spatial mean current density, linear response current and direct current conductivity as well as alternating current conductivity. In Definitions 8.1 and 8.4 we set

$$j_{\omega,k,r}(t,y;E,\beta,\mu) := \rho^{(E,\beta,\mu)}_{\omega,t,r,-}(J^{(E)}_{\omega,k,-}(t,y))\ , \tag{2.25}$$

$$j_r(t;E,\beta,\mu) := \mathbb{E}[j_r(t,0;E,\beta,\mu)]\ , \tag{2.26}$$

$$j(t;E,\beta,\mu) := \lim_{r\to-\infty} j_r(t;E,\beta,\mu) \tag{2.27}$$

for all $\omega \in \Omega$, $t, r \in \mathbb{R}$, $y \in \mathbb{Z}^d$ and $k \in \{1, ..., d\}$ for the current density and the spatial mean current density, respectively. A transformation law for the current density is proven in Theorem 8.2. It is the basis for Theorem 8.5 which provides a justification for the terminology spatial mean current density. Then, in Definition 8.6 the linear response current is defined formally as a derivative of the spatial mean current density with respect to the electric field. Precisely, the linear response current $j_{\text{res}}(t; E, \beta, \mu)$ at time t is given by

$$j_{\text{res}}(t; E, \beta, \mu) := \partial_\lambda j(t; \lambda E, \beta, \mu)|_{\lambda=0} \tag{2.28}$$

whenever the derivative on the right hand side exists. Then, the direct current (DC) conductivity $\sigma^{\text{DC}}(\eta, \beta, \mu)$ is defined in Definition 8.7 via

$$j_{\text{res}}(0; E^{\text{DC}}_\eta, \beta, \mu) =: \sigma^{\text{DC}}(\eta, \beta, \mu)(E) \,. \tag{2.29}$$

Here, $E^{\text{DC}}_\eta(t) := E\, \mathrm{e}^{\eta t}$ for all $t \in \mathbb{R}$ with some constant electric field $E \in \mathbb{R}^d$ and adiabatic switching parameter $\eta > 0$.
Neither the existence of the linear response current nor the existence of the conductivity tensor is guaranteed. In Chapter 9 we prove their existence for the special case of a non-interacting electron gas. In Theorems 9.1, 9.2 and 9.4 we connect our algebraic approach to the results of (BGKS05). In order to do so, we have to make the localisation assumption

$$\mathcal{X}_k(F^{(\beta)}(H^{(\mu)})) := \mathrm{i}[X_k, F^{(\beta)}(H^{(\mu)})] \in \mathcal{K}^2 \,. \tag{2.30}$$

In Theorem 9.4 we obtain an integral formula for the mean current density as in (BGKS05). Next, the linear response of the system is derived and leads to the expressions known from (BGKS05). This formula, which is presented in Theorem 9.5, suffers from the fact that it contains one-particle quantities. Therefore one cannot expect the formula to hold the same way for interacting electron gases. This is why we derive another Kubo formula for the linear response current, purely containing many-particle quantities, in Theorem 9.8. Namely, for an electron gas as described above at inverse temperature $\beta \in [0, \infty]$ with chemical potential $\mu \in \mathbb{R}$ and external electric field $E \in \mathcal{E}(\mathbb{R}, \mathbb{R}^d) := \{E \in C(\mathbb{R}, \mathbb{R}^d) : \forall t \in \mathbb{R} : \int_{-\infty}^t |E(r)|\, \mathrm{d}r < \infty\}$ for all $k \in \{1, ..., d\}$ and at time $t \in \mathbb{R}$ we have

$$j_{\text{res},k}(t; E, \beta, \mu) = \sum_{l=1}^{d} \int_{-\infty}^{t} E_l(r)\, \mathbb{E}[\varrho_-^{(\beta,\mu)}(\mathcal{X}_{l,-}(\tau^{(\mu)}_{r-t,-}(J_{k,-}(0))))]\, \mathrm{d}r \tag{2.31}$$

for the linear response current, where for $l \in \{1, ..., d\}$ the linear functional $\mathcal{X}_{l,-}$ is defined via taking the commutator of the position operator on Fock space $X_{l,-} := \mathrm{d}\Gamma_-(X_l)$. Directly from this for $k, l \in \{1, ..., d\}$ one obtains the components of the direct current (DC) conductivity at adiabatic switching $\eta > 0$

$$\sigma^{\text{DC}}_{k,l}(\eta, \beta, \mu) = \int_{-\infty}^{0} \mathrm{e}^{\eta r}\, \mathbb{E}[\varrho_-^{(\beta,\mu)}(\mathcal{X}_{l,-}(\tau^{(\mu)}_{r,-}(J_{k,-}(0))))]\, \mathrm{d}r \,. \tag{2.32}$$

Since Equations (2.31) and (2.32) only contain objects which have formal analogues for interacting quantum gases, namely $\varrho_-^{(\beta,\mu)}$, $\mathcal{X}_{l,-}$, $\tau^{(\mu)}_{r,-}$ and $J_{k,-}(0)$, one may suggest that the linear response current and the DC conductivity are the same as in Equations (2.31) and (2.32) but with the objects above replaced by the corresponding ones for the interacting system. At least, formal calculations promote this suggestion. The analysis of Chapter 10 is motivated by this idea. We explain this in more detail.

The derivation of the linear response current in Chapter 9 makes use of the localisation condition (2.30). Obviously, this localisation assumption is highly specific for non-interacting electron gases. It needs to be replaced in order to carry out a similar linear response theory for interacting electron gases. In Chapter 10 we present two approaches towards a generalisation of this localisation assumption, which we name strong and weak localisation criterion, respectively. However, we are not able to carry out a linear response theory in full generality for interacting electron gases, where the analysis is purely based on either the weak or the strong localisation criterion. Our approaches are closely related to the well-known Lieb-Robinson bounds (LR72, NS06, NS10, KGE13). First, we state the criteria.
By $f : \mathfrak{h}\times\mathfrak{h} \to [0, \infty]$, $(\phi, \psi) \mapsto \mathrm{dist}(\mathrm{supp}(\phi), \mathrm{supp}(\psi))$ we denote the support distance mapping and by $N_-(\psi) := a^*_-(\psi)a_-(\psi)$ we denote the particle number operator of $\psi \in \mathfrak{h}$. Then, an interacting system is said to satisfy the strong localisation criterion whenever there are constants $M, \varepsilon > 0$ and $\kappa > d + 1$, such that for any $t \in \mathbb{R}$ and $\phi, \psi \in \mathfrak{h}$ the following estimate holds

$$\mathbb{E}[\|[N_-(\phi), \tau^{(\mu)}_{t,-}(N_-(\psi))]\|] \leq \frac{M\ \|\phi\|^2\ \|\psi\|^2}{(1 + \varepsilon f(\phi, \psi))^\kappa}\ . \tag{2.33}$$

In Theorem 10.2, we prove that (2.33) is satisfied by any non-interacting electron gas which is totally localised, where the latter property implies the existence of constants $M', \varepsilon' > 0$ and $\kappa' > d + 1$ such that for any $t \in \mathbb{R}$ and $\phi, \psi \in \mathfrak{h}$ the following estimate holds

$$\mathbb{E}[|\langle\phi, \mathrm{e}^{-\mathrm{i}tH^{(\mu)}}\psi\rangle|] \leq \frac{M'\ \|\phi\|\ \|\psi\|}{(1 + \varepsilon' f(\phi, \psi))^{\kappa'}}\ . \tag{2.34}$$

Similarly, we say that the system satisfies the weak localisation criterion, if there are constants $M, \varepsilon > 0$ and $\kappa > d + 1$ such that for any $t \in \mathbb{R}$ and $\phi, \psi \in \mathfrak{h}$ the following estimate holds

$$\mathbb{E}[|\varrho^{(\beta,\mu)}_-([N_-(\phi), \tau^{(\mu)}_{t,-}(N_-(\psi))])|] \leq \frac{M\ \|\phi\|^2\ \|\psi\|^2}{(1 + \varepsilon f(\phi, \psi))^\kappa}\ . \tag{2.35}$$

Analogously to Theorem 10.2 for the strong localisation criterion, in Theorem 10.4, considering the weak localisation criterion, we prove that (2.35) is satisfied by any non-interacting electron gas in a region of localisation of the chemical potential $\mu \in \mathbb{R}$. The latter property states the existence of constants $M', \varepsilon' > 0$ and $\kappa' > d + 1$, such that for any $t \in \mathbb{R}$ and $\phi, \psi \in \mathfrak{h}$ the following estimate holds

$$\mathbb{E}[|\langle\phi, \chi_{]-\infty,0]}(H^{(\mu)})\mathrm{e}^{-\mathrm{i}tH^{(\mu)}}\psi\rangle|] \leq \frac{M'\ \|\phi\|\ \|\psi\|}{(1 + \varepsilon' f(\phi, \psi))^{\kappa'}}\ . \tag{2.36}$$

As mentioned above, we have not been able to carry out a linear response theory for interacting electron gases based on either the strong or the weak localisation criterion. But instead, since we suggest the linear response current of interacting electron gases to possess an analogous structure as in Equation (2.31) but with the objects $\varrho^{(\beta,\mu)}_-$, $\mathcal{X}_{l,-}$, $\tau^{(\mu)}_{r-t,-}$ and $J_{k,-}(0)$ replaced by the corresponding ones for interacting gases, in Theorem 10.5, based on the localisation criteria, for interacting electron gases we may define the quantity, called linear current by

$$j_{\mathrm{lin},k}(t; E, \beta, \mu) := \sum_{l=1}^{d} \int_{-\infty}^{t} E_l(r)\ \mathbb{E}[\varrho^{(\beta,\mu)}_-(\mathcal{X}_{l,-}(\tau^{(\mu)}_{r-t,-}(J_{k,-}(0))))]\ \mathrm{d}r\ , \tag{2.37}$$

in a sensible way for each $k \in \{1, ..., d\}$. According to the arguments mentioned above, we claim that linear current is the linear response current, whenever the latter may be derived for interacting electron gases from linear response theory, i.e. we conjecture the identity

$$j_{\mathrm{res}}(t; E, \beta, \mu) = j_{\mathrm{lin}}(t; E, \beta, \mu)\ . \tag{2.38}$$

Finally, as a check for consistency, in Theorem (10.6) we prove that this identity at least holds for the special case of a localised non-interacting electron gas. This statement is non-trivial, since the term $\mathbb{E}[\varrho_{-}^{(\beta,\mu)}(\mathcal{X}_{l,-}(\tau_{r-t,-}^{(\mu)}(J_{k,-}(0))))]$ in the integral of the Kubo formulas (2.31) and (2.37) is defined in two different ways in Chapters 9 and 10, respectively.

3 Operator Algebras

A large part of mathematics which becomes useful developed with absolutely no desire to be useful, and in a situation where nobody could possibly know in what area it would become useful; and there were no general indications that it ever would be so.

(John von Neumann)

Typically the formalism for many-electron systems is based on Fock spaces[1]. But this formalism can be identified with the language of operator algebras which is an abstract but also very powerful as well as elegant method to face the problems we have in view. This is why in this chapter we briefly introduce the language of operator algebras[2].
We define the operator algebras of interest in Section 3.1. In Section 3.2 we focus on morphisms between these algebras, i.e. mappings between different operator algebras that respect the algebraic structure. Section 3.3 is about the normalised, positive functionals on operator algebras, the so called states. The name is motivated by the fact that in quantum physics these objects, indeed, are identified with the state of a physical system.

3.1. Algebras

Definition 3.1 (*Algebras and *-Algebras*)

An *algebra* $\mathfrak{A}$ is a complex vector space equipped with a product $\mathfrak{A} \times \mathfrak{A} \to \mathfrak{A},\ (A, B) \mapsto AB$ such that for all $\alpha, \beta \in \mathbb{C}$ and all $A, B, C \in \mathfrak{A}$ the following relations are satisfied

$$A(BC) = (AB)C\ , \tag{3.1}$$
$$A(B + C) = AB + AC\ , \tag{3.2}$$
$$(\alpha A)(\beta B) = (\alpha\beta)(AB)\ . \tag{3.3}$$

A *-*algebra* $\mathfrak{A}$ is an algebra equipped with a mapping $^* : \mathfrak{A} \to \mathfrak{A},\ A \mapsto A^*$ called involution or adjoint operation such that for all $\alpha, \beta \in \mathbb{C}$ and all $A, B \in \mathfrak{A}$ the following properties are satisfied

$$(A^*)^* = A\ , \tag{3.4}$$
$$(AB)^* = B^* A^*\ , \tag{3.5}$$
$$(\alpha A + \beta B)^* = \overline{\alpha} A^* + \overline{\beta} B^*\ . \tag{3.6}$$

[1]The Fock space formalism is displayed in Appendix B.
[2]For a comprehensive overview on the topic of operator algebras we refer the reader to (BR87).

In *-algebras the so called *positive* elements are of certain interest. These are the elements $A \in \mathfrak{A}$ that are of the form $A = B^*B$ for some $B \in \mathfrak{A}$. In addition, for $A, B \in \mathfrak{A}$ such that $A - B$ is positive one writes $A \geq B$. If $A \geq B$, then for any $C \in \mathfrak{A}$ one has

$$C^*AC \geq C^*BC \,. \tag{3.7}$$

Now assume that we are given an identity element for the multiplication in the algebra $\mathfrak{A}$, i.e. an element E such that $EA = AE = A$ for all $A \in \mathfrak{A}$. This element is uniquely determined, because, if $E' \in \mathfrak{A}$ is also an identity element of $\mathfrak{A}$, we have $E = EE' = E'$. Moreover, if $\mathfrak{A}$ is a *-algebra , we have $E^*A = (A^*E)^* = (A^*)^* = A$ as well as $AE^* = (EA^*)^* = (A^*)^* = A$, so by uniqueness one obtains $E^* = E$.

Definition 3.2 (B^**-Algebras and* C^**-Algebras*)

A *Banach* **-algebra* or just B^**-algebra* is a *-algebra $\mathfrak{A}$ which is a Banach space with respect to a norm $\|\cdot\| : \mathfrak{A} \to [0, \infty[,\ A \mapsto \|A\|$ such that for all $\alpha, \beta \in \mathbb{C}$ and all $A, B \in \mathfrak{A}$ the following properties are satisfied

$$\|A\| = 0 \Leftrightarrow A = 0 \,, \tag{3.8}$$

$$\|\alpha A\| = |\alpha| \, \|A\| \,, \tag{3.9}$$

$$\|A + B\| \leq \|A\| + \|B\| \,, \tag{3.10}$$

$$\|AB\| \leq \|A\| \, \|B\| \,, \tag{3.11}$$

$$\|A^*\| = \|A\| \,. \tag{3.12}$$

A C^**-algebra* is a B^*-algebra, where in addition for all $A \in \mathfrak{A}$ the following property of the norm is satisfied

$$\|A^*A\| = \|A\|^2 \,. \tag{3.13}$$

Assume that we are given a C^*-algebra with identity element E. Then, for any $A, B \in \mathfrak{A}$ with $A \geq B \geq 0$ one has (BR87)

$$\|A\| \geq \|B\| \,, \tag{3.14}$$

$$\|A\| \, E \geq A \,, \tag{3.15}$$

$$\|A\| \, A \geq A^2 \,. \tag{3.16}$$

Moreover, from Equation (3.13) we get $\|E\| = \|EE\| = \|E^*E\| = \|E\|^2$. From this equation one obtains that either $\|E\| = 0$, so $E = 0$, or $\|E\| = 1$. But in the former case, one would get $\|A\| \leq \|AE\| \leq \|A\| \, \|E\| = 0$ for all $A \in \mathfrak{A}$, which is only possible if $\mathfrak{A} = \{0\}$. We like to exclude this situation in the following.

- A generic example of a C^*-algebra with an identity element is the set $\mathscr{B}(\mathfrak{H})$ of bounded operators on a Hilbert space $\mathfrak{H}$, where the involution is taken to be the mapping that maps an operator A to its adjoint A^* and the norm is the standard operator norm on $\mathscr{B}(\mathfrak{H})$. Thus, $\mathscr{B}(\mathfrak{H})$ is also an example of any other type of algebra introduced so far.

- A second example of a C^*-algebra is the set $C_0(X)$ of complex-valued continuous functions on a locally compact Hausdorff space X that vanish at infinity, where the algebra $C_0(X)$ is equipped with sup-norm $\|\cdot\|_\infty$ and with complex conjugation of functions as adjoint operation. This particular example also has the feature that $C_0(X)$ is a commutative C^*-algebra, so one has $fg = gf$ for all $f, g \in C_0(X)$.

3.2. Morphisms and Derivations

Definition 3.3 (*Morphisms and *-Morphisms*)

A *morphism* between two algebras $\mathfrak{A}$ and $\mathfrak{B}$ is a mapping $\pi : \mathfrak{A} \to \mathfrak{B}$ such that for all $\alpha, \beta \in \mathbb{C}$ and all $A, B \in \mathfrak{A}$ the following properties are satisfied

$$\pi(\alpha A + \beta B) = \alpha\pi(A) + \beta\pi(B) , \tag{3.17}$$

$$\pi(AB) = \pi(A)\pi(B) . \tag{3.18}$$

A *-*morphism* between two *-algebras $\mathfrak{A}$ and $\mathfrak{B}$ is a morphism $\pi : \mathfrak{A} \to \mathfrak{B}$ such that for all $A \in \mathfrak{A}$ the following property is satisfied

$$\pi(A^*) = \pi(A)^* . \tag{3.19}$$

In particular, if $\mathfrak{A}$ is a C^*-algebra and $\mathfrak{B} = \mathscr{B}(\mathfrak{h})$ for some Hilbert space $\mathfrak{h}$, one also calls a *-morphism $\pi : \mathfrak{A} \to \mathscr{B}(\mathfrak{h})$ a *-*representation* of $\mathfrak{A}$.
Obviously, any composition of morphisms or *-morphisms is a morphism or *-morphism, respectively. Of course, the image $\pi(\mathfrak{A})$ is a subalgebra or a *-subalgebra of $\mathfrak{B}$, respectively. Moreover, if $\mathfrak{A}$ has an identity element with respect to the algebra multiplication, because of $\pi(E)\pi(A) = \pi(EA) = \pi(A)$, the element $\pi(E)$ is an identity with respect to the multiplication in the algebra $\pi(\mathfrak{A})$.
Each *-morphism $\pi : \mathfrak{A} \to \mathfrak{B}$ between *-algebras $\mathfrak{A}, \mathfrak{B}$ is *positivity preserving*. This means that $\pi(A) \geq 0$ whenever $A > 0$. Positivity preservation can be seen easily, since for any $B \in \mathfrak{A}$

$$\pi(B^*B) = \pi(B^*)\pi(B) = \pi(B)^*\pi(B) .$$

In addition, if $\mathfrak{A}$ and $\mathfrak{B}$ are C^*-algebras, we get that π is continuous with $\|\pi\| \leq 1$, since for all $A \in \mathfrak{A}$ the element A^*A is self-adjoint, i.e. $(A^*A)^* = A^*A$, such that $(A^*A)^2 = (A^*A)^*(A^*A)$ is positive. From Equation (3.16) one has $0 \leq (A^*A)^2 \leq \|A^*A\|\, A^*A = \|A\|^2\, A^*A$. From positivity preservation of π one obtains

$$\begin{aligned}
\|\pi(A)\|^4 &= (\|\pi(A)\|^2)^2 = \|\pi(A)^*\pi(A)\|^2 \\
&= \|(\pi(A)^*\pi(A))^2\| = \|(\pi(A^*A))^2\| \\
&= \|\pi((A^*A)^2)\| \leq \|\pi(\|A\|^2\, A^*A)\| \\
&\leq \|A\|^2\, \|\pi(A^*A)\| = \|\pi(A^*)\pi(A)\|\, \|A\|^2 \\
&= \|\pi(A)\|^2\|A\|^2 .
\end{aligned}$$

In any case, $\pi(\mathfrak{A})$ is a C^*-algebra. If π is injective, one gets that $\pi^{-1} : \pi(\mathfrak{A}) \to \mathfrak{A}$ exists and is a *-morphism. Because of $A = \pi^{-1}(\pi(A))$ for any $A \in \mathfrak{A}$, one obtains

$$\|A\| = \|\pi^{-1}(\pi(A))\| \leq \|\pi^{-1}\|\, \|\pi(A)\| \leq \|\pi(A)\| \leq \|\pi\|\, \|A\| \leq \|A\| ,$$

leading to the fact that any injective morphism of C^*-algebras is continuous with norm $\|\pi\| = 1$.
The set of *-automorphisms of a *-algebra $\mathfrak{A}$, i.e bijective *-morphisms $\pi : \mathfrak{A} \to \mathfrak{A}$ will be denoted by $\mathrm{Aut}(\mathfrak{A})$.
Next, we are interested in mappings from a locally compact group[3] G into $\mathrm{Aut}(\mathfrak{A})$, where $\mathfrak{A}$ is a C^*-algebra.

[3] A locally compact group is a topological group equipped with a locally compact topology. A topological group is a topological space equipped with a group structure such that the group multiplication as well as the inverse operation are continuous.

Definition 3.4 (*C^*-Dynamical Systems*)

A *C^*-dynamical system* is a triple $(\mathfrak{A}, G, \alpha)$, where $\mathfrak{A}$ is a C^*-algebra, G is a locally compact group and $\alpha : G \to \mathrm{Aut}(\mathfrak{A})$, $g \mapsto \alpha_g$ is a strongly continuous representation of G in the automorphism group $\mathrm{Aut}(\mathfrak{A})$, i.e. $\alpha_g : \mathfrak{A} \to \mathfrak{A}$ is a *-automorphism for any $g \in G$ and

$$\alpha_e = \mathrm{id} , \tag{3.20}$$

$$\alpha_{g_1} \circ \alpha_{g_2} = \alpha_{g_1 g_2} , \tag{3.21}$$

where e denotes the identity element of G and $g_1, g_2 \in G$ are arbitrary. Moreover, for each $A \in \mathfrak{A}$ the mapping $G \to \mathfrak{A}$, $g \mapsto \alpha_g(A)$ is continuous with respect to the norm on $\mathfrak{A}$.

The situation we are most interested in is where the locally compact group is given by $\mathbb{R}$ equipped with the addition as a group multiplication. In this case, we write $(\mathfrak{A}, \tau)$ instead of $(\mathfrak{A}, \mathbb{R}, \tau)$ for the C^*-dynamical system. C^*-dynamical systems of this type describe the time evolution of physical systems.

There is another important class of mappings on algebras. Instead of preserving the algebraic structure, these satisfy a certain type of product rule.

Definition 3.5 (*Derivations*)

Let $\mathfrak{S}$ be a subalgebra of an algebra $\mathfrak{A}$. A mapping $\delta : \mathfrak{S} \to \mathfrak{A}$ is called a *derivation*, if it satisfies

$$\delta(\lambda A + \mu B) = \lambda\delta(A) + \mu\delta(B) , \tag{3.22}$$

$$\delta(AB) = \delta(A)B + A\delta(B) \tag{3.23}$$

for any $\lambda, \mu \in \mathbb{C}$ and $A, B \in \mathfrak{S}$. Moreover, if $\mathfrak{S}$ and $\mathfrak{A}$ are *-algebras, a derivation $\delta : \mathfrak{S} \to \mathfrak{A}$ is said to be *symmetric* whenever $\delta(A^*) = \delta(A)^*$ holds for all $A \in \mathfrak{S}$. The set of derivations on $\mathfrak{S}$ will be denoted by $\mathrm{Der}(\mathfrak{S})$.

3.3. States

Definition 3.6 (*Positive Functional*)

A linear functional $\rho : \mathfrak{A} \to \mathbb{C}$ over a *-algebra $\mathfrak{A}$ is said to be *positive*, if it is positivity preserving, i.e. if it satisfies $\rho(A^*A) \geq 0$ for all $A \in \mathfrak{A}$.

Now, if ρ is a positive linear functional over the *-algebra $\mathfrak{A}$, then for any $\beta \in \mathbb{C}$ and $A, B \in \mathfrak{A}$ one has

$$\begin{aligned} 0 &\leq \rho((A + \beta B)^*(A + \beta B)) \\ &= \rho((A^* + \overline{\beta}B^*)(A + \beta B)) \\ &= \rho(A^*A + \beta A^*B + \overline{\beta}B^*A + \overline{\beta}\beta B^*B) \\ &= \rho(A^*A) + \beta\rho(A^*B) + \overline{\beta}\rho(B^*A) + |\beta|^2\rho(B^*B) . \end{aligned}$$

Since this holds true for any $\beta \in \mathbb{C}$, positive linear functionals necessarily satisfy

$$\rho(A^*B) = \overline{\rho(B^*A)} , \tag{3.24}$$

$$|\rho(A^*B)|^2 \leq \rho(A^*A)\rho(B^*B) . \tag{3.25}$$

Lemma 3.7

Let ρ be a positive linear functional on a C^*-algebra $\mathfrak{A}$ with identity element E. Then, ρ is continuous with $\|\rho\| = \rho(E)$ and for all $A, B \in \mathfrak{A}$ one has

$$\rho(A^*) = \overline{\rho(A)} , \tag{3.26}$$

$$|\rho(A)|^2 \leq \|\rho\|\, \rho(A^*A) , \tag{3.27}$$

$$|\rho(A^*BA)| \leq \|B\|\, \rho(A^*A) . \tag{3.28}$$

Proof: For $A \in \mathfrak{A}$ arbitrary from the fact that $A^*A \leq \|A\|^2 E$ by an application of the Cauchy-Schwarz inequality (3.25) one gets that ρ is continuous with $\|\rho\| \leq \rho(E)$, because

$$|\rho(A)|^2 = |\rho(E^*A)|^2 \leq \rho(E^*E)\rho(A^*A) = \rho(E)\rho(A^*A) \leq \rho(E)\rho(\|A\|^2 E) = \|A\|^2(\rho(E))^2 .$$

But since $\|E\| = 1$, one also has $\rho(E) \leq \|\rho\|$ which proves equality. In addition, we get the Identities (3.26) and (3.27) from the Identities (3.24) and (3.25), respectively, by

$$\rho(A^*) = \rho(EA^*) = \overline{\rho(AE^*)} = \overline{\rho(AE)} = \overline{\rho(A)} ,$$

$$|\rho(A)|^2 = |\rho(E^*A)|^2 \leq \rho(E^*E)\, \rho(A^*A) = \rho(E)\, \rho(A^*A) = \|\rho\|\, \rho(A^*A).$$

Finally, from the fact that for $A, B \in \mathfrak{A}$ arbitrary one has $B^*B \leq \|B\|^2 E$. Therefore $A^*B^*BA \leq \|B\|^2 A^*A$ and one gets Equation (3.28) from

$$|\rho(A^*BA)|^2 \leq \rho(A^*A)\rho(A^*B^*BA) \leq \|B\|^2(\rho(A^*A))^2 .$$

■

Lemma 3.8

Let $\lambda, \mu \geq 0$ and ρ and η be positive linear functionals over the C^*-algebra $\mathfrak{A}$ with identity element E. Then, $\lambda\rho + \mu\eta$ is a positive linear functional and

$$\|\lambda\rho + \mu\eta\| = \lambda\|\rho\| + \mu\|\eta\| . \tag{3.29}$$

Proof: Clearly, we have that $\lambda\rho + \mu\eta$ is a linear functional and for $A \in \mathfrak{A}$ arbitrary first positivity and second Equation (3.29) follow from

$$(\lambda\rho + \mu\eta)(A^*A) = \lambda\rho(A^*A) + \mu\eta(A^*A) \geq 0 ,$$

$$\|\lambda\rho + \mu\eta\| = (\lambda\rho + \mu\eta)(E) = \lambda\rho(E) + \mu\eta(E) = \lambda\|\rho\| + \mu\|\eta\| .$$

■

Definition 3.9 (*States*)

A positive linear functional ρ over a C^*-algebra $\mathfrak{A}$ is called a *state*, if it satisfies $\|\rho\| = 1$.

Considering the set of states over a C^*-algebra $\mathfrak{A}$ with identity element E, as a direct consequence of Lemma 3.8, one has that the states form a convex subset of the bounded linear functionals on $\mathfrak{A}$. Given any states ρ and η, for all $t \in [0, 1]$ the functional $t\rho + (1 - t)\eta$ is positive and by Lemma 3.8

$$\|t\rho + (1 - t)\eta\| = (t\rho + (1 - t)\eta)(E) = t\rho(E) + (1 - t)\eta(E) = t + (1 - t) = 1 .$$

The set of states on $\mathfrak{A}$ will be denoted by $\mathrm{Sta}(\mathfrak{A})$. Any composition $\rho \circ \pi$ of a state ρ over a C^*-algebra $\mathfrak{A}$ with a *-automorphism $\pi \in \mathrm{Aut}(\mathfrak{A})$ is a state.

Description of Physical Systems

The language of operator algebras may be used for the description of physical systems in the following way (Haa92, BR87, BR97). Given a physical system, measurements are implemented by the self-adjoint elements of a C^*-algebra $\mathfrak{A}$. The latter is characteristic for the system. Often, these elements will be called *observables*. The system itself at time $t \in \mathbb{R}$ is described by a state ρ_t over $\mathfrak{A}$. Then, the states at the times $t, r \in \mathbb{R}$ are related via

$$\rho_t = \rho_r \circ \tau_{r,t} , \tag{3.30}$$

where, $\tau_{r,t} \in \mathrm{Aut}(\mathfrak{A})$ is the *-automorphism that describes the time evolution of the state. If a system is in thermal equilibrium, the time evolution just depends on the difference of the times $t, r \in \mathbb{R}$, i.e. one has

$$\tau_{r,t} = \tau_{r-t} . \tag{3.31}$$

In that case, the pair $(\mathfrak{A}, \tau)$ forms a C^*-dynamical system. In addition, there is a symmetric derivation[4] $\mathcal{H} : \mathfrak{S} \to \mathfrak{S}$ on a dense subalgebra $\mathfrak{S} = D(\mathcal{H})$ of $\mathfrak{A}$ such that

$$\tau_t(A) = \mathrm{e}^{t\mathcal{H}}(A) \tag{3.32}$$

holds for any $t \in \mathbb{R}$ and any $A \in \mathfrak{A}$. In that case, $\mathcal{H}$ will be called the *generator* of $(\mathfrak{A}, \tau)$. So far we have not explained rigorously the meaning of the term thermal equilibrium. But the following chapter focuses on this situation.

Remarks

At the end of Section 3.1 we gave two examples of C^*-algebras. In fact, one can show that any C^*-algebra $\mathfrak{A}$ can be identified with a norm closed subalgebra of $\mathscr{B}(\mathfrak{H})$ for some Hilbert space $\mathfrak{H}$. In addition, one can also show that every commutative C^*-algebra can be identified with a norm closed subalgebra of $C_0(X)$ for some locally compact Hausdorff space X. Both identifications are the statement of a theorem by Israel Gelfand and Mark Naimark (GN43). They are closely related to what is known as GNS construction[5]. The latter was achieved by Irving **S**egal (Seg47) as a refinement of the work by **G**elfand and **N**aimark.

Assumption

All algebras in subsequent chapters of this thesis will be separable C^*-algebras with identity element. Because of this, we will eventually denote *-morphisms just as morphisms. Moreover, the identity element eventually will be identified with the complex identity. Redundantly for the identity element we use the notation

$$1 = \mathbb{1} = \mathrm{id} . \tag{3.33}$$

[4]The operator $\mathcal{L} := -\mathrm{i}\mathcal{H}$ is also called the *Liouville operator* or just *Liouvillian* of the system (BGKS05, KLM07, KM08).

[5]For comprehensive overviews on that topic see (BR87, Wer11).

4 KMS States

Diese spekulative Unterscheidung von Gleichgewicht, Spannung und Bewegung ist wesentlicher für das praktische Handeln, als es auf den ersten Augenblick scheinen möchte. Im Zustand der Ruhe und des Gleichgewichts kann mancherlei Tätigkeit herrschen, nämlich die, welche bloß von Gelegenheitsursachen und nicht von dem Zweck einer großen Veränderung ausgeht.

(Carl von Clausewitz)

The starting point of linear response theory is a physical system in thermal equilibrium. Physical systems are described by states. But, of course, not every state describes a physical system in thermal equilibrium. Typically, there are many other possible configurations of a physical system than thermal equilibrium which have to be described by states as well. So, there is a request to characterise the thermal equilibrium states of a physical system by a property additional to the one of being a state. This is done by the concept of KMS condition named after Ryogo **K**ubo, Paul **M**artin and Julian **S**chwinger[1]. The present chapter focuses on the states satisfying this condition, the so called KMS states.

KMS states can be characterised in many different equivalent ways. We choose one of these characterisations for definition. However, having certain problems, such as thermodynamical limits in view, one of the equivalent characterisations may be more natural to use or have technical advantages compared to the other characterisations. This is why, after giving a definition of KMS states, we also state an alternative characterisation in Theorem 4.2.

After the rather technical definition and the alternative characterisations of KMS states we motivate these states as the right description of systems in thermal equilibrium. The first motivation is the fact that for systems described by KMS states the expectation values of observables are time independent whenever the observables do not depend on time. This is the statement of Theorem 4.4.

The second motivation is given by the generic example of KMS states. We will present this in a subsequent section to Theorem 4.4. It relates KMS states to a certain type of density matrices that most mathematical physicists are much more familiar with than with the concept of KMS states.

Moreover, in Section 4.4 we focus on convergence properties of sequences of KMS states. These play a key-role for the construction of KMS states for thermal systems. This is the central idea used in Chapter 7. More specifically, in Chapter 7 for a concrete model of an interacting electron gas on a lattice in dimension $d = 1$ we construct KMS states. For the same model in arbitrary dimension $d \in \mathbb{N}$ but without interaction we also construct KMS states.

[1] Kubo was the first to introduce the condition in 1957 in (Kub57). In 1959 Martin and Schwinger used the KMS condition in (MS59). The name KMS condition first appeared in 1967 in (HHW67). A detailed overview on the topic is given in (BR97).

4.1. Characterisation

First, we introduce strips of width β above or below the real axis in $\mathbb{C}$, since we need them for our definition of KMS states. For $\beta \in \mathbb{R}$ we set $\mathfrak{C}_\beta := \{z \in \mathbb{C} : \min(0,\beta) < \mathrm{Im}(z) < \max(0,\beta)\}$. Moreover, for $\beta \in \mathbb{R} \setminus \{0\}$ we define $\mathfrak{D}_\beta$ to be the closure of $\mathfrak{C}_\beta$. For $\beta = 0$ we set $\mathfrak{D}_\beta := \mathbb{R}$.

Definition 4.1 (*KMS States*)

Let $\beta \in \mathbb{R}$ and $(\mathfrak{A}, \tau)$ be a C^*-dynamical system. A state $\varrho^{(\beta)}$ over $\mathfrak{A}$ is called (τ,β)-*KMS state*, if for all $A, B \in \mathfrak{A}$ there exists a continuous function $F_{A,B} : \mathfrak{D}_\beta \to \mathbb{C}$ which is analytic on $\mathfrak{C}_\beta$ such that for all $t \in \mathbb{R}$

$$F_{A,B}(t) = \varrho^{(\beta)}(A\tau_t(B)) \,, \tag{4.1}$$

$$F_{A,B}(t + \mathrm{i}\beta) = \varrho^{(\beta)}(\tau_t(B)A) \,. \tag{4.2}$$

Since for all $t \in \mathbb{R}$ one has $|F_{A,B}(t)| \leq \|A\| \, \|B\|$ and $|F_{A,B}(t + \mathrm{i}\beta)| \leq \|A\| \, \|B\|$, the function $F_{A,B}$ is bounded on $\mathfrak{D}_\beta \setminus \mathfrak{C}_\beta$. As an immediate consequence from Hadamard's three-lines theorem (RS75) one obtains $|F_{A,B}(z)| \leq \|A\| \, \|B\|$ for all $z \in \mathfrak{D}_\beta$. Thus, in the definition of KMS states the term continuous could be replaced by bounded and continuous.
Let $f : \mathbb{R} \to \mathbb{C}$ be a function with Fourier transform $\hat{f} := \mathscr{F}(f) \in C_c^\infty(\mathbb{R})$. More precisely, let $\mathrm{supp}(\hat{f}) \subset [-a, a]$ for some $a > 0$. An application of the Paley-Wiener theorem (Rud87) yields that there is an entire analytic extension of f which is given by

$$f(z) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{f}(p) \, \mathrm{e}^{\mathrm{i}pz} \, \mathrm{d}p \tag{4.3}$$

for $z \in \mathbb{C}$. In addition, for any $n \in \mathbb{N}$ there is a constant C_n such that the following estimate is satisfied for all $z \in \mathbb{C}$

$$|f(z)| \leq C_n \, \frac{\mathrm{e}^{a|\mathrm{Im}(z)|}}{(1 + |z|)^n} \,. \tag{4.4}$$

Now we are able to state the second alternative characterisation of KMS states, which is of interest especially in view of thermodynamic limits. Detailed proof of Theorem 4.2 can be found in (BR97, HHW67).

Theorem 4.2 (*Alternative Characterisation of KMS States*)

Let $\beta \in \mathbb{R}$ and $(\mathfrak{A}, \tau)$ be a C^*-dynamical system. A state $\varrho^{(\beta)}$ over $\mathfrak{A}$ is a (τ,β)-KMS state if and only if for all $A, B \in \mathfrak{A}$ and all f with $\hat{f} \in C_c^\infty(\mathbb{R})$ one has

$$\int_{\mathbb{R}} f(t) \, \varrho^{(\beta)}(A\tau_t(B)) \, \mathrm{d}t = \int_{\mathbb{R}} f(t + \mathrm{i}\beta) \, \varrho^{(\beta)}(\tau_t(B)A) \, \mathrm{d}t \,. \tag{4.5}$$

Proof : Let $f \in \mathscr{S}(\mathbb{R})$ with $\hat{f} \in C_c^\infty(\mathbb{R})$, $\varrho^{(\beta)}$ be a (τ,β)-KMS state and $A, B \in \mathfrak{A}$. Then, $z \mapsto f(z) \, F_{A,B}(z)$ defines a bounded analytic function on $\mathfrak{C}_\beta$, continuous on $\mathfrak{D}_\beta$ and, provided $|\mathrm{Im}(z)| \leq \beta$, we obtain $\lim_{|\mathrm{Re}(z)| \to \infty} z^2 f(z) \, F_{A,B}(z) = 0$. An application of the Cauchy theorem yields

$$\begin{aligned}
\int_{\mathbb{R}} f(t) \, \varrho^{(\beta)}(A\tau_t(B)) \, \mathrm{d}t &= \int_{\mathbb{R}} f(t) \, F_{A,B}(t) \, \mathrm{d}t \\
&= \int_{\mathbb{R}} f(t + \mathrm{i}\beta) \, F_{A,B}(t + \mathrm{i}\beta) \, \mathrm{d}t \\
&= \int_{\mathbb{R}} f(t + \mathrm{i}\beta) \, \varrho^{(\beta)}(\tau_t(B)A) \, \mathrm{d}t \,.
\end{aligned}$$

Now assume that $A, B \in \mathfrak{A}$ and that Equation (4.5) holds for any $f \in \mathscr{S}(\mathbb{R})$ with $\hat{f} \in C_c^\infty(\mathbb{R})$. Then, for $t \in \mathbb{R}$ we define $F_{A,B}(t) := \varrho^{(\beta)}(A\tau_t(B))$ and $G_{A,B}(t) := \varrho^{(\beta)}(\tau_t(B)A)$. The functions $F_{A,B}$ and $G_{A,B}$ as well as their Fourier transforms $\hat{F}_{A,B}$ and $\hat{G}_{A,B}$ can be considered as distributions on $\mathscr{S}(\mathbb{R})$. Since $F_{A,B}$ and $G_{A,B}$ are bounded and continuous, from Equation (4.5) we get that

$$\hat{F}_{A,B}(p) = e^{\beta p}\hat{G}_{A,B}(p) \tag{4.6}$$

in the sense of distributions on $C_c^\infty(\mathbb{R})$. Since $C_c^\infty(\mathbb{R})$ is a totalising subset of $\mathscr{S}(\mathbb{R})$, Equation (4.6) even holds in the sense of distributions on $\mathscr{S}(\mathbb{R})$. This implies that via a Laplace transform $F_{A,B}$ can be extended to a function that is analytic on $\mathfrak{C}_\beta$ and continuous on $\mathfrak{D}_\beta$ (SW80). Analogously, $G_{A,B}$ can be extended to a function that is analytic on $\mathfrak{C}_{-\beta}$ and continuous on $\mathfrak{D}_{-\beta}$. From the definition of $F_{A,B}$, the Cauchy theorem and the fact that Equation (4.5) holds for any $f \in \mathscr{S}(\mathbb{R})$ with $\hat{f} \in C_c^\infty(\mathbb{R})$ we get that for all $t \in \mathbb{R}$

$$\begin{aligned} F_{A,B}(t) &= \varrho^{(\beta)}(A\tau_t(B))\,, \\ F_{A,B}(t + i\beta) &= G_{A,B}(t) = \varrho^{(\beta)}(\tau_t(B)A)\,. \end{aligned}$$

■

Definition 4.3 (*Ground States and Ceiling States*)

Let $(\mathfrak{A}, \tau)$ be a C^*-dynamical system with $\mathcal{H}$ being the generator of τ. A state ϱ over $\mathfrak{A}$ is called a τ *ground state* or alternatively a (τ, ∞)-KMS state, if for all $A \in D(\mathcal{H})$

$$-i\varrho(A^*\mathcal{H}(A)) \geq 0\,. \tag{4.7}$$

Similarly, a state ϱ over $\mathfrak{A}$ is called a τ *ceiling state* or alternatively a $(\tau, -\infty)$-KMS state, if for all $A \in D(\mathcal{H})$

$$i\varrho(A^*\mathcal{H}(A)) \geq 0\,. \tag{4.8}$$

4.2. Generic Property

A reason for the fact that the KMS condition provides the right characterisation of thermal equilibrium is that the quantum mechanical expectation value of measurements of explicitly time independent quantities for systems described by a KMS state is time independent. The precise statement is the content of the following theorem (BR87)[Proposition 5.3.3.].

Theorem 4.4 (*Generic Property*)

Let $\beta \in \mathbb{R} \setminus \{0\}$ and $(\mathfrak{A}, \tau)$ be a C^*-dynamical system. Moreover, let $\varrho^{(\beta)}$ be a (τ, β)-KMS state over the C^*-algebra $\mathfrak{A}$. Then, $\varrho^{(\beta)}$ is τ-invariant, i.e. for all $A \in \mathfrak{A}$ and $t \in \mathbb{R}$ one has

$$\varrho^{(\beta)}(\tau_t(A)) = \varrho^{(\beta)}(A)\,. \tag{4.9}$$

Proof: Let $A \in \mathfrak{A}$ be arbitrary. Then, the KMS condition for the special case that $B = \mathbb{1}$, states that $F_A(t) := F_{B,A}(t) = \varrho^{(\beta)}(\tau_t(A)) = F_A(t + i\beta)$, i.e. F_A is periodic. Moreover, $|F_A|$ is bounded by $\|A\|$. One can extend F_A to a bounded function, that is holomorphic on $\mathbb{C}$ except for the lines $L_{n,\beta} = \{t + in\beta : t \in \mathbb{R}\}$ for $n \in \mathbb{Z}$, where F_A only is continuous. By an application of Morera's theorem (FL08) one concludes that F_A is a bounded entire function. From Liouville's theorem we get that it is constant. In particular, one has $\varrho^{(\beta)}(\tau_t(A)) = F_A(t) = F_A(0) = \varrho^{(\beta)}(A)$ for all $t \in \mathbb{R}$. ■

4.3. Generic Example

Generic Example for Positive Temperature

Typically, confined systems in thermal equilibrium are described by a self-adjoint Hamilton operator H on a Hilbert space $\mathfrak{H}$ such that the operator $\mathrm{e}^{-\beta H}$ is trace class for all $\beta \in]0, \infty[$. In this situation, one can define

$$P^{(\beta)} := \frac{\mathrm{e}^{-\beta H}}{\mathrm{Tr}(\mathrm{e}^{-\beta H})}\,, \tag{4.10}$$

$$\varrho^{(\beta)}(A) := \mathrm{Tr}(BP^{(\beta)}) = \frac{\mathrm{Tr}(A\mathrm{e}^{-\beta H})}{\mathrm{Tr}(\mathrm{e}^{-\beta H})} \tag{4.11}$$

for $B \in \mathfrak{B} := \mathscr{B}(\mathfrak{H})$. Then, $\varrho^{(\beta)}$ is a state on the C^*-algebra $\mathfrak{B}$ for the fact that $P^{(\beta)}$ is a positive operator and normalised in trace norm, i.e. $P^{(\beta)}$ is a density matrix. States induced by density matrices are called *normal*. Moreover, one obtains a one parameter group of automorphisms τ_t on $\mathfrak{B}$ via

$$\tau_t(B) := \mathrm{e}^{\mathrm{i}tH} B \mathrm{e}^{-\mathrm{i}tH} \tag{4.12}$$

for arbitrary $t \in \mathbb{R}$ and $B \in \mathfrak{B}$. For $A, B \in \mathfrak{B}$ we define a function $F_{A,B}$ of the complex variable $z = t + \mathrm{i}\sigma$ by

$$F_{A,B}(z) := \frac{\mathrm{Tr}\left(A\mathrm{e}^{-\sigma H}\mathrm{e}^{\mathrm{i}tH} B \mathrm{e}^{-\mathrm{i}tH}\mathrm{e}^{-(\beta-\sigma)H}\right)}{\mathrm{Tr}(\mathrm{e}^{-\beta H})}\,. \tag{4.13}$$

This is a continuous function defined on $\mathfrak{D}_\beta$, analytic on $\mathfrak{C}_\beta$ and at least formally given by $F_{A,B}(z) = \varrho^{(\beta)}(A\tau_z(B))$. From Equation (4.13) and cyclicity one obtains $F_{A,B}(t) = \varrho^{(\beta)}(A\tau_t(B))$ and $F_{A,B}(t + \mathrm{i}\beta) = \varrho^{(\beta)}(\tau_t(B)A)$ for all $t \in \mathbb{R}$. Thus, $\varrho^{(\beta)}$ is a (τ,β)-KMS state.
Conversely, assume that we are given a C^*-dynamical system $(\mathfrak{B}, \tau)$ where $\mathfrak{B} := \mathscr{B}(\mathfrak{H})$ is the algebra of bounded operators on a Hilbert space $\mathfrak{H}$ and τ_t is given by $\tau_t(B) = \mathrm{e}^{\mathrm{i}tH} B\mathrm{e}^{-\mathrm{i}tH}$ for some self-adjoint operator H on $\mathfrak{H}$ with discrete spectrum such that $\mathrm{e}^{-\beta H}$ is trace class for $\beta \in]0, \infty[$. Moreover, assume that $\varrho^{(\beta)}$ is a normal state on $\mathfrak{B}$, i.e. one has $\varrho^{(\beta)}(B) = \mathrm{Tr}(P^{(\beta)}B)$ for some density matrix $P^{(\beta)}$. In this situation, whenever $\varrho^{(\beta)}$ is a (τ,β)-KMS state its density matrix $P^{(\beta)}$ is given by Equation (4.10).
We give a heuristic justification (Haa92, HHW67). Let $A \in \mathfrak{B}$ be arbitrary and $B \in \mathfrak{B}$ be an arbitrary element that commutes with $\mathrm{e}^{\mathrm{i}tH}$ for all $t \in \mathbb{R}$. From $\tau_t(B) = \mathrm{e}^{\mathrm{i}tH} B\mathrm{e}^{-\mathrm{i}tH} = B$ for all $t \in \mathbb{R}$ we get $\varrho^{(\beta)}(A\tau_t(B)) = \varrho^{(\beta)}(AB)$ so that $F_{A,B}(z)$ becomes independent of $z \in \mathfrak{D}_\beta$. In particular, $F_{A,B}(t) = F_{A,B}(t + \mathrm{i}\beta)$ for all $t \in \mathbb{R}$ so that

$$\begin{aligned}
0 &= F_{A,B}(t + \mathrm{i}\beta) - F_{A,B}(t)\\
&= \varrho^{(\beta)}(\tau_t(B)A) - \varrho^{(\beta)}(A\tau_t(B))\\
&= \varrho^{(\beta)}(BA) - \varrho^{(\beta)}(AB)\\
&= \mathrm{Tr}(P^{(\beta)}BA) - \mathrm{Tr}(P^{(\beta)}AB)\\
&= \mathrm{Tr}(P^{(\beta)}BA) - \mathrm{Tr}(BP^{(\beta)}A)\\
&= \mathrm{Tr}([P^{(\beta)}, B]A)\,.
\end{aligned}$$

Since this holds true for all $A \in \mathfrak{B}$, one obtains $[P^{(\beta)}, B] = 0$ for all $B \in \mathfrak{B}$ that commute with all $\mathrm{e}^{\mathrm{i}tH}$ for all $t \in \mathbb{R}$. From this one concludes that $P^{(\beta)} = F(H)$ for some function F on $\mathbb{R}$.

That this function is of the form $F(x) = C\mathrm{e}^{-\beta x}$ for some $C > 0$ follows from a special choice of $A, B \in \mathfrak{B}$. Let $\psi_k, \psi_l \in \mathfrak{H}$ be arbitrary vectors of an orthonormal basis $(\psi_n)_{n\in\mathbb{N}}$ of $\mathfrak{H}$ consisting of eigenvectors of H and let $\varepsilon_k, \varepsilon_l \in \mathbb{R}$ be the corresponding eigenvalues. We choose $A = P_{\psi_k,\psi_l}$ and $B = P_{\psi_l,\psi_k}$ where $P_{\phi,\psi}(\eta) := \phi\langle\psi, \eta\rangle$ for all $\phi, \psi, \eta \in \mathfrak{H}$. Then, for any $t \in \mathbb{R}$

$$\begin{aligned}
\varrho^{(\beta)}(A\tau_t(B)) &= \mathrm{Tr}(P^{(\beta)}A\tau_t(B)) \\
&= \sum_{n\in\mathbb{N}} \langle\psi_n, F(H)P_{\psi_k,\psi_l}\mathrm{e}^{\mathrm{i}tH}P_{\psi_l,\psi_k}\mathrm{e}^{-\mathrm{i}tH}\psi_n\rangle \\
&= \sum_{n\in\mathbb{N}} \langle\psi_n, F(\varepsilon_k)\psi_k\rangle\, \langle\psi_l, \mathrm{e}^{\mathrm{i}t\varepsilon_l}\psi_l\rangle\, \langle\psi_k, \mathrm{e}^{-\mathrm{i}t\varepsilon_n}\psi_n\rangle \\
&= \sum_{n\in\mathbb{N}} \mathrm{e}^{\mathrm{i}t(\varepsilon_l-\varepsilon_n)}F(\varepsilon_k)\, \langle\psi_n, \psi_k\rangle\langle\psi_l, \psi_l\rangle\, \langle\psi_k, \psi_n\rangle \\
&= \mathrm{e}^{\mathrm{i}t(\varepsilon_l-\varepsilon_k)}F(\varepsilon_k)\,.
\end{aligned}$$

Analogously, one shows that $\varrho^{(\beta)}(\tau_t(B)A) = \mathrm{e}^{\mathrm{i}t(\varepsilon_l-\varepsilon_k)}F(\varepsilon_l)$. So, the function one has to look at is given by $F_{A,B}(z) = \mathrm{e}^{\mathrm{i}z(\varepsilon_l-\varepsilon_k)}F(\varepsilon_k)$ for $z \in \mathfrak{D}_\beta$ and the KMS condition is satisfied if $\mathrm{e}^{-\beta(\varepsilon_l-\varepsilon_k)}\mathrm{e}^{\mathrm{i}t(\varepsilon_l-\varepsilon_k)}F(\varepsilon_k) = F_{A,B}(t + \mathrm{i}\beta) = \mathrm{e}^{\mathrm{i}t(\varepsilon_l-\varepsilon_k)}F(\varepsilon_l)$. Thus, $\mathrm{e}^{\beta\varepsilon_k}F(\varepsilon_k) = \mathrm{e}^{\beta\varepsilon_l}F(\varepsilon_l)$ which implies $F(x) = C\mathrm{e}^{-\beta x}$ for all $x \in \mathbb{R}$. Finally, $C = (\mathrm{Tr}(\mathrm{e}^{-\beta H}))^{-1}$ follows from $\varrho(\mathbb{1}) = 1$.

So for confined systems the notion of KMS state is equivalent to normal states with density matrices $P^{(\beta)}$ as in Equation (4.10). Of course, in the above situation $\mathrm{e}^{-\beta H}$ has to be a trace class operator. But this typically does not hold for extended systems.

This demonstrates the brilliant idea behind the concept of KMS condition. Even if $\mathrm{e}^{-\beta H}$ is no trace class operator, say, because the system described by the Hamiltonian H on the Hilbert space $\mathfrak{H}$ is an extended one, the system still may be described by an equilibrium state $\varrho^{(\beta)}$, i.e. a normalised, positive and linear functional on the algebra $\mathfrak{B} = \mathscr{B}(\mathfrak{H})$, and time translation automorphisms τ_t given by $\tau_t(B) := \mathrm{e}^{\mathrm{i}tH}B\mathrm{e}^{-\mathrm{i}tH}$. In general this state will not be normal, i.e. $\varrho^{(\beta)}$ will not be given by a density matrix P, so that the system in equilibrium at inverse temperature β cannot be characterised by a density matrix as in Equation (4.10). However, the state $\varrho^{(\beta)}$ still may be a (τ, β)-KMS state, since the KMS condition avoids the language of density matrices.

Generic Example for Ground States

We illustrate the basic idea behind the concept of ground states in Definition 4.3. For simplicity we consider a system described by a bounded Hamilton operator H on a Hilbert space $\mathfrak{H}$ with discrete spectrum $\sigma(H) \subset \mathbb{R}$. Let $\varepsilon_0 := \inf(\sigma(H))$ be the lowest eigenvalue of the spectrum of H and let $\psi_0 \in \mathfrak{H}$ be a corresponding normalised eigenvector. On the C^*-algebra $\mathfrak{B} := \mathscr{B}(\mathfrak{H})$ we consider the state ϱ defined by

$$\varrho(B) := \langle\psi_0, B\psi_0\rangle \tag{4.14}$$

for all $B \in \mathfrak{B}$. Common understanding of quantum mechanics dictates that ϱ as defined above should be the generic candidate for a ground state of the system. Indeed, it is a ground state in the sense of Definition 4.3 as we will explain in more detail. Analogously to Equation (4.12) the time evolution τ of the system is given by

$$\tau_t(B) := \mathrm{e}^{\mathrm{i}tH}B\mathrm{e}^{-\mathrm{i}tH} \tag{4.15}$$

for all $t \in \mathbb{R}$ and $B \in \mathfrak{B}$. Then, the generator $\mathcal{H}$ of the time evolution τ is defined on the full algebra $\mathfrak{B}$ and is given by

$$\mathcal{H}(B) := \mathrm{i}[H, B] \tag{4.16}$$

for all $B \in \mathfrak{B}$. We show that ϱ is a τ ground state in the sense of Definition 4.3. Since ψ_0 is a normalised eigenvector of H corresponding to eigenvalue ε_0, for all $B \in \mathfrak{B}$ one obtains

$$\begin{aligned} -\mathrm{i}\varrho(B^*\mathcal{H}(B)) &= \langle \psi_0, B^*[H,B]\psi_0\rangle \\ &= \langle B\psi_0, HB\psi_0\rangle - \langle B\psi_0, BH\psi_0\rangle \\ &= \langle B\psi_0, HB\psi_0\rangle - \varepsilon_0\langle B\psi_0, B\psi_0\rangle \\ &= \langle B\psi_0, (H-\varepsilon_0)B\psi_0\rangle \, . \end{aligned}$$

Clearly, in the calculation above the right hand side is non-negative, since ε_0 is the infimum of the spectrum of $\mathfrak{H}$, so $(H - \varepsilon_0)$ is a positive operator. So indeed, ϱ as given by Equation (4.14) defines a ground state in the sense of Definition 4.3 for the time evolution τ as given by Equation (4.15). In an analogous way one constructs the generic example of a τ ceiling state.

4.4. Convergence Properties

For the construction of KMS states for concrete model systems in subsequent chapters we will use the following theorem (BR97)[Proposition 5.3.25.]. We consider a situation, where one is given a sequence of time evolutions $(\tau_n)_{n\in\mathbb{N}}$ on some C^*-algebra $\mathfrak{A}$. In more detail, for each $n \in \mathbb{N}$ the mapping $\tau_n : \mathbb{R} \to \mathrm{Aut}(\mathfrak{A})$, $t \mapsto \tau_{n,t}$ forms a strongly continuous one-parameter group of automorphisms of $\mathfrak{A}$. Moreover, for each time $t \in \mathbb{R}$ in the sense of strong operator topology on $\mathrm{Aut}(\mathfrak{A})$ the sequence $(\tau_{n,t})_{n\in\mathbb{N}}$ is supposed to converge to τ_t, the values of a one-parameter group $\tau : \mathbb{R} \to \mathrm{Aut}(\mathfrak{A})$, $t \mapsto \tau_t$ on $\mathfrak{A}$.

Theorem 4.5 (*Convergence of Sequences of KMS States*)

Let $\mathfrak{A}$ be a C^*-algebra, and $(\tau_n)_{n\in\mathbb{N}}$ be a sequence of strongly continuous one-parameter groups of automorphisms of $\mathfrak{A}$ converging strongly to a one-parameter group τ, i.e.

$$\lim_{n\to\infty} \|\tau_{n,t}(A) - \tau_t(A)\| = 0 \tag{4.17}$$

for each $t \in \mathbb{R}$ and $A \in \mathfrak{A}$. Moreover, let $\beta \in [-\infty, \infty]$ and $(\beta_n)_{n\in\mathbb{N}}$ be a sequence in $[-\infty, \infty]$ with

$$\lim_{n\to\infty} \beta_n = \beta \, .$$

Assume that for each $n \in \mathbb{N}$ there exists a (τ_n, β_n)-KMS state $\varrho^{(\beta_n)}$ on $\mathfrak{A}$. It follows that each weak*-limit point $\varrho^{(\beta)}$ of the sequence $(\varrho^{(\beta_n)})_{n\in\mathbb{N}}$ is a (τ, β)-KMS state on $\mathfrak{A}$.

Proof: We only prove the statement for $\beta \in \mathbb{R}$. A complete proof of the theorem including the cases $\beta \in \{-\infty, \infty\}$ can be found in (BR97, HHW67). We may assume that $(\beta_n)_{n\in\mathbb{N}}$ is a bounded sequence in $\mathbb{R}$. Let $\varrho^{(\beta)}$ be a weak*-limit point of $(\varrho^{(\beta_n)})_{n\in\mathbb{N}}$, i.e. there exists a subsequence $(\varrho^{(\beta_{n_k})})_{k\in\mathbb{N}}$, such that for all $A \in \mathfrak{A}$ we have $\lim_{k\to\infty} \varrho^{(\beta_{n_k})}(A) = \varrho^{(\beta)}(A)$. Then, because of the strong convergence of $(\tau_{n,t})_{n\in\mathbb{N}}$ to τ_t for any given $A, B \in \mathfrak{A}$, we have

$$\lim_{k\to\infty} \|A\tau_{n_k,t}(B) - A\tau_t(B)\| = \lim_{k\to\infty} \|\tau_{n_k,t}(B)A - \tau_t(B)A\| = 0 \, .$$

Because of the weak*-convergence of the sequence $(\varrho^{(\beta_{n_k})})_{k\in\mathbb{N}}$ to $\varrho^{(\beta)}$ and the fact that $\varrho^{(\beta_n)}$ is a state for each $n \in \mathbb{N}$, which implies $\|\varrho^{(\beta_n)}\| = 1$, we have

$$\begin{aligned} \lim_{k\to\infty} \varrho^{(\beta_{n_k})}(A\tau_{n_k,t}(B)) &= \varrho^{(\beta)}(A\tau_t(B)) \, , \\ \lim_{k\to\infty} \varrho^{(\beta_{n_k})}(\tau_{n_k,t}(B)A) &= \varrho^{(\beta)}(\tau_t(B)A) \, . \end{aligned}$$

In addition, one has $|\varrho^{(\beta_{n_k})}(A\tau_{n_k,t}(B))| \leq \|A\|\,\|B\|$ as well as $|\varrho^{(\beta_{n_k})}(\tau_{n_k,t}(B)A)| \leq \|A\|\,\|B\|$. Let $f \in \mathscr{S}(\mathbb{R})$ be a function with $\hat{f} \in C_c^\infty(\mathbb{R})$. Then, from dominated convergence theorem, which applies due to the fact that f satisfies the estimate (4.4), for each $A, B \in \mathfrak{A}$ we get[2]

$$\begin{aligned}
\int_{\mathbb{R}} f(t)\, \varrho(A\tau_t(B))\, \mathrm{d}t &= \int_{\mathbb{R}} \lim_{k\to\infty} f(t)\, \varrho^{(\beta_{n_k})}(A\tau_{n_k,t}(B))\, \mathrm{d}t \\
&= \lim_{k\to\infty} \int_{\mathbb{R}} f(t)\, \varrho^{(\beta_{n_k})}(A\tau_{n_k,t}(B))\, \mathrm{d}t \\
&= \lim_{k\to\infty} \int_{\mathbb{R}} f(t+\mathrm{i}\beta_{n_k})\, \varrho^{(\beta_{n_k})}(\tau_{n_k,t}(B)A)\, \mathrm{d}t \\
&= \int_{\mathbb{R}} \lim_{k\to\infty} f(t+\mathrm{i}\beta_{n_k})\, \varrho^{(\beta_{n_k})}(\tau_{n_k,t}(B)A)\, \mathrm{d}t \\
&= \int_{\mathbb{R}} f(t+\mathrm{i}\beta)\, \varrho^{(\beta)}(\tau_t(B)A)\, \mathrm{d}t\,.
\end{aligned}$$

Since this holds for any $f \in \mathscr{S}(\mathbb{R})$ with $\hat{f} \in C_c^\infty(\mathbb{R})$, from Theorem 4.2 we get that $\varrho^{(\beta)}$ is a (τ,β)-KMS state. ■

[2]The function f is extended to an entire function by Equation (4.3). The extended function is also denoted by f.

5 Ergodic Systems

The human story does not always unfold like a mathematical calculation on the principle that two and two make four. Sometimes in life they make five or minus three; and sometimes the blackboard topples down in the middle of the sum and leaves the class in disorder and the pedagogue with a black eye.

(Winston Churchill)

Materials that appear in nature are not ideal in the sense that the atomic structure be given by a perfectly periodic crystal. In the latter case, the atomic structure of a sample could be known completely, at least in principle. Reality confronts us with the fact that solid states may have impurities or may be alloys of different materials. Even the case of amorphous materials that have no periodic structure at all, such as glasses, may appear. In these cases, the atomic structure of a given sample of a material is known only on average. For example, one knows the ratios of the constituent pure materials of a given alloy.

Therefore, we want to cover disordered materials by our model. This is done by considering all possible configurations of the atomic structure of a given sample of a solid state as well as the probability of these configurations. On the mathematical level this is done by identifying each configuration with an element ω of a probability space Ω.

Despite the fact that the exact atomic structure of a given material cannot be known completely, we would expect certain quantities, such as electric and thermal conductivity, to be independent of the exact realisation, i.e. two samples of the same mixture of glass should also have the same electrical conductivity even though they certainly will not be exact duplicates up to the level of their atomic structure.

On the mathematical side, this phenomenon, which is dictated by common sense, is a result of an application of Birkhoff's theorem from ergodic theory. The latter applies, since we consider materials that possess a certain type of disorder. More concretely, we consider solid states, where in each neighbourhood of any point the disorder looks the same on average over all possible realisations.

This chapter defines the meaning of covariance for various operator algebraic objects. Of course, this is done in order to achieve an operator algebraic language for the description of random systems. Similar problems also appeared in (BF04, BF11, Fid06, BSPK13a). Most important we introduce the concepts of covariant states and covariant automorphisms. Assuming that the underlying physical system at a given temperature only has one phase, we can combine the concepts of covariance and KMS states to construct covariant states for interacting electron gases. This is done in Theorem 5.6.

The concepts mentioned above are motivated by the fact that for non-interacting electron gases in random media one can construct the objects explicitly. The constructions of Chapters 6 and 7 should be seen in this context.

5.1. Covariant Algebraic Objects

We consider a probability space $(\Omega, \mathcal{F}, \mathbb{P})$. Maps defined on Ω that agree almost everywhere are identified. Moreover, we assume that Ω is equipped[1] with an *ergodic group* of *measure preserving* transformations $\{\phi_a : \Omega \to \Omega : a \in \mathbb{Z}^d\}$. We want to explain this in more detail[2]. The group structure is reflected in the relations

$$\phi_a \circ \phi_b = \phi_{a+b}\,, \tag{5.1}$$

$$\phi_0 = \mathrm{id}\,, \tag{5.2}$$

which are required to hold for any $a, b \in \mathbb{Z}^d$. The term *measure preserving* is defined by the property that for any $a \in \mathbb{Z}^d$ the mapping $\phi_a : \Omega \to \Omega$ is measurable and satisfies

$$\mathbb{P}(\phi_a(M)) = \mathbb{P}(M) \tag{5.3}$$

for each $M \in \mathcal{F}$. A set $M \in \mathcal{F}$ is called *invariant* with respect to the group $\{\phi_a : a \in \mathbb{Z}^d\}$ whenever the relation

$$\phi_a(M) = M \tag{5.4}$$

holds for all $a \in \mathbb{Z}^d$. Finally, the term *ergodic* is defined by the property that every invariant set $M \in \mathcal{F}$ of the group $\{\phi_a : a \in \mathbb{Z}^d\}$ satisfies either $\mathbb{P}(M) = 1$ or $\mathbb{P}(M) = 0$. In short, invariant sets are either of full or of vanishing probability.
In addition to that probabilistic structure, let $\mathfrak{A}$ be a C^*-algebra and let φ be a representation of the additive group $\mathbb{Z}^d$ on the algebra $\mathfrak{A}$, i.e. the mapping $\varphi : \mathbb{Z}^d \to \mathrm{Aut}(\mathfrak{A})$, $a \mapsto \varphi_a$ satisfies the relations

$$\varphi_a \circ \varphi_b = \varphi_{a+b}\,, \tag{5.5}$$

$$\varphi_0 = \mathrm{id} \tag{5.6}$$

for any $a, b \in \mathbb{Z}^d$. The following definitions all contain maps $\Omega \to V$, where V is a vector space. Similar formalisms were achieved in (BF11, BSPK13a).

Definition 5.1 (*Covariant Elements*)

A *covariant element* is a bounded measurable map $A : \Omega \to \mathfrak{A}$, $\omega \mapsto A_\omega$ such that for almost every $\omega \in \Omega$ and all $a \in \mathbb{Z}^d$ the following transformation law is satisfied

$$\varphi_a(A_\omega) = A_{\phi_a(\omega)}\,. \tag{5.7}$$

Note that by Pettis theorem[3] $A : \Omega \to \mathfrak{A}$, $\omega \mapsto A_\omega$ is measurable, if and only if for any continuous linear functional $\eta : \mathfrak{A} \to \mathbb{C}$ the map $\eta \circ A : \Omega \to \mathbb{C}$, $\omega \mapsto \eta(A_\omega)$ is measurable.

Definition 5.2 (*Covariant States*)

A *covariant state* is a mapping $\rho : \Omega \to \mathrm{Sta}(\mathfrak{A})$, $\omega \mapsto \rho_\omega$ such that for all measurable mappings $\Omega \to \mathfrak{A}$, $\omega \mapsto A_\omega$ the mapping $\Omega \to \mathbb{C}$, $\omega \mapsto \rho_\omega(A_\omega)$ is measurable and for almost every $\omega \in \Omega$ and all $a \in \mathbb{Z}^d$ the following transformation law is satisfied

$$\rho_\omega = \rho_{\phi_a(\omega)} \circ \varphi_a\,. \tag{5.8}$$

[1] Here, for later purposes we just consider the additive group $\mathbb{Z}^d$. In general, one could also consider representations of other groups on Ω and $\mathfrak{A}$, even non-abelian ones.
[2] For reference see (Sto01, Kir07, CL90).
[3] See for example (AE01).

Definition 5.3 (*Covariant Automorphisms*)

A *covariant automorphism* π is a mapping $\pi : \Omega \to \mathrm{Aut}(\mathfrak{A})$, $\omega \mapsto \pi_\omega$ such that for all measurable mappings $\Omega \to \mathfrak{A}$, $\omega \mapsto A_\omega$ the mapping $\Omega \to \mathfrak{A}$, $\omega \mapsto \pi_\omega(A_\omega)$ is measurable and for almost every $\omega \in \Omega$ and all $a \in \mathbb{Z}^d$ the following transformation law is satisfied

$$\varphi_a \circ \pi_\omega = \pi_{\phi_a(\omega)} \circ \varphi_a \,. \tag{5.9}$$

Definition 5.4 (*Covariant Derivations*)

A *covariant derivation* δ is a mapping $\delta : \Omega \to \mathrm{Der}(\mathfrak{S})$, $\omega \mapsto \delta_\omega$ to the symmetric derivations $\mathrm{Der}(\mathfrak{S})$ defined on a dense subalgebra $\mathfrak{S}$ of $\mathfrak{A}$ such that for all measurable mappings $\Omega \to \mathfrak{A}$, $\omega \mapsto A_\omega$ the mapping $\Omega \to \mathfrak{A}$, $\omega \mapsto \delta_\omega(A)$ is measurable and for almost every $\omega \in \Omega$ and all $a \in \mathbb{Z}^d$ one has $\varphi_a(\mathfrak{S}) = \mathfrak{S}$ and the following transformation law is satisfied

$$\varphi_a \circ \delta_\omega = \delta_{\phi_a(\omega)} \circ \varphi_a \,. \tag{5.10}$$

Heuristically, these concepts are motivated by the following situation. Consider the C^*-algebra $\mathfrak{B} := \mathscr{B}(\mathfrak{H})$ of bounded operators on some Hilbert space $\mathfrak{H}$. In addition, consider that T is a *projective unitary representation* of $\mathbb{Z}^d$ on $\mathfrak{H}$. The latter is a map $T : \mathbb{Z}^d \to \mathscr{U}(\mathfrak{H})$, $a \mapsto T(a)$, where $\mathscr{U}(\mathfrak{H})$ is the set of unitary operators on $\mathfrak{H}$. In addition, T satisfies

$$T(a)T(b) = \mathrm{e}^{\mathrm{i}f(a,b)}T(a+b) \,, \tag{5.11}$$

$$T(0) = \mathrm{id} \tag{5.12}$$

for any $a, b \in \mathbb{Z}^d$, where $f : \mathbb{Z}^d \times \mathbb{Z}^d \to \mathbb{R}$ is some real-valued mapping. For $f = 0$ the map T is called a *unitary representation*. From that we obtain a representation of $\mathbb{Z}^d$ as in Equations (5.5) and (5.6) via

$$\varphi_a(B) := T(a)BT(a)^* \tag{5.13}$$

for any $a \in \mathbb{Z}^d$ and $B \in \mathfrak{B}$. This is the statement of the following lemma.

Lemma 5.5

The mapping $\varphi : \mathbb{Z}^d \to \mathrm{Aut}(\mathfrak{B})$, $a \mapsto \varphi_a$ gives a representation of $\mathbb{Z}^d$ on the C^*-algebra $\mathfrak{B}$.

Proof: Clearly, $\varphi_a : \mathfrak{B} \to \mathfrak{B}, B \mapsto T(a)BT(a)^*$ is linear for any $a \in \mathbb{Z}^d$ and we have $\varphi_0 = \mathrm{id}$. From the fact that $T(a)$ is a unitary operator for any $a \in \mathbb{Z}^d$ we get that φ_a is a morphism of $\mathfrak{B}$, because

$$\varphi_a(BC) = T(a)BCT(a)^* = (T(a)BT(a)^*)(T(a)CT(a)^*) = \varphi_a(B)\varphi_a(C) \,,$$
$$\varphi_a(B)^* = (T(a)BT(a)^*)^* = T(a)B^*T(a)^* = \varphi_a(B^*)$$

for any $B, C \in \mathfrak{B}$. Finally, one has $\varphi_a \circ \varphi_b = \varphi_{a+b}$ for all $a, b \in \mathbb{Z}^d$, since for all $B \in \mathfrak{B}$ one has

$$\begin{aligned}\varphi_a(\varphi_b(B)) &= T(a)(T(b)BT(b)^*)T(a)^* = (T(a)T(b))B(T(a)T(b))^* \\ &= \mathrm{e}^{\mathrm{i}f(a,b)}T(a+b)B(\mathrm{e}^{\mathrm{i}f(a,b)}T(a+b))^* \\ &= \mathrm{e}^{\mathrm{i}f(a,b)}T(a+b)B\mathrm{e}^{-\mathrm{i}f(a,b)}T(a+b)^* \\ &= T(a+b)BT(a+b)^* \\ &= \varphi_{a+b}(B) \,.\end{aligned}$$

■

In this situation, the elements in Definition 5.1 transform as one expects covariant operators to transform having for example (Kir07, Sto01, KLM07, KM08, BGKS05, CL90) in mind. Similarly, one might consider normal states on $\mathfrak{B}$ with a density matrix that transforms covariantly as an operator on $\mathfrak{H}$. Then, a simple calculation shows that the state as a linear functional transforms as in Definition 5.2. Analogously, Definitions 5.3 and 5.4 are motivated.
Immediate but important implications of Definitions 5.1 - 5.4 are for example that any composition of covariant automorphisms forms a covariant automorphism and any composition of a covariant state and a covariant automorphism forms a covariant state.

5.2. Covariant KMS States

It seems to be a natural desire to combine the concepts of covariant states and KMS states, i.e. one considers covariant states $\varrho^{(\beta)} : \Omega \to \mathrm{Sta}(\mathfrak{A}),\ \omega \mapsto \varrho^{(\beta)}_\omega$, where $\varrho^{(\beta)}_\omega$ is a KMS state each single realisation $\omega \in \Omega$ This is done in a natural in the following theorem. Even though this theorem is elementary, it seems new in literature.

Theorem 5.6 (*Covariant KMS States*)

Let $\beta \in \mathbb{R} \cup \{\infty\}$ and $\tau_t : \Omega \to \mathrm{Aut}(\mathfrak{A}),\ \omega \mapsto \tau_{\omega,t}$ be a covariant automorphism for each $t \in \mathbb{R}$ such that $(\mathfrak{A}, \tau_\omega)$ is a C^*-dynamical system for all $\omega \in \Omega$. Moreover, assume that for each $\omega \in \Omega$ there is a unique (τ_ω,β)-KMS state $\varrho^{(\beta)}_\omega$ and that $\varrho^{(\beta)} : \Omega \to \mathrm{Sta}(\mathfrak{A}),\ \omega \mapsto \varrho^{(\beta)}_\omega$ is a measurable mapping. Then, $\varrho^{(\beta)}$ is a covariant state.

Proof: For $\omega \in \Omega$ and $a \in \mathbb{Z}^d$ arbitrary let $\varrho^{(\beta)}_{\omega,a} := \varrho^{(\beta)}_\omega \circ \varphi_{-a}$. We show that $\varrho^{(\beta)}_{\omega,a}$ is a $(\tau_{\phi_a(\omega)},\beta)$-KMS state. Then, by uniqueness of the $(\tau_{\phi_a(\omega)},\beta)$-KMS state we get $\varrho^{(\beta)}_\omega \circ \varphi_{-a} = \varrho^{(\beta)}_{\phi_a(\omega)}$. First we assume that $\beta \neq \infty$. Then, for all f with $\hat{f} \in C^\infty_c(\mathbb{R})$ and all $A, B \in \mathfrak{A}$ we obtain

$$\begin{aligned}
\int_{\mathbb{R}} f(t)\, \varrho^{(\beta)}_{\omega,a}(A\tau_{\phi_a(\omega),t}(B))\, \mathrm{d}t &= \int_{\mathbb{R}} f(t)\, \varrho^{(\beta)}_\omega(\varphi_{-a}(A\varphi_a(\tau_{\omega,t}(\varphi_{-a}(B)))))\, \mathrm{d}t \\
&= \int_{\mathbb{R}} f(t)\, \varrho^{(\beta)}_\omega(\varphi_{-a}(A)\tau_{\omega,t}(\varphi_{-a}(B)))\, \mathrm{d}t \\
&= \int_{\mathbb{R}} f(t+\mathrm{i}\beta)\, \varrho^{(\beta)}_\omega(\tau_{\omega,t}(\varphi_{-a}(B))\varphi_{-a}(A))\, \mathrm{d}t \\
&= \int_{\mathbb{R}} f(t+\mathrm{i}\beta)\, \varrho^{(\beta)}_\omega(\varphi_{-a}(\varphi_a(\tau_{\omega,t}(\varphi_{-a}(B))))\varphi_{-a}(A))\, \mathrm{d}t \\
&= \int_{\mathbb{R}} f(t+\mathrm{i}\beta)\, \varrho^{(\beta)}_\omega(\varphi_{-a}(\tau_{\phi_a(\omega),t}(B)A))\, \mathrm{d}t \\
&= \int_{\mathbb{R}} f(t+\mathrm{i}\beta)\, \varrho^{(\beta)}_{\omega,a}(\tau_{\phi_a(\omega),t}(B)A)\, \mathrm{d}t\,.
\end{aligned}$$

From Theorem 4.2 and uniqueness we get the statement of Theorem 5.6. Analogously, we will proceed in the case $\beta = \infty$. For each $\omega \in \Omega$ let $\mathcal{H}_\omega$ be the generator of $\tau_{\omega,t}$ on a subalgebra $\mathfrak{S}$ of $\mathfrak{A}$, which is invariant with respect to $\{\varphi_a : a \in \mathbb{Z}^d\}$. The mapping $\mathcal{H} : \Omega \to \mathrm{Der}(\mathfrak{S}),\ \omega \mapsto \mathcal{H}_\omega$ forms a covariant derivation. Then, for all $A \in D(\mathcal{H})$ we obtain

$$-\mathrm{i}\, \varrho^{(\beta)}_{\omega,a}(A^*\mathcal{H}_{\phi_a(\omega)}(A)) = -\mathrm{i}\, \varrho^{(\beta)}_\omega(\varphi_{-a}(A^*\varphi_a(\mathcal{H}_\omega(\varphi_{-a}(A))))) = -\mathrm{i}\, \varrho^{(\beta)}_\omega(\varphi_{-a}(A)^*\mathcal{H}_\omega(\varphi_{-a}(A))) \geq 0\,.$$

■

6 Model System

In physics we have dealt hitherto only with periodic crystals. To a humble physicist's mind, these are very interesting and complicated objects; they constitute one of the most fascinating and complex material structures by which inanimate nature puzzles his wits. Yet, compared with the aperiodic crystal, they are rather plain and dull. The difference in structure is of the same kind as that between an ordinary wallpaper in which the same pattern is repeated again and again in regular periodicity and a masterpiece of embroidery, say a Raphael tapestry, which shows no dull repetition, but an elaborate, coherent, meaningful design traced by the great master.

(Erwin Schrödinger)

So far we have introduced an abstract language in terms of operator algebras which we claimed to be an adequate playground for the description of quantum many-particle systems. However, we have not focused on concrete examples of such systems illustrating the power of the formalism achieved in the previous chapters. The underlying chapter is about the elimination of this drawback.

In particular, we present a discrete model of an interacting electron gas that is trapped in the environment of a random solid state. This solid state is considered to inherit ergodicity. More concretely, one may think of a solid state that is an alloy of two different metals, for instance brass, which is an isotropic mixture of the metals copper and zinc. On a microscopic scale this solid state has no periodic structure at all. Nevertheless, in a certain sense of average its disorder is the same around each of its points.

In Section 6.1 we start with the basic definitions for the system of a single electron in the solid state. We introduce the underlying Hilbert space, describe an external electric field, implement randomness and present an alloy type model as a generic special case. Then, the Schrödinger operator of the disordered system is introduced and is used to define the velocity operator. Next, we introduce the useful concept of a current density operator, which is an operator only acting in a finite neighbourhood of some point in the solid state. At this point the current density operator measures the presence and velocity of the electron. Finally, we describe the time evolution of the system by its unitary propagator. In parallel to all these Hilbert space objects we define the corresponding operator algebraic quantities. Essentially this means that from unitary operators implementing spatial shifts, electric field and time evolution on the one-particle Hilbert space we get automorphisms implementing the corresponding objects on the C^*-algebra of bounded linear operators on the one-particle Hilbert space. These structures form a specific example of the algebraic formalism introduced in Chapters 3 - 5.

In Section 6.2 we construct the analogous model of an interacting electron gas using the formalism of Appendix B. Furthermore, the operator algebraic concepts of Section 6.1 are transported to the corresponding concepts for a many-electron system.

6.1. Framework for One-Electron Systems

6.1.1. Hilbert Space

On the one-particle level we follow the model of (BGKS05, KLM07, KM08). Our notation is similar to (BSPK13a). As the Hilbert space of a single electron we consider $\mathfrak{h} := \ell^2(\mathbb{Z}^d)$ equipped with the standard scalar product given by

$$\langle \phi, \psi \rangle := \sum_{x \in \mathbb{Z}^d} \overline{\phi(x)}\, \psi(x)$$

for $\phi, \psi \in \mathfrak{h}$ arbitrary. Important subspaces of $\mathfrak{h}$ are $\mathfrak{h}_\Lambda$, the space of elements with support in Λ, where Λ is any subset of $\mathbb{Z}^d$, and $\mathfrak{h}_c := \ell^2_c(\mathbb{Z}^d)$, the space of elements with finite support. Note that $\mathfrak{h}_c$ is a dense subspace of $\mathfrak{h}$.
In this situation, the space $\mathfrak{B} := \mathscr{B}(\mathfrak{h})$ of bounded linear operators on $\mathfrak{h}$ becomes a C^*-algebra. Moreover, for any subset $\Lambda \subset \mathbb{Z}^d$ we define[1] $\mathfrak{B}_\Lambda$, the algebra of operators with support in Λ, as the set of all bounded linear operators such that $B\psi = 0$ for all $\psi \in \mathfrak{h}_{\Lambda^c}$. Analogously, $\mathfrak{B}_c$ is the subalgebra of operators with finite support. Note that $\mathfrak{h}$ has a countable orthonormal basis in $\{\delta_x : x \in \mathbb{Z}^d\}$, where

$$\delta_x(y) := \begin{cases} 1 & \text{for } y = x \\ 0 & \text{otherwise} \end{cases} . \tag{6.1}$$

Associated to the $\mathbb{Z}^d$ structure there are linear operators $T(a) : \mathfrak{h} \to \mathfrak{h}$ for any $a \in \mathbb{Z}^d$ whose action on arbitrary elements $\psi \in \mathfrak{h}$ is defined pointwise for all $x \in \mathbb{Z}^d$ by

$$(T(a)\psi)(x) := \mathrm{e}^{\mathrm{i}\langle a, S\,x\rangle}\psi(x-a)\,, \tag{6.2}$$

where S is a given real $d \times d$-matrix and the scalar product in the exponent on the right hand side of Equation (6.2) is the standard scalar product on $\mathbb{R}^d$. We will refer to these operators as *magnetic shifts*. Note that the magnetic shifts map $\mathfrak{h}_c$ onto itself.

Lemma 6.1

The mapping $T : \mathbb{Z}^d \to \mathscr{U}(\mathfrak{h})$, $a \mapsto T(a)$ defines a projective unitary representation of $\mathbb{Z}^d$.

Proof: The well-definedness of T follows from the fact that for all $\phi, \psi \in \mathfrak{h}$ and $a \in \mathbb{Z}^d$ we have

$$\begin{aligned}
\langle T(a)\phi, T(a)\psi \rangle &= \sum_{x\in\mathbb{Z}^d} \overline{\mathrm{e}^{\mathrm{i}\langle a,S\,x\rangle}\phi(x-a)}\, \mathrm{e}^{\mathrm{i}\langle a,S\,x\rangle}\psi(x-a) \\
&= \sum_{x\in\mathbb{Z}^d} \mathrm{e}^{-\mathrm{i}\langle a,S\,x\rangle}\overline{\phi(x-a)}\, \mathrm{e}^{\mathrm{i}\langle a,S\,x\rangle}\psi(x-a) \\
&= \sum_{x\in\mathbb{Z}^d} \overline{\phi(x-a)}\, \psi(x-a) = \sum_{x\in\mathbb{Z}^d} \overline{\phi(x)}\, \psi(x) \; = \langle \phi, \psi \rangle\,.
\end{aligned}$$

Thus, for any $a \in \mathbb{Z}^d$ the operator $T(a)$ preserves scalar products. Obviously, $T(0) = \mathrm{id}$ and for any $a, b \in \mathbb{Z}^d$

$$\begin{aligned}
(T(a)(T(b)\psi))(x) &= \mathrm{e}^{\mathrm{i}\langle a,S\,x\rangle}(T(b)\psi)(x-a) \\
&= \mathrm{e}^{\mathrm{i}\langle a,S\,x\rangle}\mathrm{e}^{\mathrm{i}\langle b,S\,(x-a)\rangle}\psi((x-a)-b) \\
&= \mathrm{e}^{-\mathrm{i}\langle b,S\,a\rangle}\mathrm{e}^{\mathrm{i}\langle a+b,S\,x\rangle}\psi(x-(a+b)) = \mathrm{e}^{-\mathrm{i}\langle b,S\,a\rangle}(T(a+b)\psi)(x)
\end{aligned}$$

for all $\psi \in \mathfrak{h}$ and $x \in \mathbb{Z}^d$, so $T(a)T(b) = \mathrm{e}^{-\mathrm{i}\langle b,S\,a\rangle}T(a+b)$. From this we directly obtain that $T(a)$ is invertible with $T(a)^{-1} = T(a)^* = \mathrm{e}^{-\mathrm{i}\langle a,S\,a\rangle}T(-a)$. ■

[1] For $B \in \mathfrak{B}_\Lambda$ one has $B = \sum_{x\in\Lambda}\sum_{y\in\mathbb{Z}^d} b_{y,x}\,|\delta_y\rangle\langle\delta_x|$ with coefficients $b_{y,x}$ such that $\sum_{y\in\mathbb{Z}^d}|b_{y,x}|^2 < \infty$ for all $x \in \Lambda$.

For any $a \in \mathbb{Z}^d$ the magnetic shift operators induce linear mappings $\varphi_a : \mathscr{L}(\mathfrak{h}_c, \mathfrak{h}) \to \mathscr{L}(\mathfrak{h}_c, \mathfrak{h})$ defined on the linear maps between $\mathfrak{h}_c$ and $\mathfrak{h}$. These are given by

$$\varphi_a(B) := T(a)BT(a)^* \tag{6.3}$$

for any $B \in \mathscr{L}(\mathfrak{h}_c, \mathfrak{h})$. Since $\mathfrak{B} = \mathscr{B}(\mathfrak{h}) \subset \mathscr{L}(\mathfrak{h}_c, \mathfrak{h})$, for any $a \in \mathbb{Z}^d$ the restriction $\varphi_a : \mathfrak{B} \to \mathfrak{B}$ forms an automorphism on the C^*-algebra $\mathfrak{B}$. The position operator $X = (X_1, ..., X_d)$ is the self-adjoint operator given by the action of its components on arbitrary $\psi \in \mathfrak{h}_c$ which is

$$(X_k\psi)(x) := x_k\psi(x) \tag{6.4}$$

for $k \in \{1, ..., d\}$ and $x \in \mathbb{Z}^d$. Using $X_k(\mathfrak{h}_c) \subset \mathfrak{h}_c$ we have $(T(a)X_kT(a)^*\psi)(x) = (x_k - a_k)\psi(x)$ for any $x, a \in \mathbb{Z}^d$, $k \in \{1, ..., d\}$ and $\psi \in \mathfrak{h}_c$, the components of the position operator transform

$$\varphi_a(X_k) = T(a)X_kT(a)^* := X_k - a_k\ . \tag{6.5}$$

On the algebra of operators with finite support the components of the position operator define derivations $\mathcal{X} = (\mathcal{X}_1, ..., \mathcal{X}_d)$ via the commutator

$$\mathcal{X}_k(B) := \mathrm{i}[X_k, B] \tag{6.6}$$

for any $k \in \{1, ..., d\}$ and $B \in \mathfrak{B}_c$. Since one has $\varphi_a(\mathfrak{B}_c) = \mathfrak{B}_c$, for any $a \in \mathbb{Z}^d$, $k \in \{1, ..., d\}$ and $B \in \mathfrak{B}_c$ one obtains the transformation law

$$\varphi_a(\mathcal{X}_k(B)) = \mathrm{i}[\varphi_a(X_k), \varphi_a(B)] = \mathrm{i}[X_k - a_k, \varphi_a(B)] = \mathrm{i}[X_k, \varphi_a(B)] = \mathcal{X}_k(\varphi_a(B))\ . \tag{6.7}$$

6.1.2. Disorder

We model the random background by a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ with expectation value $\mathbb{E}[Y]$ for random variables Y. Then, each $\omega \in \Omega$ represents a specific realisation of the random system. In addition, we assume that we are given an ergodic group $\{\phi_a : \Omega \to \Omega : a \in \mathbb{Z}^d\}$ of measure preserving transformations as introduced in Chapter 5.
Next, we introduce spaces of covariant operators as in (BGKS05). By $\mathcal{M}(\Omega, \mathscr{L}(\mathfrak{h}_c, \mathfrak{h}))$ we denote the space of measurable operators $B : \Omega \to \mathscr{L}(\mathfrak{h}_c, \mathfrak{h})$, $\omega \mapsto B_\omega$. We also consider the space $\mathcal{BM}(\Omega, \mathscr{L}(\mathfrak{h}_c, \mathfrak{h}))$ of essentially bounded mappings with the norm

$$|||B|||_\infty := \operatorname{ess\,sup}\{\ \|B_\omega\| : \omega \in \Omega\ \}\ . \tag{6.8}$$

$\mathcal{BM}(\Omega, \mathscr{L}(\mathfrak{h}_c, \mathfrak{h}))$ forms a C^*-algebra. Furthermore, a measurable[2] mapping $B \in \mathcal{M}(\Omega, \mathscr{L}(\mathfrak{h}_c, \mathfrak{h}))$ is called a *covariant operator*, if for all $a \in \mathbb{Z}^d$ and almost every $\omega \in \Omega$ the relation

$$\varphi_a(B_\omega) = B_{\phi_a(\omega)} \tag{6.9}$$

is satisfied. The space of measurable covariant operators is denoted by $\mathcal{MC}(\Omega, \mathscr{L}(\mathfrak{h}_c, \mathfrak{h}))$ and we define $\mathcal{K}^\infty := \mathcal{BMC}(\Omega, \mathscr{L}(\mathfrak{h}_c, \mathfrak{h}))$ as the subset of bounded, measurable[3] and covariant mappings. In particular, $\mathcal{K}^\infty$ is an example of a C^*-algebra consisting of covariant elements in the sense of Definition 5.1. For example, the potential energy of one single electron is implemented by a covariant multiplication operator $V \in \mathcal{K}^\infty$, i.e. for each $\omega \in \Omega$ the operator V_ω is a multiplication operator on $\mathfrak{h}$ induced by a bounded mapping $v_\omega : \mathbb{Z}^d \to \mathbb{R}$. Via

$$\langle\langle B, C\rangle\rangle := \mathbb{E}\,[\langle B\delta_0, C\delta_0\rangle] \tag{6.10}$$

[2] $B \in \mathcal{M}(\Omega, \mathscr{L}(\mathfrak{h}_c, \mathfrak{h}))$ is measurable, if for all $\phi, \psi \in \mathfrak{h}_c$ the mapping $\Omega \to \mathbb{C}$, $\omega \mapsto \langle\phi, B_\omega\psi\rangle$ is measurable.
[3] For $B \in \mathcal{K}^\infty$ measurability is understood in the sense of Definition 5.1.

for any $B, C \in \mathcal{K}^\infty$ a scalar product is defined on $\mathcal{K}^\infty$ (BGKS05). Positivity follows from considering $\mathbb{E}[\|B\delta_x\|^2]$ for general $x \in \mathbb{Z}^d$ using the covariance property of operators $B \in \mathcal{K}^\infty$. Note that $\mathcal{K}^\infty$ is no Hilbert space, because it lacks completeness with respect to the norm

$$|||B|||_2 := (\mathbb{E}[\|B\delta_0\|^2])^{\frac{1}{2}} \tag{6.11}$$

induced by the scalar product in Equation (6.10). The closure of $\mathcal{K}^\infty$ with respect to the norm in Equation (6.11) within the space $\mathcal{MC}(\Omega, \mathscr{L}(\mathfrak{h}_c, \mathfrak{h}))$ is denoted by $\mathcal{K}^2$. For any $B \in \mathcal{MC}(\Omega, \mathscr{L}(\mathfrak{h}_c, \mathfrak{h}))$ one has $\mathfrak{h}_c \subset D(B^*_\omega)$ for almost every $\omega \in \Omega$ (BGKS05, KLM07, KM08). Thus, the operator $B^\star_\omega := B^*_\omega|_{\mathfrak{h}_c}$ is well-defined and induces a conjugation on $\mathcal{MC}(\Omega, \mathscr{L}(\mathfrak{h}_c, \mathfrak{h}))$. In addition, for any $B, C \in \mathcal{K}^2$ the identity

$$\langle\langle B, C\rangle\rangle = \langle\langle C^\star, B^\star\rangle\rangle \tag{6.12}$$

holds. This can be seen formally by writing an identity between the operators in the scalar product on the right hand side of Equation (6.10). The identity is then expressed as a sum of orthogonal projections with respect to the basis $\{\delta_x : x \in \mathbb{Z}^d\}$. Using the covariance of B and C one obtains Equation (6.12). We prove the following useful lemma (BGKS05)[Lemma 3.9].

Lemma 6.2

Let $(B_n)_{n\in\mathbb{N}}$ be a bounded sequence in $\mathcal{BM}(\Omega, \mathfrak{B})$ converging pointwise strongly to zero, i.e. for each $\omega \in \Omega$ and all $\psi \in \mathfrak{h}$ one has $\lim_{n\to\infty} \|B_{n,\omega}\psi\| = 0$. Then, for all $C \in \mathcal{K}^2$

$$\lim_{n\to\infty} \mathbb{E}[\|B_n C\delta_0\|^2] = 0\ . \tag{6.13}$$

Proof: We prove the statement by use of the dominated convergence theorem. For $n \in \mathbb{N}$ and $C \in \mathcal{K}^2$ arbitrary let $f_n : \Omega \to [0, \infty[,\ \omega \mapsto \|B_{n,\omega}C_\omega\delta_0\|^2$. Because of the pointwise strong convergence of $(B_n)_{n\in\mathbb{N}}$, for all $\omega \in \Omega$ we have

$$\lim_{n\to\infty} f_n(\omega) = \lim_{n\to\infty} \|B_{n,\omega}C_\omega\delta_0\|^2 = 0\ .$$

So, the sequence of random variables $(f_n)_{n\in\mathbb{N}}$ converges pointwise to zero. Moreover, due to the fact that $(B_n)_{n\in\mathbb{N}}$ is a bounded sequence in $\mathcal{BM}(\Omega, \mathfrak{B})$, there is a constant $M > 0$ such that

$$|f_n(\omega)| \leq \|B_{n,\omega}C_\omega\delta_0\|^2 \leq |||B_n|||^2_\infty\ \|C_\omega\delta_0\|^2 \leq M\|C_\omega\delta_0\|^2\ ,$$

i.e. the sequence $(f_n)_{n\in\mathbb{N}}$ is dominated by an integrable mapping. Then, from the dominated convergence theorem we get

$$\lim_{n\to\infty} \mathbb{E}[\|B_n C\delta_0\|^2] = \lim_{n\to\infty} \mathbb{E}[f_n] = \lim_{n\to\infty} \int_\Omega f_n(\omega)\, \mathrm{d}\mathbb{P}(\omega) = \int_\Omega \lim_{n\to\infty} f_n(\omega)\, \mathrm{d}\mathbb{P}(\omega) = 0\ .$$

■

Generic Example

The canonical example the reader should have in mind is the Anderson model[4]. Consider the space $\Omega = \mathbb{R}^{(\mathbb{Z}^d)}$ equipped with the σ-algebra $\mathcal{F}$ generated by the ring of cylinder sets, i.e. all sets which are of the form

$$M := \left\{\omega \in \mathbb{R}^{(\mathbb{Z}^d)} : \omega_{i_1} \in I_1,\ \omega_{i_2} \in I_2, ...,\ \omega_{i_n} \in I_n\right\} \tag{6.14}$$

[4] This model first was considered by Philip Warren Anderson in 1958 in (And58).

for some $n \in \mathbb{N}$, where $I_1, ..., I_n \in \mathcal{B}([0,1])$ are Borel sets and $i_1, ..., i_n \in \mathbb{Z}^d$ differ pairwise. Now, if $\mu : \mathcal{B}([0,1]) \to [0,1]$ is a probability measure on $[0,1]$, there is a unique probability measure $\mathbb{P} : \mathcal{F} \to [0,1]$ on Ω defined by

$$\mathbb{P}(M) := \prod_{k=1}^{n} \mu(I_k) \tag{6.15}$$

for all $M \in \mathcal{F}$ that are of the form as in Equation (6.14) (Kir07). Obviously, in this situation, for each $a \in \mathbb{Z}^d$ the mapping $\phi_a : \Omega \to \Omega$ defined by the property

$$(\phi_a(\omega))_b := \omega_{b-a} \tag{6.16}$$

for all $\omega \in \Omega$ and $b \in \mathbb{Z}^d$ is bijective and measurable, because it maps cylinder sets to cylinder sets. Moreover, with respect to $\mathbb{P}$, as defined by Equation (6.15), it is a measure preserving transformation of Ω and one can show that the family $\{\phi_a : a \in \mathbb{Z}^d\}$ is ergodic (Kir07). Finally, given a mapping $u : \mathbb{Z}^d \to \mathbb{R}$ of finite support, for each $\omega \in \Omega$ we define a bounded mapping $v_\omega : \mathbb{Z}^d \to \mathbb{R}$ pointwise by

$$v_\omega(x) := \sum_{b \in \mathbb{Z}^d} \omega_b \, u(x-b) \, .$$

The mapping u is also called the *single site potential*. The term $u(x-b)$ describes the effect of a single atomic core that is centred at $b \in \mathbb{Z}^d$ on the electron at position $x \in \mathbb{Z}^d$. Because for $\omega \in \Omega$ and all $x, a \in \mathbb{Z}^d$ we have

$$\begin{aligned} v_\omega(x-a) &= \sum_{b \in \mathbb{Z}^d} \omega_b \, u((x-a)-b) = \sum_{b \in \mathbb{Z}^d} \omega_b \, u(x-(a+b)) \\ &= \sum_{b \in \mathbb{Z}^d} \omega_{b-a} \, u(x-b) = \sum_{b \in \mathbb{Z}^d} (\phi_a(\omega))_b \, u(x-b) = v_{\phi_a(\omega)}(x) \, , \end{aligned}$$

we obtain a covariant transformation law for the potential energy of one electron, i.e one has

$$\varphi_a(V_\omega) = T(a) v_\omega(X) T(a)^* = v_\omega(T(a) X T(a)^*) = v_\omega(X-a) = v_{\phi_a(\omega)}(X) = V_{\phi_a(\omega)} \, . \tag{6.17}$$

6.1.3. Electric Field

We consider the space $\mathcal{E}(\mathbb{R}, \mathbb{R}^d) := \{E \in C(\mathbb{R}, \mathbb{R}^d) : \|\chi_{]-\infty,t]} E\|_1 < \infty, \forall t \in \mathbb{R}\}$, where $\|\cdot\|_1$ denotes the norm on $L^1(\mathbb{R}, \mathbb{R}^d)$ and χ_I the characteristic function of a subset $I \subset \mathbb{R}$, and we implement time dependence by switching on an external spatially homogeneous electric field $E \in \mathcal{E}(\mathbb{R}, \mathbb{R}^d)$ starting at time $s \in \mathbb{R} \cup \{-\infty\}$. For any $t \in \mathbb{R}$ we set

$$F^{(E)}(t) := \int_{-\infty}^{t} E(r) \, \mathrm{d}r \, , \tag{6.18}$$

$$G^{(E)}(t) := \mathrm{e}^{\mathrm{i}\langle F^{(E)}(t), X \rangle} \, . \tag{6.19}$$

The unitary operators in the Equation (6.19) are gauge transformations that implement the effect of an electric field on the level of the Hilbert space $\mathfrak{h}$.

Lemma 6.3

For any $\psi \in \mathfrak{h}_c$ the mapping $\mathbb{R} \to \mathfrak{h}_c, \; t \mapsto G(t)\psi$ is differentiable with respect to t and

$$\partial_t G^{(E)}(t)\psi = \mathrm{i}\langle E(t), X \rangle G^{(E)}(t)\psi = \mathrm{i} G^{(E)}(t) \langle E(t), X \rangle \psi \, . \tag{6.20}$$

Proof: Let $\psi \in \mathfrak{h}_c$ be arbitrary. We have $G^{(E)}(t)\psi = \sum_{x\in\mathbb{Z}^d} \psi(x)\, G^{(E)}(t)\delta_x = \sum_{x\in\mathbb{Z}^d} \psi(x)\, \mathrm{e}^{\mathrm{i}\langle F^{(E)}(t),x\rangle}\delta_x$ only including a finite sum. Thus, we can differentiate $G^{(E)}(t)\psi$ with respect to t and obtain

$$\begin{aligned}\partial_t G^{(E)}(t)\psi &= \sum_{x\in\mathbb{Z}^d} \psi(x)\, \partial_t \mathrm{e}^{\mathrm{i}\langle F^{(E)}(t),x\rangle}\delta_x \\ &= \mathrm{i}\sum_{x\in\mathbb{Z}^d} \psi(x)\mathrm{e}^{\mathrm{i}\langle F^{(E)}(t),x\rangle}\langle E(t),x\rangle\delta_x \\ &= \mathrm{i}G^{(E)}(t)\langle E(t),X\rangle\psi = \mathrm{i}\langle E(t),X\rangle G^{(E)}(t)\psi\ .\end{aligned}$$

■

Analogously, one proves $\partial_t G^{(E)}(t)^*\psi = -\mathrm{i}G^{(E)}(t)^*\langle E(t),X\rangle\psi = -\mathrm{i}\langle E(t),X\rangle G^{(E)}(t)^*\psi$ for any $\psi \in \mathfrak{h}_c$ and $t \in \mathbb{R}$.
Using the fact that the gauge transformations in Equation (6.19) do not change the support of an element $\psi \in \mathfrak{h}$, for any $t \in \mathbb{R}$ we can define a linear mapping $\gamma_t^{(E)} : \mathscr{L}(\mathfrak{h}_c,\mathfrak{h}) \to \mathscr{L}(\mathfrak{h}_c,\mathfrak{h})$ by

$$\gamma_t^{(E)}(B) := G^{(E)}(t)BG^{(E)}(t)^* \tag{6.21}$$

for any $B \in \mathscr{L}(\mathfrak{h}_c,\mathfrak{h})$. In addition, the restrictions $\gamma_t^{(E)} : \mathfrak{B} \to \mathfrak{B}$ are automorphisms. We have $\varphi_a(G^{(E)}(t)) = \varphi_a(\mathrm{e}^{\mathrm{i}\langle F^{(E)}(t),X\rangle}) = \mathrm{e}^{\mathrm{i}\langle F^{(E)}(t),X-a\rangle} = \mathrm{e}^{-\mathrm{i}\langle F^{(E)}(t),a\rangle}G^{(E)}(t)$ for any $a \in \mathbb{Z}^d$ and $t \in \mathbb{R}$ which yields the following transformation law for the gauge automorphisms

$$\varphi_a \circ \gamma_t^{(E)} = \gamma_t^{(E)} \circ \varphi_a\ . \tag{6.22}$$

This transformation law is important, because it leads to the result that the automorphisms defined in Equation (6.21) naturally provide linear mappings on $\mathcal{K}^\infty$ as well as on $\mathcal{K}^2$. Moreover, on $\mathcal{K}^\infty$ these linear mappings are *-automorphisms. Obviously, $\gamma_t^{(E)}$ defines an isometry on $\mathcal{K}^\infty$ for any $t \in \mathbb{R}$, but it also defines an isometry on $\mathcal{K}^2$, since for any $B, C \in \mathcal{K}^2$ and $t \in \mathbb{R}$

$$\begin{aligned}\langle\langle\gamma_t^{(E)}(B),\gamma_t^{(E)}(C)\rangle\rangle &= \mathbb{E}[\langle\gamma_t^{(E)}(B)\delta_0,\gamma_t^{(E)}(C)\delta_0\rangle] \\ &= \mathbb{E}[\langle G^{(E)}(t)BG^{(E)}(t)^*\delta_0, G^{(E)}(t)CG^{(E)}(t)^*\delta_0\rangle] \\ &= \mathbb{E}[\langle G^{(E)}(t)B\delta_0, G^{(E)}(t)C\delta_0\rangle] \\ &= \mathbb{E}[\langle B\delta_0, C\delta_0\rangle] \\ &= \langle\langle B,C\rangle\rangle\ .\end{aligned}$$

Lemma 6.4

For any $B \in \mathfrak{B}_c$ the mapping $\mathbb{R} \to \mathfrak{B}_c,\ t \mapsto \gamma_t^{(E)}(B)$ is differentiable with respect to t and with the derivation $\langle E(t),\mathcal{X}\rangle := \sum_{k=1}^d E_k(t)\mathcal{X}_k$ for any $t \in \mathbb{R}$ one has

$$\partial_t\gamma_t^{(E)}(B) = \langle E(t),\mathcal{X}\rangle(\gamma_t^{(E)}(B)) = \gamma_t^{(E)}(\langle E(t),\mathcal{X}\rangle(B))\ . \tag{6.23}$$

Proof: Let $B \in \mathfrak{B}_c$ and $\Lambda := \mathrm{supp}(B)$. Since $\gamma_t^{(E)}(B)\psi = 0$ for all $t \in \mathbb{R}$ and $\psi \in \mathfrak{h}_{\Lambda^c}$ and since Λ is finite, it is sufficient to differentiate the mappings $\mathbb{R} \to \mathfrak{h}_\Lambda,\ t \mapsto \gamma_t^{(E)}(B)\psi$ for all $\psi \in \mathfrak{h}_\Lambda$. For all $t \in \mathbb{R}$ and $\psi \in \mathfrak{h}_\Lambda$ we obtain

$$\begin{aligned}\partial_t\gamma_t^{(E)}(B)\psi &= \mathrm{i}\langle E(t),X\rangle G^{(E)}(t)BG^{(E)}(t)^*\psi - \mathrm{i}G^{(E)}(t)BG^{(E)}(t)^*\langle E(t),X\rangle\psi \\ &= \mathrm{i}[\langle E(t),X\rangle, G^{(E)}(t)BG^{(E)}(t)^*]\psi = \langle E(t),\mathcal{X}\rangle(\gamma_t^{(E)}(B))\psi \\ &= \mathrm{i}G^{(E)}(t)[\langle E(t),X\rangle, B]G^{(E)}(t)^*\psi = \gamma_t^{(E)}(\langle E(t),\mathcal{X}\rangle(B))\psi\ .\end{aligned}$$

■

We prove several lemmas concerning the gauge transformations (BGKS05)[Lemma 4.13]. These will be used in the context of the linear response theory in Chapter 9.

Lemma 6.5

For any $B \in \mathcal{K}^2$ the mapping $\mathbb{R} \to \mathcal{K}^2,\ t \mapsto \gamma_t^{(E)}(B)$ is norm-continuous and one has

$$\lim_{t\to-\infty} |||\gamma_t^{(E)}(B) - B|||_2 = 0 . \tag{6.24}$$

Proof : For any $t, h \in \mathbb{R}$ we define the mapping $\gamma_{t,h}^{(E)} := \gamma_{t+h}^{(E)} \circ (\gamma_t^{(E)})^{-1}$ on $\mathcal{K}^2$. Then, the norm-continuity of the mapping $\mathbb{R} \to \mathcal{K}^2,\ t \mapsto \gamma_t^{(E)}(B)$ is equivalent to

$$\lim_{h\to 0} |||\gamma_{t,h}^{(E)}(B) - B|||_2^2 = 0$$

for all $t \in \mathbb{R}$ and $B \in \mathcal{K}^2$. We define unitary operators $G^{(E)}(t,h) := G^{(E)}(t+h)G^{(E)}(t)^* = \mathrm{e}^{\mathrm{i}\langle F^{(E)}(t+h)-F^{(E)}(t),X\rangle}$ on $\mathfrak{h}$ for any $t, h \in \mathbb{R}$. Using this notation one has $\gamma_{t,h}^{(E)}(B) = G^{(E)}(t,h)BG^{(E)}(t,h)^*$ for all $t, h \in \mathbb{R}$ and $B \in \mathscr{L}(\mathfrak{h}_c, \mathfrak{h})$. Moreover, for any $\psi \in \mathfrak{h}$ one has $\lim_{h\to 0} \|(1 - G^{(E)}(t,h)^*)\psi\| = 0$. One also has the identity

$$\gamma_{t,h}^{(E)}(B) - B = G^{(E)}(t,h)((1 - G^{(E)}(t,h)^*)B + B(G^{(E)}(t,h)^* - 1)) ,$$

which holds for any $t, h \in \mathbb{R}$ and any $B \in \mathscr{L}(\mathfrak{h}_c, \mathfrak{h})$. Using the unitarity of $G^{(E)}(t,h)$, for any $t, h \in \mathbb{R}$ and $B \in \mathcal{K}^2$ one obtains

$$\begin{aligned} |||\gamma_{t,h}^{(E)}(B) - B|||_2^2 &= \mathbb{E}[\|G^{(E)}(t,h)((1 - G^{(E)}(t,h)^*)B + B(G^{(E)}(t,h)^* - 1))\delta_0\|^2] \\ &= \mathbb{E}[\|G^{(E)}(t,h)(1 - G^{(E)}(t,h)^*)B\delta_0\|^2] \\ &= \mathbb{E}[\|(1 - G^{(E)}(t,h)^*)B\delta_0\|^2] . \end{aligned}$$

Now, the norm-continuity follows from an application of Lemma 6.2. Moreover, Equation (6.24) is just norm-continuity at the point $t = -\infty$ and is proven the same way. ∎

Lemma 6.6

Assume that $B \in \mathcal{K}^2$ satisfies $\mathcal{X}_k(B) := \mathrm{i}[X_k, B] \in \mathcal{K}^2$ for all $k \in \{1, ..., d\}$. Then, the mapping $\mathbb{R} \to \mathcal{K}^2,\ t \mapsto \gamma_t^{(E)}(B)$ is continuously differentiable and for all $t \in \mathbb{R}$ one has

$$\partial_t \gamma_t^{(E)}(B) = \langle E(t), \mathcal{X}\rangle(\gamma_t^{(E)}(B)) = \gamma_t^{(E)}(\langle E(t), \mathcal{X}\rangle(B)) . \tag{6.25}$$

Proof : We use the notation introduced in the proof of Lemma 6.5. Since we have $\mathcal{X}_k(B) \in \mathcal{K}_2$ for all $k \in \{1, ..., d\}$, we also have $\langle E(t), \mathcal{X}\rangle(B) \in \mathcal{K}^2$ for all $t \in \mathbb{R}$. So, for any $t, h \in \mathbb{R}$ the following $\mathcal{K}^2$-valued integral exists in a Bochner sense

$$\eta_{t,h} := \int_0^h \gamma_{t,r}^{(E)}(\langle E(t+r), \mathcal{X}\rangle(B))\, \mathrm{d}r .$$

In addition, because of Lemma 6.5, the integral includes a continuous integral mapping. This implies $\partial_h \eta_{t,h} = \gamma_{t,h}^{(E)}(\langle E(t+h), \mathcal{X}\rangle(B))$ for any $t, h \in \mathbb{R}$. Moreover, one has

$$\langle \delta_x, \eta_{\omega,t,h}\delta_y\rangle = \langle \delta_x, (\gamma_{t,h}^{(E)}(B_\omega) - B_\omega)\delta_y\rangle$$

for any $t, h \in \mathbb{R}$, $x, y \in \mathbb{Z}^d$ and almost every $\omega \in \Omega$. This follows from the fact that both sides vanish for $h = 0$ (Lemma 6.5) and posses the same derivatives (Lemma 6.4). Altogether, equivalently to Equation (6.25) for any $t \in \mathbb{R}$ we get

$$\lim_{h\to 0} \frac{1}{h}(\gamma_{t,h}^{(E)}(B) - B) = \partial_h \eta_{t,h}|_{h=0} = \langle E(t), \mathcal{X}\rangle(B) .$$

∎

Lemma 6.7

Let $(E_n)_{n\in\mathbb{N}}$ be a sequence in $\mathcal{E}(\mathbb{R},\mathbb{R}^d)$ such that $\lim_{n\to\infty}\|\chi_{]-\infty,t]}E_n\|_1 = 0$ for any $t\in\mathbb{R}$. Then, for any $t\in\mathbb{R}$ and $B\in\mathcal{K}^2$ one has

$$\lim_{n\to\infty}|||\gamma_t^{(E_n)}(B)-B|||_2 = 0\,. \tag{6.26}$$

Proof: For any $t\in\mathbb{R}$ and $\psi\in\mathfrak{h}$ we have $\lim\limits_{n\to\infty}\|(1-G^{(E_n)}(t)^*)\psi\| = 0$. Moreover, as in the proof of Lemma 6.5 the identity

$$\gamma_t^{(E_n)}(B)-B = G^{(E_n)}(t)((1-G^{(E_n)}(t)^*)B + B(G^{(E_n)}(t)^*-1)) \tag{6.27}$$

holds for any $n\in\mathbb{N}$, $t\in\mathbb{R}$ and $B\in\mathscr{L}(\mathfrak{h}_c,\mathfrak{h})$. An analogous calculation as in the proof of Lemma 6.5 leads to the identity

$$|||\gamma_t^{(E_n)}(B)-B|||_2^2 = \mathbb{E}[\|(1-G^{(E_n)}(t)^*)B\delta_0\|^2]\,, \tag{6.28}$$

which holds for any $n\in\mathbb{N}$, $t\in\mathbb{R}$ and $B\in\mathcal{K}^2$. Then, the statement of Lemma 6.7 follows from an application of Lemma 6.2. ■

6.1.4. Schrödinger Operator

We define the random Schrödinger operator that describes the total energy of a single electron in the disordered solid state. In a first step we introduce the random magnetic Laplacian.
Let ϑ be a mapping from a probability space Ω to the real-valued mappings on the oriented edges of $\mathbb{Z}^d$, so for each $\omega\in\Omega$ the value ϑ_ω is such a real-valued mapping. This mapping implements the effect of a random magnetic field on the electron. In addition, for each $\omega\in\Omega$ the magnetic potential is assumed to satisfy the symmetry condition $\vartheta_\omega(x,y) = -\vartheta_\omega(y,x)$ whenever $x,y\in\mathbb{Z}^d$ are neighbouring vertices. In this case, for each $\omega\in\Omega$ the discrete magnetic Laplacian $\Delta(\vartheta_\omega)$ on $\mathfrak{h}$ is defined by

$$(\Delta(\vartheta_\omega)\psi)(x) := -\sum_{\substack{y\in\mathbb{Z}^d,\\ |x-y|=1}} \mathrm{e}^{-\mathrm{i}\vartheta_\omega(x,y)}\,\psi(y)\,. \tag{6.29}$$

for all $\psi\in\mathfrak{h}$ and $x\in\mathbb{Z}^d$. The random magnetic Laplacian models the kinetic energy of a single electron in a random magnetic field.

Lemma 6.8

For each $\omega\in\Omega$ the magnetic Laplacian $\Delta(\vartheta_\omega)$ is a bounded, linear and self-adjoint operator.

Proof: Let $\omega\in\Omega$ be arbitrary. The boundedness of the magnetic Laplacian is a consequence of the following estimate which is valid for all $\psi\in\mathfrak{h}$

$$\begin{aligned}
\|\Delta(\vartheta_\omega)\psi\|^2 &= \sum_{x\in\mathbb{Z}^d}|\Delta(\vartheta_\omega)\psi(x)|^2 = \sum_{x\in\mathbb{Z}^d}\Big|\sum_{\substack{y\in\mathbb{Z}^d,\\ |x-y|=1}}\mathrm{e}^{-\mathrm{i}\vartheta_\omega(x,y)}\psi(y)\Big|^2\\
&\le \sum_{x\in\mathbb{Z}^d}\Big(\sum_{\substack{y\in\mathbb{Z}^d,\\ |x-y|=1}}\big|\mathrm{e}^{-\mathrm{i}\vartheta_\omega(x,y)}\big|^2\Big)\Big(\sum_{\substack{y\in\mathbb{Z}^d,\\ |x-y|=1}}|\psi(y)|^2\Big) = 2d\sum_{x\in\mathbb{Z}^d}\sum_{\substack{y\in\mathbb{Z}^d,\\ |x-y|=1}}|\psi(y)|^2\\
&= (2d)^2\sum_{x\in\mathbb{Z}^d}|\psi(x)|^2 = 4d^2\|\psi\|^2\,.
\end{aligned}$$

The self-adjointness of the magnetic Laplacian then follows from the fact that for all $\phi, \psi \in \mathfrak{h}$ we have

$$\begin{aligned}\langle \phi, \Delta(\vartheta_\omega)\psi\rangle &= \sum_{x\in\mathbb{Z}^d} \overline{\phi(x)}(\Delta(\vartheta_\omega)\psi)(x) = -\sum_{x\in\mathbb{Z}^d} \overline{\phi(x)}\Big(\sum_{\substack{y\in\mathbb{Z}^d,\\ |x-y|=1}} \mathrm{e}^{-\mathrm{i}\vartheta_\omega(x,y)}\psi(y)\Big)\\ &= -\sum_{\substack{x,y\in\mathbb{Z}^d,\\ |x-y|=1}} \mathrm{e}^{-\mathrm{i}\vartheta_\omega(x,y)}\overline{\phi(x)}\,\psi(y) = -\sum_{y\in\mathbb{Z}^d}\Big(\sum_{\substack{x\in\mathbb{Z}^d,\\ |x-y|=1}} \overline{\mathrm{e}^{\mathrm{i}\vartheta_\omega(x,y)}\phi(x)}\Big)\psi(y)\\ &= -\sum_{y\in\mathbb{Z}^d}\Big(\overline{\sum_{\substack{x\in\mathbb{Z}^d,\\ |x-y|=1}} \mathrm{e}^{-\mathrm{i}\vartheta_\omega(y,x)}\phi(x)}\Big)\psi(y) = \sum_{y\in\mathbb{Z}^d}\overline{(\Delta(\vartheta_\omega)\phi)(y)}\,\psi(y) = \langle\Delta(\vartheta_\omega)\phi,\psi\rangle\ .\end{aligned}$$

■

We consider the action of the gauge automorphisms on the magnetic Laplacian. Introducing the mapping $R : \mathbb{Z}^d \times \mathbb{Z}^d \to \mathbb{R}^d, (x, y) \mapsto y - x$, for any $\omega \in \Omega$, $t \in \mathbb{R}$ and $\psi \in \mathfrak{h}$ we obtain

$$\begin{aligned}(\gamma_t^{(E)}(\Delta(\vartheta_\omega))\psi)(x) &= (G^{(E)}(t)\Delta(\vartheta_\omega)G^{(E)}(t)^*\psi)(x) = -\mathrm{e}^{\mathrm{i}\langle F^{(E)}(t),x\rangle}\sum_{\substack{y\in\mathbb{Z}^d,\\ |y-x|=1}} \mathrm{e}^{-\mathrm{i}\vartheta_\omega(x,y)}\mathrm{e}^{-\mathrm{i}\langle F^{(E)}(t),y\rangle}\psi(y)\\ &= -\sum_{\substack{y\in\mathbb{Z}^d,\\ |y-x|=1}} \mathrm{e}^{-\mathrm{i}(\vartheta_\omega(x,y)+\langle F^{(E)}(t),y-x\rangle)}\psi(y) = (\Delta(\vartheta_\omega + \langle F^{(E)}(t),R\rangle)\psi)(x)\ .\end{aligned}$$

Thus, we found the transformation law for the magnetic Laplacian with respect to the gauge automorphisms, i.e. for any $\omega \in \Omega$ and all $t \in \mathbb{R}$ one has

$$\gamma_t^{(E)}(\Delta(\vartheta_\omega)) = \Delta(\vartheta_\omega + \langle F^{(E)}(t), R\rangle)\ . \tag{6.30}$$

We define the random Schrödinger operator $H^{(E,\mu)}(t) : \Omega \to \mathfrak{B}, \omega \mapsto H_\omega^{(E,\mu)}(t)$ at time $t \in \mathbb{R}$ as a sum of the magnetic Laplacian that appeared in Equation (6.30), a constant $\mu \in \mathbb{R}$ called the *chemical potential* and a random potential $V \in \mathcal{K}^\infty$ as considered in Subsection 6.1.2. Namely, for each $\omega \in \Omega$ and $t \in \mathbb{R}$ we set

$$H_\omega^{(E,\mu)}(t) := -\Delta(\vartheta_\omega + \langle F^{(E)}(t), R\rangle) - \mu + V_\omega\ . \tag{6.31}$$

For each $\omega \in \Omega$ the Schrödinger operator $H_\omega^{(E,\mu)}(t)$ is self-adjoint. For the special case of a vanishing electric field the Schrödinger operator becomes time independent. Thus, we just write $H_\omega^{(\mu)}$. Using this notation we have $H_\omega^{(E,\mu)}(t) = \gamma_t^{(E)}(H_\omega^{(\mu)})$ for all $\omega \in \Omega$ and $t \in \mathbb{R}$.
We want the Schrödinger operator to transform covariantly, so for all $t \in \mathbb{R}$, $a \in \mathbb{Z}^d$ and almost every $\omega \in \Omega$ we assume that the equation

$$\varphi_a(H_\omega^{(E,\mu)}(t)) = H_{\phi_a(\omega)}^{(E,\mu)}(t) \tag{6.32}$$

holds. For example, this is satisfied, if in Equation (6.2) we set $S = 0$ and if for any $x, y, a \in \mathbb{Z}^d$ and $\omega \in \Omega$ one has $\vartheta_\omega(x - a, y - a) = \vartheta_{\phi_a(\omega)}(x, y)$. In this case, chemical and electric potential in Equation (6.31) already transform covariantly. Thus, covariance just needs to be checked for the magnetic Laplacian. Since the shift automorphisms and the gauge automorphisms commute, only the special case of vanishing electric field needs to be considered. For the time independent magnetic Laplacian covariance holds, because for any $\psi \in \mathfrak{h}$, $x, a \in \mathbb{Z}^d$ and almost every $\omega \in \Omega$ we have

$$\begin{aligned}(\varphi_a(\Delta(\vartheta_\omega))\psi)(x) &= (T(a)\Delta(\vartheta_\omega)T(a)^*\psi)(x) = -\sum_{\substack{y\in\mathbb{Z}^d,\\ |y-(x-a)|=1}} \mathrm{e}^{-\mathrm{i}\vartheta_\omega(x-a,y)}\psi(y+a)\\ &= -\sum_{\substack{y\in\mathbb{Z}^d,\\ |y-x|=1}} \mathrm{e}^{-\mathrm{i}\vartheta_\omega(x-a,y-a)}\psi(y) = -\sum_{\substack{y\in\mathbb{Z}^d,\\ |y-x|=1}} \mathrm{e}^{-\mathrm{i}\vartheta_{\phi_a(\omega)}(x,y)}\psi(y) = (\Delta(\vartheta_{\phi_a(\omega)})\psi)(x)\ .\end{aligned}$$

We are also interested in restricting the system to arbitrary subsets $\Lambda \subset \mathbb{Z}^d$. Therefore, given any $\Lambda \subset \mathbb{Z}^d$ and a specific type of boundary condition, we define the restricted Schrödinger operator $H^{(E,\mu)}_{\Lambda,\omega}(t)$ at time $t \in \mathbb{R}$, in realisation $\omega \in \Omega$ as the bounded, linear and self-adjoint operator that is uniquely determined by

$$\langle \delta_x, H^{(E,\mu)}_{\Lambda,\omega}(t)\delta_y\rangle := \begin{cases} \langle \delta_x, H^{(E,\mu)}_{\omega}(t)\delta_y\rangle + f(x)\,\delta_{x,y} & \text{for } x,y \in \Lambda \\ 0 & \text{otherwise} \end{cases}, \tag{6.33}$$

where f is a bounded real-valued mapping on Λ vanishing in the interior of Λ and $\delta_{x,y}$ is Kronecker's delta. If $f = 0$, the boundary conditions are called *simple*. Another type, called *Dirichlet boundary conditions*, are defined by $f(x) = 2d - \mathrm{neigh}_\Lambda(x)$ for any $x \in \Lambda$, where $\mathrm{neigh}_\Lambda(x)$ is the number of neighbouring vertices $x \in \Lambda$ that are also located in Λ (Kir07) . Finally, the case, where $f(x) = \mathrm{neigh}_\Lambda(x) - 2d$ for any $x \in \Lambda$, will be denoted as *Neumann boundary conditions* (Kir07). For each $\Lambda \subset \mathbb{Z}^d$, $\omega \in \Omega$ and $t \in \mathbb{R}$ the Schrödinger operator induces a derivation $\mathcal{H}^{(E)}_{\Lambda,\omega,t} : \mathfrak{B} \to \mathfrak{B}$ by

$$\mathcal{H}^{(E)}_{\Lambda,\omega,t}(B) := \mathrm{i}[H^{(E,\mu)}_{\Lambda,\omega}(t), B] \tag{6.34}$$

for any $B \in \mathfrak{B}$. For $\Lambda = \mathbb{Z}^d$ we just write $\mathcal{H}^{(E)}_{\omega,t}$. In this case, for each $t \in \mathbb{R}$ the mapping $\mathcal{H}^{(E)}_t : \Omega \to \mathrm{Der}(\mathfrak{B})$, $\omega \mapsto \mathcal{H}^{(E)}_{\omega,t}$ forms a covariant derivation, since for any $a \in \mathbb{Z}^d$, $B \in \mathfrak{B}$ and almost every $\omega \in \Omega$ one has

$$\begin{aligned}\varphi_a(\mathcal{H}^{(E)}_{\omega,t}(B)) &= \mathrm{i}\varphi_a([H^{(E,\mu)}_{\omega}(t), B]) = \mathrm{i}[\varphi_a(H^{(E,\mu)}_{\omega}(t)), \varphi_a(B)] \\ &= \mathrm{i}[H^{(E,\mu)}_{\phi_a(\omega)}(t), \varphi_a(B)] = \mathcal{H}^{(E)}_{\phi_a(\omega),t}(\varphi_a(B))\,.\end{aligned}$$

6.1.5. Velocity Operator

For each $\omega \in \Omega$, $\Lambda \subset \mathbb{Z}^d$ and $t \in \mathbb{R}$ the velocity operator $D^{(E)}_{\Lambda,\omega}(t) := (D^{(E)}_{\Lambda,\omega,1}(t), ..., D^{(E)}_{\Lambda,\omega,d}(t))$ is defined as the closure of the commutator of the Schrödinger operator with the components of the position operator, precisely[5]

$$D^{(E)}_{\Lambda,\omega,k}(t)\psi := \frac{\mathrm{i}}{2}[H^{(E,\mu)}_{\Lambda,\omega}(t), X_k]\psi \tag{6.35}$$

for each $k \in \{1, ..., d\}$ and $\psi \in \mathfrak{h}_c$. For the time independent case of vanishing electric field, we just write $D_{\Lambda,\omega}$. We drop the label Λ for $\Lambda = \mathbb{Z}^d$. Clearly, for finite volume $\Lambda \subset \mathbb{Z}^d$ the velocity operator is bounded. But also for the case $\Lambda = \mathbb{Z}^d$, the velocity operator is bounded. This is the statement of the following lemma. Let $\{e_k : k \in \{1, ..., d\}\}$ be the canonical basis of $\mathbb{R}^d$.

Lemma 6.9

For all $\omega \in \Omega$, $k \in \{1, ..., d\}$ and $t \in \mathbb{R}$, the components of the velocity operator are bounded self-adjoint operators on $\mathfrak{h}$ and for any $\omega \in \Omega$, $k \in \{1, ..., d\}$, $\psi \in \mathfrak{h}$ and $x \in \mathbb{Z}^d$ we have

$$(D_{\omega,k}\psi)(x) = \frac{\mathrm{i}}{2}(\mathrm{e}^{-\mathrm{i}\vartheta_\omega(x,x+e_k)}\psi(x + e_k) - \mathrm{e}^{-\mathrm{i}\vartheta_\omega(x,x-e_k)}\psi(x - e_k))\,. \tag{6.36}$$

[5] The factor $\frac{1}{2}$ in the definition of the velocity operator was introduced for convenience.

Proof: First we show boundedness of D_ω for any $\omega \in \Omega$. Therefore, let $\psi \in \mathfrak{h}_c$. Then, for all $\omega \in \Omega$, $k \in \{1, ..., d\}$ and $x \in \mathbb{Z}^d$ we obtain

$$\begin{aligned}(D_{\omega,k}\psi)(x) &= \frac{\mathrm{i}}{2}([H_\omega^{(\mu)}, X_k]\psi)(x) = \frac{\mathrm{i}}{2}([-\Delta(\vartheta_\omega) - \mu + V_\omega, X_k]\psi)(x) = \frac{\mathrm{i}}{2}([-\Delta(\vartheta_\omega), X_k]\psi)(x)\\ &= \frac{\mathrm{i}}{2}\Big(\sum_{\substack{y\in\mathbb{Z}^d,\\ |x-y|=1}} \mathrm{e}^{-\mathrm{i}\vartheta_\omega(x,y)} y_k\psi(y) - x_k \sum_{\substack{y\in\mathbb{Z}^d,\\ |x-y|=1}} \mathrm{e}^{-\mathrm{i}\vartheta_\omega(x,y)}\psi(y)\Big) = \frac{\mathrm{i}}{2}\sum_{\substack{y\in\mathbb{Z}^d,\\ |x-y|=1}} \mathrm{e}^{-\mathrm{i}\vartheta_\omega(x,y)}(y-x)_k\psi(y)\\ &= \frac{\mathrm{i}}{2}\Big(\sum_{l=1}^d \mathrm{e}^{-\mathrm{i}\vartheta_\omega(x,x+e_l)}(e_l)_k\psi(x+e_l) - \sum_{l=1}^d \mathrm{e}^{-\mathrm{i}\vartheta_\omega(x,x-e_l)}(e_l)_k\psi(x-e_l)\Big)\\ &= \frac{\mathrm{i}}{2}(\mathrm{e}^{-\mathrm{i}\vartheta_\omega(x,x+e_k)}\psi(x+e_k) - \mathrm{e}^{-\mathrm{i}\vartheta_\omega(x,x-e_k)}\psi(x-e_k))\,.\end{aligned}$$

From this one directly obtains the boundedness of the operator, since

$$\|D_{\omega,k}\psi\|^2 = \sum_{x\in\mathbb{Z}^d} |D_{\omega,k}\psi(x)|^2 \le \sum_{x\in\mathbb{Z}^d} 2(|\psi(x+e_k)|^2 + |\psi(x-e_k)|^2) = 4\,\|\psi\|^2\,.$$

From the fact that $D_{\omega,k}^{(E)}(t) = \frac{\mathrm{i}}{2}[H_\omega^{(E,\mu)}(t), X_k] = \frac{\mathrm{i}}{2}[\gamma_t^{(E)}(H_\omega^{(\mu)}), \gamma_t^{(E)}(X_k)] = \gamma_t^{(E)}(D_{\omega,k})$ for any $t \in \mathbb{R}$ we get uniform boundedness of the velocity operator in time. Since $H_\omega^{(E,\mu)}$ is a bounded and self-adjoint operator with $H_\omega^{(E,\mu)}(\mathfrak{h}_c) \subset \mathfrak{h}_c$ for each $\omega \in \Omega$ and since the position operator is essentially self-adjoint on $\mathfrak{h}_c$, one gets that the velocity operator defined by Equation (6.35) is self-adjoint. ■

Given the bounded velocity operator, for any $\Lambda \subset \mathbb{Z}^d$, $\omega \in \Omega$, $k \in \{1, ..., d\}$ pointwise for any $B \in \mathfrak{B}$ one can define bounded derivations $\mathcal{D}_{\Lambda,\omega,k,t}^{(E)} : \mathfrak{B} \to \mathfrak{B}$ by

$$\mathcal{D}_{\Lambda,\omega,k,t}^{(E)}(B) := \mathrm{i}[D_{\Lambda,\omega,k}^{(E)}(t), B]\,. \tag{6.37}$$

If $\Lambda = \mathbb{Z}^d$, we drop the label Λ. Note that the velocity operator transforms covariantly. Therefore the mappings $\mathcal{D}_{k,t}^{(E)} : \Omega \to \mathrm{Der}(\mathfrak{B})$ form covariant derivations for all $k \in \{1, ..., d\}$ and $t \in \mathbb{R}$. All this follows from the fact that for almost all $\omega \in \Omega$, $k \in \{1, ..., d\}$, $t \in \mathbb{R}$ and $\psi \in \mathfrak{h}_c$ we have

$$\begin{aligned}\varphi_a(D_{\omega,k}^{(E)}(t))\psi &= \frac{\mathrm{i}}{2}\varphi_a([H_\omega^{(E,\mu)}(t), X_k])\psi\\ &= \frac{\mathrm{i}}{2}[\varphi_a(H_\omega^{(E,\mu)}(t)), \varphi_a(X_k)]\psi\\ &= \frac{\mathrm{i}}{2}[H_{\phi_a(\omega)}^{(E,\mu)}(t), X_k - a_k]\psi = \frac{\mathrm{i}}{2}[H_{\phi_a(\omega)}^{(E,\mu)}(t), X_k]\psi = D_{\phi_a(\omega),k}^{(E)}(t)\psi\,.\end{aligned}$$

The following lemma investigates the time dependence of the Schrödinger operator induced by the electric field. Its usefulness will become evident in the proof of Lemma 6.13, where a Duhamel formula for the unitary propagator is achieved. This will be of importance for the linear response theory in Chapter 9.

Lemma 6.10

For all electric fields $E \in \mathcal{E}(\mathbb{R}, \mathbb{R}^d)$, chemical potentials $\mu \in \mathbb{R}$, times $t, r \in \mathbb{R}$ and realisations $\omega \in \Omega$ of the system the following identities hold

$$H_\omega^{(E,\mu)}(t) - H_\omega^{(E,\mu)}(r) = -2\int_r^t \langle E(q), D_\omega^{(E)}(q)\rangle\,\mathrm{d}q\,, \tag{6.38}$$

$$H_\omega^{(E,\mu)}(t) - H_\omega^{(\mu)} = -2\int_{-\infty}^t \langle E(q), D_\omega^{(E)}(q)\rangle\,\mathrm{d}q\,. \tag{6.39}$$

Proof: First assume $\psi \in \mathfrak{h}_c$. Then, because we have $H_\omega^{(E,\mu)}(t)\psi = G^{(E)}(t)H_\omega^{(\mu)}G^{(E)}(t)^*\psi$ for any $\omega \in \Omega$ and $t \in \mathbb{R}$, one obtains

$$\begin{aligned}\partial_t H_\omega^{(E,\mu)}(t)\psi &= \partial_t G^{(E)}(t)H_\omega^{(\mu)}G^{(E)}(t)^*\psi \\ &= \mathrm{i}\,\langle E(t), X\rangle G^{(E)}(t)H_\omega^{(\mu)}G^{(E)}(t)^*\psi - \mathrm{i}\,G^{(E)}(t)H_\omega^{(\mu)}G^{(E)}(t)^*\,\langle E(t), X\rangle\psi \\ &= \mathrm{i}\,[\langle E(t), X\rangle, H_\omega^{(E,\mu)}(t)]\psi = -2\big\langle E(t), D_\omega^{(E)}(t)\big\rangle\psi\,.\end{aligned}$$

Because of the estimate[6] $\|\langle E(t), D_\omega^{(E)}(t)\rangle\| \leq |E(t)|\,\|D_\omega\|$, the following equalities including Bochner integrals hold for all $t, r \in \mathbb{R}$

$$\begin{aligned}H_\omega^{(E,\mu)}(t)\psi - H_\omega^{(E,\mu)}(r)\psi &= \int_r^t \partial_q H_\omega^{(E,\mu)}(q)\psi\,\mathrm{d}q = -2\int_r^t \big\langle E(q), D_\omega^{(E)}(q)\big\rangle\psi\,\mathrm{d}q \\ &= -2\int_r^t \big\langle E(q), D_\omega^{(E)}(q)\big\rangle\,\mathrm{d}q\,\psi\,.\end{aligned}$$

This still holds taking the limit $r \to -\infty$ on both sides, because $\lim_{r\to-\infty} G^{(E)}(r)\psi = \psi$ and $E \in \mathcal{E}(\mathbb{R}, \mathbb{R}^d)$ resulting $\lim_{r\to-\infty} H_\omega^{(E,\mu)}(r)\psi = H_\omega^{(\mu)}\psi$ and $\int_{-\infty}^t \langle E(q), D_\omega^{(E)}(q)\rangle\,\mathrm{d}q\,\psi = \lim_{r\to-\infty}\int_r^t \langle E(q), D_\omega^{(E)}(q)\rangle\,\mathrm{d}q\,\psi$ by dominated convergence, respectively. Finally, since both sides of this equation describe bounded linear operators on $\mathfrak{h}$, we get the statement of the lemma. ■

6.1.6. Current Density Operator

In this subsection we introduce the random current density operator which is an operator of finite support depending on the realisation $\omega \in \Omega$, time $t \in \mathbb{R}$, and a position of measurement $y \in \mathbb{Z}^d$. For its precise definition we let χ_y denote the multiplication operator on $\mathfrak{h}$ induced by the characteristic function of the point $y \in \mathbb{Z}^d$.

Definition 6.11 (*Current Density Operator*)

For any $\Lambda \subset \mathbb{Z}^d$, $\omega \in \Omega$, $t \in \mathbb{R}$ and $y \in \mathbb{Z}^d$ the *current density operator* is defined as the anti-commutator of the velocity operator $D_{\Lambda,\omega}^{(E)}(t)$ and the multiplication operator χ_y, i.e. for any $k \in \{1, ..., d\}$

$$J_{\Lambda,\omega,k}^{(E)}(t, y) := \{D_{\Lambda,\omega,k}^{(E)}(t), \chi_y\}\,. \tag{6.40}$$

The interpretation of the current density operator $J_{\Lambda,\omega}^{(E)}(t, y) = (J_{\Lambda,\omega,1}^{(E)}(t, y), ..., J_{\Lambda,\omega,d}^{(E)}(t, y))$ in terms of a self-adjoint operator representing a measurement is, that it incorporates the presence as well as the velocity of an electron at time $t \in \mathbb{R}$ and at position $y \in \mathbb{Z}^d$ in a random solid state in realisation $\omega \in \Omega$. Once again, for the case $\Lambda = \mathbb{Z}^d$, we drop the label Λ. If there is no electric field, the arguments E and t are dropped.
For any $x, y \in \mathbb{Z}^d$ we have that $J_{\Lambda,\omega}^{(E)}(t, y)\delta_x = 0$ for all $\omega \in \Omega$ and $t \in \mathbb{R}$, unless x and y both are in Λ and are nearest neighbours. Since the support of the current density operator is finite and is given by a box centred at $y \in \mathbb{Z}^d$ of side length 2, we have that for simple, for Dirichlet and for Neumann boundary conditions the operators $J_\omega^{(E)}(t, y)$ and $J_{\Lambda,\omega}^{(E)}(t, y)$ agree for any $y \in \Lambda$ in a fixed “safety distance“ from the boundary of Λ. This is important having a thermodynamical limit in view.
Also, we are interested in a transformation law for the current density operator with respect to the shift automorphisms, i.e. for fixed $t \in \mathbb{R}$ and $y \in \mathbb{Z}^d$ we investigate the action of shift

[6] For $B = (B_1, ..., B_d)$, where $B_k : \mathfrak{B} \to \mathfrak{B}$ for any $k \in \{1, ..., d\}$, we set $\|B\|^2 := \sum_{k=1}^d \|B_k\|^2$.

automorphisms on the mapping $J_k^{(E)}(t,y) : \Omega \to \mathfrak{B}_c,\ \omega \mapsto J_{\omega,k}^{(E)}(t,y)$ for $k \in \{1,...,d\}$. Note that due to the appearance of a characteristic function in the definition of the current density operator, $J_k^{(E)}(t,y)$ does not define a covariant mapping. However, there is a transformation law which is stated in the following lemma.

Theorem 6.12 (*Transformation Law of the Current Density Operator*)

Let $t,r \in \mathbb{R}$ and $y,a \in \mathbb{Z}^d$. Then, for all $k \in \{1,...,d\}$ and almost every $\omega \in \Omega$, the current density operator satisfies the following transformation law

$$\varphi_a(J_{\omega,k}^{(E)}(t,y)) = J_{\phi_a(\omega),k}^{(E)}(t,y+a)\ . \tag{6.41}$$

Proof: Let $\omega \in \Omega$, $k \in \{1,...,d\}$, $t,r \in \mathbb{R}$ and $y,a \in \mathbb{Z}^d$ be arbitrary. Since one has $\varphi_a(\chi_y) = \chi_{y+a}$, the current density operator transforms

$$\begin{aligned}\varphi_a(J_{\omega,k}^{(E)}(t,y)) &= \varphi_a(\{D_{\omega,k}^{(E)}(t),\chi_y\})\\ &= \{\varphi_a(D_{\omega,k}^{(E)}(t)),\varphi_a(\chi_y)\}\\ &= \{D_{\phi_a(\omega),k}^{(E)}(t),\chi_{y+a}\}\\ &= J_{\phi_a(\omega),k}^{(E)}(t,y+a)\ .\end{aligned}$$

■

6.1.7. Time Evolution

On the Hilbert space level the time evolution of our system restricted to a volume $\Lambda \subset \mathbb{Z}^d$ and in realisation $\omega \in \Omega$ is described by the so called *unitary propagator* which is a unitary operator that is completely determined by the Schrödinger operator of the system. For the case of a vanishing electric field, the propagator is given by

$$U_{\Lambda,\omega}^{(0,\mu)}(t,r) := \mathrm{e}^{\mathrm{i}(r-t)H_{\Lambda,\omega}^{(\mu)}}\ , \tag{6.42}$$

where $r,t \in \mathbb{R}$ are the starting and the end point of the time evolution of the system, respectively. In this case, since the system is time translation invariant, the propagator just depends on the difference of the starting and the end point of the time evolution. So, using just one argument in this case, we set $U_{\Lambda,\omega}^{(\mu)}(t) := U_{\Lambda,\omega}^{(0,\mu)}(t,0)$ for any $t \in \mathbb{R}$.

For the case of a non-vanishing electric field, the unitary propagator is approximated, roughly speaking, by Riemannian sums. More concretely, for any $n \in \mathbb{N}$, $k \in \mathbb{Z}$, $\omega \in \Omega$ and times $\frac{k-1}{n} \le r \le t \le \frac{k}{n}$ we set

$$U_{n,\Lambda,\omega}^{(E,\mu)}(t,r) := \mathrm{e}^{\mathrm{i}(r-t)H_{\Lambda,\omega}^{(E,\mu)}(t_{n,k})}\ , \tag{6.43}$$

$$U_{n,\Lambda,\omega}^{(E,\mu)}(r,t) := U_{n,\Lambda,\omega}^{(E,\mu)}(t,r)^*\ , \tag{6.44}$$

where $t_{n,k} := \frac{k-1}{n}$. Moreover, for arbitrary $n \in \mathbb{N}$, $\omega \in \Omega$ and $t,r,q \in \mathbb{R}$ the operator $U_{n,\Lambda,\omega}^{(E,\mu)}(t,q)$ is defined recursively as the operator satisfying the relation

$$U_{n,\Lambda,\omega}^{(E,\mu)}(t,q) = U_{n,\Lambda,\omega}^{(E,\mu)}(t,r)U_{n,\Lambda,\omega}^{(E,\mu)}(r,q)\ . \tag{6.45}$$

As stated in (Yos80)[Theorem XIV.3.1] as well as in (BGKS05), for any $\omega \in \Omega$ and $t,r \in \mathbb{R}$ the sequence $(U_{n,\Lambda,\omega}^{(E,\mu)}(t,r))_{n\in\mathbb{N}}$ converges in norm to an operator $U_{\Lambda,\omega}^{(E,\mu)}(t,r)$, the unitary propagator of the system. The latter satisfies the following relations for all $t, r, q \in \mathbb{R}$ and every $\omega \in \Omega$

$$U^{(E,\mu)}_{\Lambda,\omega}(t,t) = \mathrm{id}\,, \tag{6.46}$$

$$U^{(E,\mu)}_{\Lambda,\omega}(t,r)U^{(E,\mu)}_{\Lambda,\omega}(r,q) = U^{(E,\mu)}_{\Lambda,\omega}(t,q)\,, \tag{6.47}$$

$$\mathrm{i}\partial_t U^{(E,\mu)}_{\Lambda,\omega}(t,r) = H^{(E,\mu)}_{\Lambda,\omega}(t)U^{(E,\mu)}_{\Lambda,\omega}(t,r)\,, \tag{6.48}$$

$$-\mathrm{i}\partial_r U^{(E,\mu)}_{\Lambda,\omega}(t,r) = U^{(E,\mu)}_{\Lambda,\omega}(t,r)H^{(E,\mu)}_{\Lambda,\omega}(r)\,. \tag{6.49}$$

Note that there is no ambiguity between the definition in (6.42) and what follows Equation (6.43) for the special case of vanishing electric field. We drop the label Λ for $\Lambda = \mathbb{Z}^d$. The following two lemmas investigate the dependence of the unitary propagator on the electric field $E \in \mathcal{E}(\mathbb{R}, \mathbb{R}^d)$. The first lemma contains the so called Duhamel formula. A similar form of this was obtained in (BGKS05)[Lemma 2.8]

Lemma 6.13 (*Duhamel Formula*)

For any $\omega \in \Omega$ and any times $t, r \in \mathbb{R}$ the following so called *Duhamel formula* holds

$$U^{(E,\mu)}_{\omega}(r,t) = U^{(\mu)}_{\omega}(r-t) - 2\mathrm{i}\int_r^t U^{(\mu)}_{\omega}(r-q)\Big(\int_{-\infty}^q \langle E(p), D^{(E)}_{\omega}(p)\rangle\,\mathrm{d}p\Big)U^{(E,\mu)}_{\omega}(r,t)\,\mathrm{d}q\,. \tag{6.50}$$

Proof: For any $\omega \in \Omega$ and $t, r \in \mathbb{R}$ we define unitary operators by $V^{(E,\mu)}_{\omega}(t,r) := U^{(\mu)}_{\omega}(t-r)U^{(E,\mu)}_{\omega}(r,t)$ and differentiate with respect to r, leading to

$$\mathrm{i}\partial_r V^{(E,\mu)}_{\omega}(t,r) = U^{(\mu)}_{\omega}(t-r)(H^{(E,\mu)}_{\omega}(r) - H^{(\mu)}_{\omega})U^{(E,\mu)}_{\omega}(r,t)\,.$$

Using the statement of Lemma 6.10 for any $t, r \in \mathbb{R}$ we obtain the following equalities, where the integrals exist in a Bochner sense.

$$\begin{aligned}
\mathrm{id} - U^{(\mu)}_{\omega}(t-r)U^{(E,\mu)}_{\omega}(r,t) = V^{(E,\mu)}_{\omega}(t,t) - V^{(E,\mu)}_{\omega}(t,r) &= \int_r^t \partial_q V^{(E,\mu)}_{\omega}(t,q)\,\mathrm{d}q \\
&= -\mathrm{i}\int_r^t U^{(\mu)}_{\omega}(t-q)(H^{(E,\mu)}_{\omega}(q) - H^{(\mu)}_{\omega})U^{(E,\mu)}_{\omega}(q,t)\,\mathrm{d}q \\
&= 2\mathrm{i}\int_r^t U^{(\mu)}_{\omega}(t-q)\Big(\int_{-\infty}^q \langle E(p), D^{(E)}_{\omega}(p)\rangle\,\mathrm{d}p\Big)U^{(E,\mu)}_{\omega}(q,t)\,\mathrm{d}q \\
&= 2\mathrm{i}\int_r^t U^{(\mu)}_{\omega}(t-q)\Big(\int_{-\infty}^q \langle E(p), D^{(E)}_{\omega}(p)\rangle\,\mathrm{d}p\Big)U^{(E,\mu)}_{\omega}(q,t)\,\mathrm{d}q\,.
\end{aligned}$$

From a multiplication on both sides with the operator $U^{(\mu)}_{\omega}(r-t)$ we obtain the statement of the lemma. ∎

Corollary 6.14 (*Convergence of Unitary Propagators on One-Electron Space*)

Let $(E_n)_{n\in\mathbb{N}}$ be a sequence in $\mathcal{E}(\mathbb{R}, \mathbb{R}^d)$ such that for any $t \in \mathbb{R}$ the sequence $(\chi_{]-\infty,t]}E_n)_{n\in\mathbb{N}}$ converges to zero with respect to $L^1(\mathbb{R}, \mathbb{R}^d)$. Then, for all $r, t \in \mathbb{R}$ uniformly on compact intervals we have

$$\lim_{n\to\infty} \|U^{(E_n,\mu)}_{\omega}(r,t) - U^{(\mu)}_{\omega}(r-t)\| = 0\,. \tag{6.51}$$

Proof: Using the Duhamel formula for any $n \in \mathbb{N}$, $\omega \in \Omega$ and $t, r \in \mathbb{R}$ we directly obtain the estimate $\|U^{(E_n)}_{\omega}(r,t) - U_{\omega}(r-t)\| \leq 2\|\chi_{]-\infty,t]}E_n\|_1\,\|D_{\omega}\|\,|t-r|$. The statement of the lemma follows immediately. ∎

Note that due to the covariance of the Schrödinger operator for any fixed $t, r \in \mathbb{R}$, the mapping $U^{(E,\mu)}(t,r) : \Omega \to \mathscr{U}(\mathfrak{h}),\ \omega \mapsto U^{(E,\mu)}_\omega(t,r)$ is covariant. On the level of the C^*-algebra $\mathfrak{B}$, for fixed $\Lambda \subset \mathbb{Z}^d$ and $\omega \in \Omega$, the time evolution between the times $t, r \in \mathbb{R}$ is implemented by automorphisms $\tau^{(E)}_{\Lambda,\omega,t,r}$ that are defined by

$$\tau^{(E)}_{\Lambda,\omega,t,r}(B) := U^{(E,\mu)}_{\Lambda,\omega}(t,r) B U^{(E,\mu)}_{\Lambda,\omega}(r,t) \tag{6.52}$$

for any $B \in \mathfrak{B}$. For fixed $B \in \mathfrak{B}$ and $t \in \mathbb{R}$ the mapping $\mathbb{R} \to \mathfrak{B},\ r \mapsto \tau^{(E)}_{\Lambda,\omega,t,r}(B)$ is differentiable. In general, using the derivation introduced in Equation (6.34) as well as the Equations (6.48) and (6.49) one obtains

$$\partial_r \tau^{(E)}_{\Lambda,\omega,t,r}(B) = \tau^{(E)}_{\Lambda,\omega,t,r}(\mathcal{H}^{(E)}_{\Lambda,\omega,r}(B)) \, . \tag{6.53}$$

For the special case of vanishing electric field, the unitary propagator defines a strongly continuous one parameter group of automorphisms $\{\tau_{\Lambda,\omega,t} : t \in \mathbb{R}\}$ on $\mathfrak{B}$ via

$$\tau_{\Lambda,\omega,t}(B) := U^{(\mu)}_{\Lambda,\omega}(t) B U^{(\mu)}_{\Lambda,\omega}(t)^* = \mathrm{e}^{-\mathrm{i}tH^{(\mu)}_{\Lambda,\omega}} B \mathrm{e}^{\mathrm{i}tH^{(\mu)}_{\Lambda,\omega}} = \mathrm{e}^{-t\mathcal{H}_{\Lambda,\omega}}(B) \, . \tag{6.54}$$

For fixed $\omega \in \Omega$ and $B \in \mathfrak{B}$, the mapping $\mathbb{R} \to \mathfrak{B},\ t \mapsto \tau_{\Lambda,\omega,t}(B)$ is differentiable with respect to t and satisfies the differential equation

$$\partial_t \tau_{\Lambda,\omega,t}(B) = \tau_{\Lambda,\omega,t}(\mathcal{H}_{\Lambda,\omega}(B)) \, . \tag{6.55}$$

We concentrate on the case $\Lambda = \mathbb{Z}^d$. Obviously, via $(\tau^{(E)}_{t,r}(B))_\omega := \tau^{(E)}_{\omega,t,r}(B_\omega)$ for any $B \in \mathcal{K}^\infty$ and $\omega \in \Omega$ a bijective isometry $\tau^{(E)}_{t,r}$ is defined on $\mathcal{K}^\infty$ for any $t, r \in \mathbb{R}$. In addition, the fact that $(\tau^{(E)}_{r,t} \circ \tau^{(E)}_{t,r})(B) = B$ for any $B \in \mathcal{K}^\infty$ yields[7] $|||\tau^{(E)}_{t,r}(B)|||_2 \le |||B|||_2 \le |||\tau^{(E)}_{t,r}(B)|||_2$. So, for any $t, r \in \mathbb{R}$ the mapping $\tau^{(E)}_{t,r}$ can be extended to a unitary operator on $\mathcal{K}^2$. Again, we set $\tau^{(0)}_{t,r} =: \tau_{t-r}$ for any $t, r \in \mathbb{R}$, but in our notation we do not distinguish between these mappings on $\mathcal{K}^\infty$ and their extensions to $\mathcal{K}^2$. We prove several lemmas concerning the unitary propagator of the system (BGKS05)[Lemma 4.9], which will be used in the context of the linear response theory in Chapter 9.

Lemma 6.15

For any $B \in \mathcal{K}^2$ the mapping $\mathbb{R}^2 \to \mathcal{K}^2,\ (t,r) \mapsto \tau^{(E)}_{t,r}(B)$ is norm-continuous.

Proof: For any $\omega \in \Omega$ and $(t,r), (t',r') \in \mathbb{R}^2$ we define the mapping $\pi^{(E)}_{\omega,t,r,t',r'} := \tau^{(E)}_{\omega,t,r} \circ \tau^{(E)}_{\omega,r',t'}$. Then, the statement of Lemma 6.15 is equivalent to

$$\lim_{|(t,r)-(t',r')| \to 0} |||\pi^{(E)}_{t,r,t',r'}(B) - B|||_2^2 = 0$$

for any $(t,r) \in \mathbb{R}^2$ and $B \in \mathcal{K}^2$. Moreover, for any $(t,r), (t',r') \in \mathbb{R}^2$ we define the unitary operators $V^{(E,\mu)}_\omega(t,r,t',r') := U^{(E,\mu)}_\omega(t,r) U^{(E,\mu)}_\omega(r',t')$. Then, for any $(t,r), (t',r') \in \mathbb{R}^2$, $\omega \in \Omega$, $B \in \mathfrak{B}$ and $\psi \in \mathfrak{h}$ we have the identity $\pi^{(E)}_{\omega,t,r,t',r'}(B) = V^{(E,\mu)}_\omega(t,r,t',r') B V^{(E,\mu)}_\omega(t,r,t',r')^*$ and from Duhamel's formula we get $\lim_{|(t,r)-(t',r')| \to 0} \|(1 - V^{(E,\mu)}_\omega(t,r,t',r')^*)\psi\|^2 = 0$. As in the proof of Lemma 6.5 one uses the identity

$$\pi^{(E)}_{\omega,t,r,t',r'}(B) = V^{(E,\mu)}_\omega(t,r,t',r')((1 - V^{(E,\mu)}_\omega(t,r,t',r')^*)B + B(V^{(E,\mu)}_\omega(t,r,t',r')^* - 1)) \, ,$$

which holds for any $\omega \in \Omega$, $(t,r), (t',r') \in \mathbb{R}^2$ and $B \in \mathfrak{B}$. From this we obtain the estimate

$$|||\pi^{(E)}_{t,r,t',r'}(B) - B|||_2^2 \le \mathbb{E}[\|(1 - V^{(E,\mu)}(t,r,t',r')^*)B\delta_0\|^2] + \mathbb{E}[\|B(V^{(E,\mu)}(t,r,t',r')^* - 1)\delta_0\|^2]$$

for any $B \in \mathcal{K}^\infty$. Then, dominated convergence arguments as in Lemma 6.2 yield the statement of Lemma 6.15 for all $B \in \mathcal{K}^\infty$. Using unitarity of $\pi^{(E)}_{t,r,t',r'}$ on $\mathcal{K}^2$ as well as a density argument leads to the fact that the statement even holds true for all $B \in \mathcal{K}^2$. ∎

[7] The proof of this inequalities in (BGKS05)[Proposition 4.7] uses Hölder type arguments.

Lemma 6.16

For any $t \in \mathbb{R}$ and $B \in \mathcal{K}^2$ the mapping $\mathbb{R} \to \mathcal{K}^2,\ r \mapsto \tau^{(E)}_{t,r}(B)$ is continuously differentiable. For any $t, r \in \mathbb{R}$ and $B \in \mathcal{K}^2$ one has

$$\partial_r \tau^{(E)}_{t,r}(B) = \tau^{(E)}_{t,r}(\mathcal{H}^{(E)}_r(B)) . \tag{6.56}$$

Proof: We just briefly present the key idea in of the proof of (BGKS05)[Proposition 4.9]. For any $\omega \in \Omega$, $t, r, h \in \mathbb{R}$ and $B \in \mathcal{K}^\infty$ one has

$$\begin{aligned}\tau^{(E)}_{\omega,t,r+h}(B_\omega) - \tau^{(E)}_{\omega,t,r}(B_\omega) &= U^{(E,\mu)}_\omega(t, r+h) B_\omega U^{(E,\mu)}_\omega(r+h, t) - U^{(E,\mu)}_\omega(t,r) B_\omega U^{(E,\mu)}_\omega(r,t) \\ (U^{(E,\mu)}_\omega(t, r+h) - U^{(E,\mu)}_\omega(t,r)) B_\omega U^{(E,\mu)}_\omega(r+h,t) &+ U^{(E,\mu)}_\omega(t,r) B_\omega (U^{(E,\mu)}_\omega(r+h,t) - U^{(E,\mu)}_\omega(r,t)) .\end{aligned} \tag{6.57}$$

Then, considering the Equations (6.48) and (6.49) in the case $\Lambda = \mathbb{Z}^d$, by arguments as in Lemma 6.2 one concludes that Equation (6.56) holds. In more detail, one uses that

$$\begin{aligned} \mathrm{i}\partial_t U^{(E,\mu)}_\omega(t,r) &= H^{(E,\mu)}_\omega(t) U^{(E,\mu)}_\omega(t,r) , \\ -\mathrm{i}\partial_r U^{(E,\mu)}_\omega(t,r) &= U^{(E,\mu)}_\omega(t,r) H^{(E,\mu)}_\omega(r) \end{aligned}$$

in the sense of Fréchet derivatives on $\mathfrak{B}$ for any $\omega \in \Omega$ and $t, r \in \mathbb{R}$. Considering the partition in Equation (6.57), arguments as in Lemma 6.2 provide that

$$\lim_{h \to 0} \frac{1}{h} (\tau^{(E)}_{t,r+h}(B) - \tau^{(E)}_{t,r}(B)) = \tau^{(E)}_{t,r}(\mathcal{H}^{(E)}_r(B))$$

for any $t, r \in \mathbb{R}$ and $B \in \mathcal{K}^2$, where the limit is understood to be taken with respect to $\mathcal{K}^2$. ■

In our model, where $H^{(E,\mu)}(r) \in \mathcal{K}^\infty$ for all $r \in \mathbb{R}$, one has $\mathcal{H}^{(E)}_r(B) = \mathrm{i}[H^{(E,\mu)}(r), B] \in \mathcal{K}^2$ for all $r \in \mathbb{R}$ and $B \in \mathcal{K}^2$. Therefore, $\mathcal{H}^{(E)}_{r_0}(B) \in \mathcal{K}^2$ for some $r_0 \in \mathbb{R}$ is no additional condition in Lemma 6.16, whereas it is in (BGKS05)[Proposition 4.9].

Lemma 6.17

Let $(E_n)_{n \in \mathbb{N}}$ be a sequence in $\mathcal{E}(\mathbb{R}, \mathbb{R}^d)$ such that $\lim_{n\to\infty} \|\chi_{]-\infty,t]} E_n\|_1 = 0$ for any $t \in \mathbb{R}$. Then, for any $t, r \in \mathbb{R}$ and $B \in \mathcal{K}^2$ one has

$$\lim_{n\to\infty} |||\tau^{(E_n)}_{t,r}(B) - \tau_{t-r}(B)|||_2^2 = 0 . \tag{6.58}$$

Proof: For any $n \in \mathbb{N}$, $\omega \in \Omega$ and $t, r \in \mathbb{R}$ we define the mapping $\pi^{(E_n)}_{t,r} := \tau_{r-t} \circ \tau^{(E_n)}_{t,r}$. Then, the statement of Lemma 6.17 is equivalent to

$$\lim_{n\to\infty} |||\pi^{(E_n)}_{t,r}(B) - B|||_2^2 = 0 . \tag{6.59}$$

In terms of the unitary operators defined by $W^{(E_n,\mu)}_\omega(t,r) := U^{(\mu)}_\omega(r-t) U^{(E_n,\mu)}_\omega(t,r)$ for any $\omega \in \Omega$ and $(t,r) \in \mathbb{R}^2$ one has

$$\pi^{(E_n)}_{\omega,t,r}(B) = W^{(E_n,\mu)}_\omega(t,r) B W^{(E_n,\mu)}_\omega(r,t)$$

for any $B \in \mathfrak{B}$. From Corollary 6.14 we directly obtain $\lim\limits_{n\to\infty} \|(1 - W^{(E_n)}_\omega(t,r)^*)\psi\|^2 = 0$ for any $\omega \in \Omega$, $t, r \in \mathbb{R}$ and $\psi \in \mathfrak{h}$. Similarly to proofs of Lemmas 6.5, 6.7 and 6.15 we have the estimate

$$|||\pi^{(E,\mu)}_{t,r}(B) - B|||_2^2 \le \mathbb{E}[\|(1 - W^{(E_n,\mu)}(t,r)^*) B \delta_0\|^2] + \mathbb{E}[\|B(W^{(E_n,\mu)}(t,r)^* - 1)\delta_0\|^2] ,$$

which holds for any $t, r \in \mathbb{R}$ and $B \in \mathcal{K}^\infty$. Dominated convergence arguments as in Lemma 6.2 yield the statement of Lemma 6.17 for all $B \in \mathcal{K}^\infty$. Using unitarity of $\pi^{(E_n)}_{t,r}$ on $\mathcal{K}^2$ as well as a density argument leads to the fact that the statement even holds true for all $B \in \mathcal{K}^2$. ■

6.2. Framework for Many-Electron Systems

6.2.1. Hilbert Space

In order to allow the description of interacting electron gases we need to introduce many-particle spaces. For a fixed number $N \in \mathbb{N}_0$ of electrons and with $\mathfrak{h} = \ell^2(\mathbb{Z}^d)$ as in Section 6.1 the Hilbert space for the N-electron system is taken as the fermionic N-particle space $\mathfrak{h}_{N,-} := \mathfrak{F}_{N,-}(\mathfrak{h})$. For the description of arbitrarily many electrons, the Hilbert space is just the fermionic Fock space $\mathfrak{h}_- := \mathfrak{F}_-(\mathfrak{h})$. The precise definition of both Hilbert spaces as well as the construction principles for operators on these spaces via second quantisation are given in Appendix B. Finally, for the definition of an electric current density within an extended random solid state, only the Fock space $\mathfrak{h}_-$ will be relevant. This is why we focus on that case. The operator algebra $\mathfrak{B}_-$ corresponding to $\mathfrak{h}_-$ then is the Fermi algebra of $\mathfrak{h}$. It is the closure of the span of products of the so called *creation operators* $a_-^*(\psi)$ with their adjoints, the so called *annihilation operators*, where $\psi \in \mathfrak{h}$. These operators are structured in Appendix B.2.4. However, we state their defining relations, the *canonical anti-commutation relations* (CAR) also at this point. For any $\phi, \psi \in \mathfrak{h}$ one has

$$\{a_-(\phi), a_-(\psi)\} = 0 \,, \tag{6.60}$$

$$\{a_-^*(\phi), a_-^*(\psi)\} = 0 \,, \tag{6.61}$$

$$\{a_-(\phi), a_-^*(\psi)\} = \langle \phi, \psi \rangle \mathbb{1}_- \,. \tag{6.62}$$

In particular, $\mathfrak{B}_-$ has the subalgebra $\mathfrak{B}_{c,-}$ of operators, that are finite linear combinations of finite products of creation and annihilation operators of the form $a_-^*(\delta_x)$ and $a_-(\delta_y)$, where $x, y \in \mathbb{Z}^d$. We say, that these operators have finite support. On $\mathfrak{h}_-$ for any $a \in \mathbb{Z}^d$ there is a magnetic shift operator $T_-(a)$ analogous to Equation (6.2) given by

$$T_-(a) := \Gamma_-(T(a)) \,. \tag{6.63}$$

Since $\Gamma_-(T(a))\Gamma_-(T(b)) = \Gamma_-(T(a)T(b))$ for any $a, b \in \mathbb{Z}^d$, from the statement of Lemma 6.1 we directly obtain that the mapping $T_- : \mathbb{Z}^d \to \mathscr{U}(\mathfrak{h}_-)$, $a \mapsto T_-(a)$ forms a projective unitary representation of $\mathbb{Z}^d$, such that the mapping $\varphi_- : \mathbb{Z}^d \to \mathrm{Aut}(\mathfrak{B}_-)$, $a \mapsto \varphi_{a,-}$ with automorphisms defined by

$$\varphi_{a,-}(B_-) := T_-(a) B_- T_-(a)^* \tag{6.64}$$

for any $a \in \mathbb{Z}^d$ and $B_- \in \mathfrak{B}_-$ forms a representation of $\mathbb{Z}^d$. The second statement is proven in Lemma 5.5. The position operator $X_- = (X_{1,-}, ..., X_{d,-})$ on $\mathfrak{h}_-$ is defined componentwise by

$$X_{k,-} := \mathrm{d}\Gamma_-(X_k) \tag{6.65}$$

for any $k \in \{1, ..., d\}$. Note that for the position operator there is no covariant transformation law. More precisely, for any $k \in \{1, ..., d\}$ and $a \in \mathbb{Z}^d$ we have

$$\begin{aligned} T_-(a) X_{k,-} T_-(a)^* &= \Gamma_-(T(a)) \mathrm{d}\Gamma_-(X_k) \Gamma_-(T(a))^* \\ &= \mathrm{d}\Gamma_-(T(a) X_k T(a)^*) \\ &= \mathrm{d}\Gamma_-(X_k - a_k) \\ &= X_{k,-} - a_k N_- \,, \end{aligned}$$

where $N_- := \mathrm{d}\Gamma_-(\mathbb{1})$ is the particle number operator. But the position operator defines derivations $\mathcal{X}_{k,-} : \mathfrak{B}_{c,-} \to \mathfrak{B}_{c,-}$ by

$$\mathcal{X}_{k,-}(B_-) := \mathrm{i}[X_{k,-}, B_-] \tag{6.66}$$

for any $k \in \{1, ..., d\}$ and $B_- \in \mathfrak{B}_{c,-}$. Of course, this derivation is completely determined by its values on annihilation and creation operators. In more detail, one has $\mathcal{X}_{k,-}(a_-^*(\delta_x)) := x_k a_-^*(\delta_x)$ for any $k \in \{1, ..., d\}$ and $x \in \mathbb{Z}^d$. Note that only on the subalgebra $\mathfrak{B}_{pc,-}$, of operators with finite support that preserve the particle number, i.e. those operators which commute with N_-, one has that the derivations in Equation (6.66) transform covariantly.

6.2.2. Electric Field

In the obvious way the electric field $E \in \mathcal{E}(\mathbb{R}, \mathbb{R}^d)$ is implemented to the system on the Fock space by defining unitary gauge transformations via second quantisation of the operators defined in Equation (6.19), i.e.

$$G_-^{(E)}(t) := \Gamma_-(G^{(E)}(t)) = \Gamma_-(\mathrm{e}^{\mathrm{i}\langle F^{(E)}(t), X\rangle}) = \mathrm{e}^{\mathrm{i}\langle F^{(E)}(t), \mathrm{d}\Gamma_-(X)\rangle} = \mathrm{e}^{\mathrm{i}\langle F^{(E)}(t), X_-\rangle} \tag{6.67}$$

for $t \in \mathbb{R}$. As in Lemma 6.3 one obtains that the mapping $\mathbb{R} \to \mathfrak{h}_-$, $t \mapsto G_-^{(E)}(t)\psi_-$ is differentiable for $\psi_- \in D(X_-)$ and one has

$$\partial_t G_-^{(E)}(t)\psi_- = \mathrm{i}\langle E(t), X_-\rangle G_-^{(E)}(t)\psi_- = \mathrm{i}G_-^{(E)}(t)\langle E(t), X_-\rangle\psi_- \tag{6.68}$$

for any $t \in \mathbb{R}$. Furthermore, we obtain gauge automorphisms $\gamma_{t,-}^{(E)}$ on the algebra $\mathfrak{B}_-$ by defining

$$\gamma_{t,-}^{(E)}(B_-) := G_-^{(E)}(t) B_- G_-^{(E)}(t)^* \tag{6.69}$$

for any $t \in \mathbb{R}$ and $B_- \in \mathfrak{B}_-$. As a consequence of Equation (6.68) one has that for any $B_- \in \mathfrak{B}_{c,-}$ the mapping $\mathbb{R} \to \mathfrak{B}_-$, $t \mapsto \gamma_{t,-}^{(E)}(B)$ is differentiable. With $\langle E(t), \mathcal{X}_-\rangle := \sum_{k=1}^d E_k(t)\mathcal{X}_{k,-}$ for any $t \in \mathbb{R}$ and $B_- \in \mathfrak{B}_{c,-}$ one obtains

$$\partial_t \gamma_{t,-}^{(E)}(B_-) = \langle E(t), \mathcal{X}_-\rangle(\gamma_{t,-}^{(E)}(B_-)) = \gamma_{t,-}^{(E)}(\langle E(t), \mathcal{X}_-\rangle(B_-)) . \tag{6.70}$$

6.2.3. Schrödinger Operator and Time Evolution

The interaction between the electrons enters the model via a two body potential $\Phi : \mathbb{Z}^d \to \mathbb{R}$. We make the following assumptions on Φ:

Assumption

(S) Φ is symmetric, i.e. $\Phi(x) = \Phi(-x)$ for all $x \in \mathbb{Z}^d$.

(C) Φ has finite support, i.e. there is an $R \geq 0$ such that $\Phi(x) = 0$ for $|x| \geq R$.

The interaction term in the Schrödinger operator is constructed in the following way. Using the notation introduced as first construction in Appendix B.1.2, for $k \neq l$ the operator $\Phi(X_{N,k} - X_{N,l})$ models the interaction between the k-th and the l-th electron. Since any two electrons interact in this way and since we do not want to consider interactions of higher order than two-body interactions, the total term in the N-electron Schödinger operator implementing the electron-electron interaction is the multiplication operator

$$W_{N,-} := \frac{1}{2} \sum_{\substack{k,l=1,\\ k\neq l}}^{N} \Phi(X_{N,k} - X_{N,l}) \tag{6.71}$$

for all $N \geq 2$ and $W_{N,-} := 0$ for $N \in \{0, 1\}$. The interaction term is a well-defined multiplication operator on $\mathfrak{h}_{N,-}$, i.e. $W_{N,-}(\mathfrak{h}_{N,-}) \subset \mathfrak{h}_{N,-}$), for the fact that it is symmetric in the components of the position operator. For $\Lambda \subset \mathbb{Z}^d$ and $N \in \mathbb{N}_0$ the random Schrödinger operator of the N-electron system that is restricted to Λ is the bounded, linear and self-adjoint operator

$$H^{(E,\mu)}_{\Lambda,\omega,N,-}(t) := \mathrm{d}\Gamma_{N,-}(H^{(E,\mu)}_{\Lambda,\omega}(t)) + W_{N,-}\Gamma_{N,-}(\chi_\Lambda) \,, \tag{6.72}$$

where $\omega \in \Omega$ and $t \in \mathbb{R}$ are arbitrary and χ_Λ is the multiplication operator induced by the characteristic function of Λ.
Due to (Yos80, BGKS05) by the same methods as presented in 6.1.7 the random Schrödinger operator in (6.72) possesses a unitary propagator, i.e. for any $\Lambda \subset \mathbb{Z}^d$, $\omega \in \Omega$ and $N \in \mathbb{N}_0$ there exists a mapping $U^{(E,\mu)}_{\Lambda,\omega,N,-} : \mathbb{R}^2 \to \mathscr{U}(\mathfrak{h}_{N,-})$, $(t, r) \mapsto U^{(E,\mu)}_{\Lambda,\omega,N,-}(t, r)$ such that for arbitrary $t, r, q \in \mathbb{R}$ the following relations are satisfied

$$\begin{aligned} U^{(E,\mu)}_{\Lambda,\omega,N,-}(t,t) &= \mathrm{id}_{N,-} \,, \\ U^{(E,\mu)}_{\Lambda,\omega,N,-}(t,r)U^{(E,\mu)}_{\Lambda,\omega,N,-}(r,q) &= U^{(E,\mu)}_{\Lambda,\omega,N,-}(t,q) \,, \\ \mathrm{i}\partial_t U^{(E,\mu)}_{\Lambda,\omega,N,-}(t,r) &= H^{(E,\mu)}_{\Lambda,\omega,N,-}(t)U^{(E,\mu)}_{\Lambda,\omega,N,-}(t,r) \,, \\ -\mathrm{i}\partial_r U^{(E,\mu)}_{\Lambda,\omega,N,-}(t,r) &= U^{(E,\mu)}_{\Lambda,\omega,N,-}(t,r)H^{(E,\mu)}_{\Lambda,\omega,N,-}(r) \,. \end{aligned}$$

So far, we described systems of a fixed number of electrons $N \in \mathbb{N}_0$. We are interested mostly in the special case $\Lambda = \mathbb{Z}^d$ for which a finite particle number corresponds to a vanishing mean electron density. However, the formalism we are trying to achieve should describe systems of finite electron density, so we transfer to Fock space. On $\mathfrak{h}_-$ for any $\Lambda \subset \mathbb{R}^d$, $\omega \in \Omega$ and $t \in \mathbb{R}$ the energy of the many-electron system is described by the random Schrödinger operator

$$H^{(E,\mu)}_{\Lambda,\omega,-}(t) := \bigoplus_{N\in\mathbb{N}_0} H^{(E,\mu)}_{\Lambda,\omega,N,-}(t) \,. \tag{6.73}$$

For the case of vanishing electric field, we just write $H^{(\mu)}_{\Lambda,\omega,-}$. Because of the existence of unitary propagators for arbitrary finite particle number $N \in \mathbb{N}_0$, there also is a unitary propagator $U^{(E,\mu)}_{\Lambda,\omega,-} : \mathbb{R}^2 \to \mathscr{U}(\mathfrak{h}_-)$, $(t, r) \mapsto U^{(E,\mu)}_{\Lambda,\omega,-}(t, r)$ for the random Schrödinger operator on Fock space (6.73) given by

$$U^{(E,\mu)}_{\Lambda,\omega,-}(t,r) = \bigoplus_{N\in\mathbb{N}_0} U^{(E,\mu)}_{\Lambda,\omega,N,-}(t,r) \,. \tag{6.74}$$

For the reason that the random Schrödinger operator in general is an unbounded operator, the propagator is only strongly differentiable, i.e. for any $t, r, q \in \mathbb{R}$ and $\psi_- \in D(H^{(\mu)}_{\Lambda,\omega,-})$

$$U^{(E,\mu)}_{\Lambda,\omega,-}(t,t) = \mathrm{id}_- \,, \tag{6.75}$$

$$U^{(E,\mu)}_{\Lambda,\omega,-}(t,r)U^{(E,\mu)}_{\Lambda,\omega,-}(r,q) = U^{(E,\mu)}_{\Lambda,\omega,-}(t,q) \,, \tag{6.76}$$

$$\mathrm{i}\partial_t U^{(E,\mu)}_{\Lambda,\omega,-}(t,r)\psi_- = H^{(E,\mu)}_{\Lambda,\omega,-}(t)U^{(E,\mu)}_{\Lambda,\omega,-}(t,r)\psi_- \,, \tag{6.77}$$

$$-\mathrm{i}\partial_r U^{(E,\mu)}_{\Lambda,\omega,-}(t,r)\psi_- = U^{(E,\mu)}_{\Lambda,\omega,-}(t,r)H^{(E,\mu)}_{\Lambda,\omega,-}(r)\psi_- \,. \tag{6.78}$$

Moreover, for vanishing electric field the unitary propagator depends only on time differences. Accordingly, for any $t \in \mathbb{R}$ we set

$$U^{(\mu)}_{\Lambda,\omega,-}(t) := U^{(0,\mu)}_{\Lambda,\omega,-}(t,0) = \mathrm{e}^{-\mathrm{i}tH^{(\mu)}_{\Lambda,\omega,-}} \,. \tag{6.79}$$

Next, we translate the above constructions to an algebraic setting. The Schrödinger operator defines a derivation on $\mathfrak{B}_{c,-}$ via

$$\mathcal{H}^{(E,\mu)}_{\Lambda,\omega,t,-}(B_-) := \mathrm{i}[H^{(E,\mu)}_{\Lambda,\omega,-}(t), B_-] \tag{6.80}$$

for any $\Lambda \subset \mathbb{Z}^d$, $\omega \in \Omega$, $t \in \mathbb{R}$ and $B_- \in \mathfrak{B}_{c,-}$. For vanishing electric field this is independent of $t \in \mathbb{R}$. Then, we suppress these arguments such that $\mathcal{H}^{(E,\mu)}_{\Lambda,\omega,t,-} = \gamma^{(E)}_{t,-} \circ \mathcal{H}^{(\mu)}_{\Lambda,\omega,-} \circ (\gamma^{(E)}_{t,-})^{-1}$ for any $t \in \mathbb{R}$.
Similarly, for any $\Lambda \subset \mathbb{Z}^d$, $\omega \in \Omega$, $t, r \in \mathbb{R}$ and $B_- \in \mathfrak{B}_-$ the unitary propagator defined in Equation (6.74) induces automorphisms $\tau^{(E,\mu)}_{\Lambda,\omega,t,r,-} : \mathfrak{B}_- \to \mathfrak{B}_-$ via

$$\tau^{(E,\mu)}_{\Lambda,\omega,t,r,-}(B_-) := U^{(E,\mu)}_{\Lambda,\omega,-}(t,r) B_- U^{(E,\mu)}_{\Lambda,\omega,-}(r,t) \,. \tag{6.81}$$

For fixed $B_- \in D(\mathcal{H}^{(\mu)}_{\Lambda,\omega,-})$ Equation (6.81) is differentiable with respect to r and because of Equations (6.77) and (6.78) one has

$$\partial_r \tau^{(E,\mu)}_{\Lambda,\omega,t,r,-}(B_-) = \tau^{(E,\mu)}_{\Lambda,\omega,t,r,-}(\mathcal{H}^{(E,\mu)}_{\Lambda,\omega,r,-}(B_-)) \,. \tag{6.82}$$

For the special case of vanishing electric field, the unitary propagator defines a strongly continuous one parameter group of automorphisms $\{\tau^{(\mu)}_{\Lambda,\omega,t,-} : t \in \mathbb{R}\}$ on $\mathfrak{B}_-$ via

$$\tau^{(\mu)}_{\Lambda,\omega,t,-}(B_-) := U^{(\mu)}_{\Lambda,\omega,-}(t) B_- U^{(\mu)}_{\Lambda,\omega,-}(t)^* = \mathrm{e}^{-\mathrm{i}tH^{(\mu)}_{\Lambda,\omega,-}} B_- \mathrm{e}^{\mathrm{i}tH^{(\mu)}_{\Lambda,\omega,-}} = \mathrm{e}^{-t\mathcal{H}^{(\mu)}_{\Lambda,\omega,-}}(B_-) \,. \tag{6.83}$$

For fixed $\omega \in \Omega$ and $B_- \in \mathfrak{B}_{c,-}$ the mapping $\mathbb{R} \to \mathfrak{B}_-,\ t \mapsto \tau^{(\mu)}_{\Lambda,\omega,t,-}(B_-)$ is differentiable with respect to the variable t and one obtains the differential equation

$$\partial_t \tau^{(\mu)}_{\Lambda,\omega,t,-}(B_-) = \tau^{(\mu)}_{\Lambda,\omega,-}(\mathcal{H}^{(\mu)}_{\Lambda,\omega,-}(B_-)) \,. \tag{6.84}$$

For $\Lambda = \mathbb{Z}^d$ we suppress the label Λ in the definitions above. Because in this case the Schrödinger operator satisfies a covariant transformation law, we get that for fixed $t \in \mathbb{R}$ the mapping $\mathcal{H}^{(E,\mu)}_{t,-} : \Omega \to \mathrm{Der}(\mathfrak{B}_{c,-}),\ \omega \mapsto\to \mathcal{H}^{(E,\mu)}_{\omega,t,-}$ is a covariant derivation, i.e.

$$\varphi_{a,-}(\mathcal{H}^{(E,\mu)}_{\omega,t,-}(B_-)) = \mathcal{H}^{(E,\mu)}_{\phi_a(\omega),t,-}(\varphi_{a,-}(B_-)) \tag{6.85}$$

for all $a \in \mathbb{Z}^d$, $t \in \mathbb{R}$, $B_- \in \mathfrak{B}_{c,-}$ and almost all $\omega \in \Omega$. Moreover, for any fixed $t, r \in \mathbb{R}$ the mapping $\tau^{(E,\mu)}_{t,r,-} : \Omega \to \mathrm{Aut}(\mathfrak{B}_-),\ \omega \mapsto\to \tau^{(E,\mu)}_{\omega,t,r,-}$ is a covariant automorphism, i.e. for all $a \in \mathbb{Z}^d$, $t, r \in \mathbb{R}$, $B_- \in \mathfrak{B}_{c,-}$ and almost all $\omega \in \Omega$ we have

$$\varphi_{a,-}(\tau^{(E,\mu)}_{\omega,t,r,-}(B_-)) = \tau^{(E,\mu)}_{\phi_a(\omega),t,r,-}(\varphi_{a,-}(B_-)) \,. \tag{6.86}$$

6.2.4. Velocity Operator and Current Density Operator

The velocity operator on Fock space is simply defined via second quantisation, so for any $\Lambda \subset \mathbb{Z}^d$, $\omega \in \Omega$ and $t \in \mathbb{R}$ one has $D^{(E)}_{\Lambda,\omega,-}(t) = (D^{(E)}_{\Lambda,\omega,1,-}(t), ..., D^{(E)}_{\Lambda,\omega,d,-}(t))$ with

$$D^{(E)}_{\Lambda,\omega,k,-}(t) := \mathrm{d}\Gamma_-(D^{(E)}_{\Lambda,\omega,k}(t)) \tag{6.87}$$

for any $k \in \{1, ..., d\}$. Of course, the components of the current density operator define derivations $\mathcal{D}^{(E)}_{\Lambda,\omega,t,-} = (\mathcal{D}^{(E)}_{\Lambda,\omega,t,1,-}, ..., \mathcal{D}^{(E)}_{\Lambda,\omega,t,d,-})$ by

$$\mathcal{D}^{(E)}_{\Lambda,\omega,t,k,-}(B_-) := \mathrm{i}[D^{(E)}_{\Lambda,\omega,k,-}(t), B_-] \tag{6.88}$$

for any $B_- \in \mathfrak{B}_{c,-}$, so that for the special case $\Lambda = \mathbb{Z}^d$, where Λ is dropped as a label, the mapping $\mathcal{D}^{(E)}_{t,k,-} : \Omega \to \mathrm{Der}(\mathfrak{B}_{c,-}),\ \omega \mapsto \mathcal{D}^{(E)}_{\omega,t,k,-}$ forms a covariant derivation for any $\Lambda \subset \mathbb{Z}^d$, $t \in \mathbb{R}$ and $k \in \{1, ..., d\}$. Similarly, the concept of a current density operator is transported to Fock space via second quantisation.

Definition 6.18 (*Current Density Operator*)

For any $\Lambda \subset \mathbb{Z}^d$, $\omega \in \Omega$, $t \in \mathbb{R}$ and $y \in \mathbb{Z}^d$ the *current density operator* on Fock space is constructed via second quantisation of the one-electron current density operator given in Definition 6.11, i.e. for any $k \in \{1, ..., d\}$ we define

$$J^{(E)}_{\Lambda,\omega,k,-}(t,y) := \mathrm{d}\Gamma_-(J^{(E)}_{\Lambda,\omega,k}(t,y)) \,. \tag{6.89}$$

The current density operator $J^{(E)}_{\Lambda,\omega,-}(t,y) := (J^{(E)}_{\Lambda,\omega,1,-}(t,y), ..., J^{(E)}_{\Lambda,\omega,d,-}(t,y))$ is a bounded linear operator on Fock space. It has finite support, so it is an element of $\mathfrak{B}_{c,-}$. These properties will be evident from the following theorem and its proof.

Theorem 6.19 (*Representation of the Current Density Operator*)

For any $\Lambda \subset \mathbb{Z}^d$, $\omega \in \Omega$, $t \in \mathbb{R}$, $y \in \mathbb{Z}^d$ and $k \in \{1, ..., d\}$ the components of the current density operator can be represented by the formula

$$J^{(E)}_{\Lambda,\omega,k,-}(t,y) = a^*_-(D^{(E)}_{\Lambda,\omega,k}(t)\delta_y)a_-(\delta_y) + a^*_-(\delta_y)a_-(D^{(E)}_{\Lambda,\omega,k}(t)\delta_y) \,. \tag{6.90}$$

Proof: Let $\Lambda \subset \mathbb{Z}^d$, $t \in \mathbb{R}$, $y \in \mathbb{Z}^d$ and $\omega \in \Omega$ be arbitrary. Then, as a second quantised quantity, the current density operator $J^{(E)}_{\Lambda,\omega,-}(t,y)$ can be expressed in terms of creation and annihilation operators. Using the eigenbasis of the position operator $\{\delta_x : x \in \mathbb{Z}^d\}$ as well as (B.75) for any $k \in \{1, ..., d\}$ we obtain

$$\begin{aligned}
J^{(E)}_{\Lambda,\omega,k,-}(t,y) &= \mathrm{d}\Gamma_-(J^{(E)}_{\Lambda,\omega,k}(t,y)) \\
&= \sum_{x\in\mathbb{Z}^d} a^*_-(J^{(E)}_{\Lambda,\omega,k}(t,y)\delta_x)a_-(\delta_x) \\
&= \sum_{x,x'\in\mathbb{Z}^d} \langle \delta_{x'}, J^{(E)}_{\Lambda,\omega,k}(t,y)\delta_x\rangle \, a^*_-(\delta_{x'})a_-(\delta_x) \\
&= \sum_{x,x'\in\mathbb{Z}^d} (\langle \delta_{x'}, D^{(E)}_{\Lambda,\omega,k}(t)\chi_y\delta_x\rangle + \langle \delta_{x'}, \chi_y D^{(E)}_{\Lambda,\omega,k}(t)\delta_x\rangle) \, a^*_-(\delta_{x'})a_-(\delta_x) \\
&= \sum_{x'\in\mathbb{Z}^d} \langle \delta_{x'}, D^{(E)}_{\Lambda,\omega,k}(t)\delta_y\rangle \, a^*_-(\delta_{x'})a_-(\delta_y) + \sum_{x\in\mathbb{Z}^d} \langle \delta_y, D^{(E)}_{\Lambda,\omega,k}(t)\delta_x\rangle \, a^*_-(\delta_y)a_-(\delta_x) \\
&= \sum_{x'\in\mathbb{Z}^d} \langle \delta_{x'}, D^{(E)}_{\Lambda,\omega,k}(t)\delta_y\rangle \, a^*_-(\delta_{x'})a_-(\delta_y) + \sum_{x\in\mathbb{Z}^d} \overline{\langle \delta_x, D^{(E)}_{\Lambda,\omega,k}(t)\delta_y\rangle} \, a^*_-(\delta_y)a_-(\delta_x) \\
&= a^*_-\Big(\sum_{x'\in\mathbb{Z}^d} \langle \delta_{x'}, D^{(E)}_{\Lambda,\omega,k}(t)\delta_y\rangle \, \delta_{x'}\Big) \, a_-(\delta_y) + a^*_-(\delta_y) \, a_-\Big(\sum_{x\in\mathbb{Z}^d} \langle \delta_x, D^{(E)}_{\Lambda,\omega,k}(t)\delta_y\rangle \, \delta_x\Big) \\
&= a^*_-(D^{(E)}_{\Lambda,\omega,k}(t)\delta_y)a_-(\delta_y) + a^*_-(\delta_y)a_-(D^{(E)}_{\Lambda,\omega,k}(t)\delta_y) \,.
\end{aligned}$$

■

Note that all sums in the proof above are finite, since the current density operator defined in Definition 6.11 has finite support.

Again, the label Λ is suppressed, if $\Lambda = \mathbb{Z}^d$. Note that for simple, Dirichlet or Neumann boundary conditions and any values of $\omega \in \Omega$, $t \in \mathbb{R}$ and $y \in \mathbb{Z}^d$ the current density operators $J^{(E)}_{\Lambda,\omega,-}(t,y)$ and $J^{(E)}_{\omega,-}(t,y)$ agree whenever $\Lambda \subset \mathbb{Z}^d$ is large enough, where large enough means $y \in \Lambda$ and y has a distance from the boundary of Λ that is bigger than some positive constant independent of the volume. Finally, we prove a transformation law for the current density operator. Again, this transformation law follows from the corresponding transformation law on one-particle space as stated in Theorem 6.12.

Theorem 6.20 (*Transformation Law of the Current Density Operator on Fock Space*)

For almost every $\omega \in \Omega$ and all $t \in \mathbb{R}$, $y, a \in \mathbb{Z}^d$ and $k \in \{1, ..., d\}$ the components of the current density operator satisfy the following transformation law

$$\varphi_{a,-}(J^{(E)}_{\omega,k,-}(t,y)) = J^{(E)}_{\phi_a(\omega),k,-}(t, y+a) \ . \tag{6.91}$$

Proof: Because of the transformation law of the current density operator for a single electron in Theorem 6.12, using Equation (B.66) with $G = S_-$ for almost every $\omega \in \Omega$ and any $t \in \mathbb{R}$, $y, a \in \mathbb{Z}^d$ and $k \in \{1, ..., d\}$ we obtain

$$\begin{aligned}
\varphi_{a,-}(J^{(E)}_{\omega,k,-}(t,y)) &= \Gamma_-(T(a))\mathrm{d}\Gamma_-(J^{(E)}_{\omega,k}(t,y))\Gamma_-(T(a))^* \\
&= \mathrm{d}\Gamma_-(T(a)J^{(E)}_{\omega,k}(t,y)T(a)^*) \\
&= \mathrm{d}\Gamma_-(\varphi_a(J^{(E)}_{\omega,k}(t,y))) \\
&= \mathrm{d}\Gamma_-(J^{(E)}_{\phi_a(\omega),k}(t,y+a)) \\
&= J^{(E)}_{\phi_a(\omega),k,-}(t,y+a) \ .
\end{aligned}$$

■

7 Construction of States

Creating molding the earth, whether it be the plains of the west or the iron ore of Penn; it's all a big game of construction, some with a brush, some with a shovel, some choose a pen.

(Jackson Pollock)

The following chapter shall eliminate the drawback that so far we have not constructed[1] covariant states for the concrete model of an electron gas on Fock space which we presented in Chapter 6. Recent works (BSPK13a, BSPK13b) face such problems in a very similar setting.
We recall that for the model of an electron gas introduced in Chapter 6 states are understood as a positive, normalised and linear functionals on the Fermi algebra. The state of the system depends on time and, since we are dealing with random systems, it also depends on the concrete realisation of the system.
In absence of an external electric field we want the system to be in thermal equilibrium. This is why in Section 7.1 we construct KMS states. The construction is possible in two different cases. The first case is a one-dimensional electron gas including interaction. The second case is a non-interacting electron gas in arbitrary space dimension.
Then, in Section 7.2, from the KMS states we construct the state for the system at arbitrary time in a given realisation. This models the situation, where an external electric field is switched on. Since we are interested in ergodic systems, considering the set of states constructed in Section 7.2 for all different realisations of the system, the collection of these states should form a covariant state. This is how ergodicity of a system is encoded on the level of operator algebras. So, all along this chapter not only we will construct states for a system in a given realisation but also we will focus on the property of the collection of these states to transform covariantly.

7.1. Construction of KMS States

We use Theorem 4.5 to construct $(\tau^{(\mu)}_{\omega,-},\beta)$-KMS states on $\mathfrak{B}_-$ by the following method. For $L \in \mathbb{N}_0$ let $\Lambda_L \subset \mathbb{Z}^d$ be the set of all vertices of $\mathbb{Z}^d$ inside a cube centred at the origin and of side length $(2L+1)$. For this cube we consider the system introduced in Chapter 6 with either simple or Dirichlet or Neumann boundary conditions and for an arbitrary but fixed realisation $\omega \in \Omega$. Then, due to the generic example presented in Chapter 4, the state $\varrho^{(\beta,\mu)}_{\Lambda_L,\omega,-}$ defined by

$$P^{(\beta,\mu)}_{\Lambda_L,\omega,-} := \frac{\mathrm{e}^{-\beta H^{(\mu)}_{\Lambda_L,\omega,-}}}{\mathrm{Tr}\Big(\mathrm{e}^{-\beta H^{(\mu)}_{\Lambda_L,\omega,-}}\Big)}\,, \tag{7.1}$$

$$\varrho^{(\beta,\mu)}_{\Lambda_L,\omega,-}(B_-) := \mathrm{Tr}(B_- P^{(\beta,\mu)}_{\Lambda_L,\omega,-}) \tag{7.2}$$

[1]There are rumours about Jackson Pollock also having said: "Some choose C^*-algebras."

for $0 \leq \beta < \infty$ and by projection onto the set of ground states of $H^{(\mu)}_{\Lambda_L,\omega,-}$ for $\beta = \infty$ is a $(\tau^{(\mu)}_{\Lambda_L,\omega,-},\beta)$-KMS state on $\mathfrak{B}_-$. This holds true, since we considered $H^{(\mu)}_{\Lambda_L,\omega,-}$ as well as $\mathrm{e}^{-\beta H^{(\mu)}_{\Lambda_L,\omega,-}}$ as bounded operators on $\mathfrak{h}_- = \mathfrak{F}_-(\ell^2(\mathbb{Z}^d))$. Both operators have support in Λ_L. Therefore, they have finite rank. In particular, $\mathrm{e}^{-\beta H^{(\mu)}_{\Lambda_L,\omega,-}}$ is a traceclass operator and $\varrho^{(\beta,\mu)}_{\Lambda_L,\omega,-}$ as given in Equation (7.2) is well-defined.

In this situation, due to Theorem 4.5, strong convergence of the time translation automorphisms implies the existence of a KMS state for the extended system. In more detail, proving that the sequence $(\tau^{(\mu)}_{\Lambda_L,\omega,t,-}(B_-))_{L\in\mathbb{N}}$ converges in norm to $\tau^{(\mu)}_{\omega,t,-}(B_-)$ for any realisation $\omega \in \Omega$, time $t \in \mathbb{R}$ and $B_- \in \mathfrak{B}_-$ implies that the sequence $(\varrho^{(\beta,\mu)}_{\Lambda_L,\omega,-})_{L\in\mathbb{N}}$ has a subsequence $(\varrho^{(\beta,\mu)}_{\Lambda_{L_n},\omega,-})_{n\in\mathbb{N}}$ that strongly converges to a state $\varrho^{(\beta,\mu)}_{\omega,-}$. In particular, $\varrho^{(\beta,\mu)}_{\omega,-}$ is a $(\tau^{(\mu)}_{\omega,-},\beta)$-KMS state due to Theorem 4.5. Note that in general the choice of the subsequence will depend on $\omega \in \Omega$. Note that this only proves existence of KMS states for extended systems. In typical situations one will have absolutely no idea of how the KMS state of an extended and interacting electron gas looks like.

One-Dimensional Interacting Electron Gas

The first application of this construction principle is the electron gas in dimension $d = 1$ including interaction as described in Chapter 6. In this case, we can proof the existence of KMS states, but there is no explicit expression for these states.

Theorem 7.1 (*Existence of KMS States in One Dimension*)

Consider the model of an interacting electron gas introduced in Chapter 6 and its restrictions to finite boxes, either with simple or with Dirichlet or with Neumann boundary conditions, for the special case $d = 1$. Then, for any $t \in \mathbb{R}$, $B_- \in \mathfrak{B}_{c,-}$ and any fixed $\omega \in \Omega$ one has

$$\lim_{L\to\infty} \|\mathcal{H}^{(\mu)}_{\Lambda_L,\omega,-}(B_-) - \mathcal{H}^{(\mu)}_{\omega,-}(B_-)\| = 0 \, , \tag{7.3}$$

$$\lim_{L\to\infty} \|\tau^{(\mu)}_{\Lambda_L,\omega,t,-}(B_-) - \tau^{(\mu)}_{\omega,t,-}(B_-)\| = 0 \, . \tag{7.4}$$

For any $\beta \in [0,\infty]$ and $\mu \in \mathbb{R}$ by Equations (7.1) and (7.2) there exists a sequence of $(\tau^{(\mu)}_{\Lambda_L,\omega,-},\beta)$-KMS states $(\varrho^{(\beta,\mu)}_{\Lambda_L,\omega,-})_{L\in\mathbb{N}}$. Moreover, there exists a subsequence $(\varrho^{(\beta,\mu)}_{\Lambda_{L_n},\omega,-})_{n\in\mathbb{N}}$ and a $(\tau^{(\mu)}_{\omega,-},\beta)$-KMS state $\varrho^{(\beta,\mu)}_{\omega,-}$ on $\mathfrak{B}_-$ such that for any $B_- \in \mathfrak{B}_-$

$$\lim_{n\to\infty} \varrho^{(\beta,\mu)}_{\Lambda_{L_n},\omega,-}(B_-) = \varrho^{(\beta,\mu)}_{\omega,-}(B_-) \, . \tag{7.5}$$

Proof: We apply theorem (BR87)[Theorem 3.1.34] to the following situation. Let $\omega \in \Omega$ be an arbitrary but fixed realisation of the system. We are given an increasing sequence of Banach spaces X_L by restriction of the Banach algebra $\mathfrak{B}_-$ to observables with support in Λ_L. Then, $\bigcup_{L\in\mathbb{N}} X_L$ is in the domain of the symmetric derivation $\mathcal{H}^{(\mu)}_{\omega,-}$. Thus, $S := -\mathcal{H}^{(\mu)}_{\omega,-}$ defines a dissipative operator on Banach space $X := \mathfrak{B}_-$. For $L, Q \in \mathbb{N}_0$ we define $S_{L,Q} : X_L \to X_{L+Q}$ via $S_{L,Q} := -\mathcal{H}^{(\mu)}_{\Lambda_{L+Q},\omega,-}|_{X_L}$. Again, since $\mathcal{H}^{(\mu)}_{\Lambda_{L+Q},\omega,-}$ is a symmetric derivation on $\mathfrak{B}_-$ for any $L, Q \in \mathbb{N}_0$, the operators $S_{L,0}$ are dissipative operators on X_L for any $L \in \mathbb{N}_0$ and from their definition one trivially obtains that for all $L, Q \in \mathbb{N}_0$

$$S_{L,Q} = -\mathcal{H}^{(\mu)}_{\Lambda_{L+Q},\omega,-}|_{X_L} = S_{L+Q,0}|_{X_L}$$

is satisfied, which is needed in order to apply (BR87)[Theorem 3.1.34]. Because the interaction potential Φ has finite support, i.e. $\mathrm{supp}(\Phi) \subset \Lambda_R$ for some $R \geq 1$, there are constants $M, \alpha > 0$ such that

$$\|S|_{X_L} - S_{L,Q}\| \leq M L \mathrm{e}^{-\alpha Q}$$

for all $L, Q \in \mathbb{N}_0$. This can be seen by the following estimate. We use the fact that $H^{(\mu)}_{\Lambda_L,\omega,-}$ and $H^{(\mu)}_{\omega,-}$ can be expressed in terms of creation and annihilation operators. The former are given by quadratic and quartic products of the latter, precisely for all $L \in \mathbb{N}_0$ and $\omega \in \Omega$ and $B_- \in X_L$ one has

$$\mathcal{H}^{(\mu)}_{\Lambda_L,\omega,-}(B_-) = \sum_{\substack{x,y\in\Lambda_L,\\ |x-y|\le R}} \mathrm{i}\Big[\langle\delta_y, H^{(\mu)}_{\Lambda_L,\omega}\delta_x\rangle\, a^*_-(\delta_y)a_-(\delta_x) + \frac{1}{2}\Phi(x-y)a^*_-(\delta_x)a^*_-(\delta_y)a_-(\delta_y)a_-(\delta_x), B_-\Big]\,,$$

$$\mathcal{H}^{(\mu)}_{\omega,-}(B_-) = \sum_{\substack{x,y\in\Lambda_{L+R},\\ |x-y|\le R}} \mathrm{i}\Big[\langle\delta_y, H^{(\mu)}_{\omega}\delta_x\rangle\, a^*_-(\delta_y)a_-(\delta_x) + \frac{1}{2}\Phi(x-y)a^*_-(\delta_x)a^*_-(\delta_y)a_-(\delta_y)a_-(\delta_x), B_-\Big]\,.$$

Both, $H^{(\mu)}_{\Lambda_L,\omega}$ and $H^{(\mu)}_{\omega}$, can be bounded by a constant $C > 0$, uniformly in $L \in \mathbb{N}_0$ and $\omega \in \Omega$. We obtain $\|S|_{X_L} - S_{L,Q}\| = 0$ for all $Q > R$. Using the fact that we treat a system in dimension $d = 1$, for $Q \le R$ we obtain that for any $B_- \in X_L$

$$\|S_{L+Q}(B_-)\| = \|\mathcal{H}^{(\mu)}_{\Lambda_{L+Q},\omega,-}(B_-)\| = \|[H^{(\mu)}_{\Lambda_{L+Q},\omega,-}, B_-]\| \le 2(2(L+R)+1)(2R+1)(C+\|\Phi\|_\infty)\|B_-\|\,,$$

$$\|S(B_-)\| = \|\mathcal{H}^{(\mu)}_{\omega,-}(B_-)\| = \|[H^{(\mu)}_{\omega,-}, B_-]\| \le 2(2(L+R)+1)(2R+1)\,(C+\|\Phi\|_\infty)\,\|B_-\|$$

by a norm estimate of the commutator. So one chooses the constants $M, \alpha > 0$ such that

$$\|S|_{X_L} - S_{L,Q}\| \le 4(2(L+R)+1)(2R+1)\,(C+\|\Phi\|_\infty) \le ML\mathrm{e}^{-\alpha R}$$

for all $L \in \mathbb{N}_0$ and $Q \in \{1, ..., R\}$. Then, all requirements to apply (BR87)[Theorem 3.1.34] are satisfied. Trivially Equation (7.3) is satisfied, because for any observable of finite support $B_- \in \mathfrak{B}_{c,-}$ and $L \in \mathbb{N}_0$ large enough we have that $\mathcal{H}^{(\mu)}_{\Lambda_L,\omega,-}(B_-) = \mathcal{H}^{(\mu)}_{\omega,-}(B_-)$. Moreover, we get that (7.4) holds from

$$\begin{aligned}\lim_{L\to\infty} \|\, \tau^{(\mu)}_{\Lambda_L,\omega,t,-}(B_-) - \tau^{(\mu)}_{\omega,t,-}(B_-)\,\| &= \lim_{L\to\infty} \Big\|\, \mathrm{e}^{-t\mathcal{H}^{(\mu)}_{\Lambda_L,\omega,-}}(B_-) - \mathrm{e}^{-t\mathcal{H}^{(\mu)}_{\omega,-}}(B_-)\,\Big\| \\ &= \lim_{L\to\infty} \|\, \mathrm{e}^{tS_{L,0}}(B_-) - \mathrm{e}^{tS}(B_-)\,\| = 0\end{aligned}$$

for all $B_- \in \mathfrak{B}_-$ with finite support. Next, let $\beta \in [0,\infty]$ and $\mu \in \mathbb{R}$. By the Banach-Alaoglu theorem the sequence $(\varrho^{(\beta,\mu)}_{\Lambda_L,\omega,-})_{L\in\mathbb{N}}$ has weak*-limit points, i.e there exists a subsequence $(L_n)_{n\in\mathbb{N}}$ of the sequence $(L)_{L\in\mathbb{N}}$ and a state $\varrho^{(\beta,\mu)}_{\omega,-}$ such that $\lim_{n\to\infty} |\varrho^{(\beta,\mu)}_{\Lambda_{L_n},\omega,-}(B_-) - \varrho^{(\beta,\mu)}_{\omega,-}(B_-)| = 0$ for all $B_- \in \mathfrak{B}_-$. From the strong convergence in (7.4) by an application of Theorem 4.5 we get that $\varrho^{(\beta,\mu)}_{\omega,-}$ is a $(\tau^{(\mu)}_{\omega,-},\beta)$-KMS state. This proves the existence of $(\tau^{(\mu)}_{\omega,-},\beta)$-KMS states for our model in dimension $d = 1$. ■

The choice of subsequence in the proof above depends on the realisation $\omega \in \Omega$. Typically, Ω will not be countable. Accordingly, there is no general way to construct a subsequence via diagonalisation, such that this subsequence converges independently of the realisation of the system. Moreover, we remark that the convergence in the theorem above is uniform on compacts in $t \in \mathbb{R}$.

Non-Interacting Electron Gas

By the same method as described above we can also prove the existence of KMS states for the model of a non-interacting electron gas in dimension $d \in \mathbb{N}$ (BR97)[Paragraph 5.2.4]. We start by proving strong convergence of time evolution automorphisms. For a non-interacting system we have important simplifications, that can be used for the construction of a KMS state. The two most essential simplifications are

$$H^{(\mu)}_{\Lambda,\omega,-} = \mathrm{d}\Gamma_-(H^{(\mu)}_{\Lambda,\omega})\,, \tag{7.6}$$

$$U^{(\mu)}_{\Lambda.\omega,-}(t) = \mathrm{e}^{-\mathrm{i}tH^{(\mu)}_{\Lambda,\omega,-}} = \mathrm{e}^{-\mathrm{i}t\mathrm{d}\Gamma_-(H^{(\mu)}_{\Lambda,\omega})} = \Gamma_-\Big(\mathrm{e}^{-\mathrm{i}tH^{(\mu)}_{\Lambda,\omega}}\Big) = \Gamma_-(U^{(\mu)}_{\Lambda,\omega}(t)) \tag{7.7}$$

for any $\Lambda \subset \mathbb{Z}^d$, $\omega \in \Omega$ and $t \in \mathbb{R}$, where the Schrödinger operator is supposed to be equipped either with simple or with Dirichlet or with Neumann boundary conditions.

Theorem 7.2 (*Strong Convergence of Time Evolutions for the Non-Interacting System*)

Consider the model of the electron gas introduced in Chapter 6 for the special case, where no interaction between the electrons is present, i.e. assume $\Phi = 0$. Then, for any fixed realisation $\omega \in \Omega$ one has strong convergence of the time evolution automorphisms $(\tau^{(\mu)}_{\Lambda_L,\omega,-})_{L\in\mathbb{N}}$ to $\tau^{(\mu)}_{\omega,-}$, i.e. for all $t \in \mathbb{R}$ and all $B_- \in \mathfrak{B}_-$ one has

$$\lim_{L\to\infty} \|\tau^{(\mu)}_{\Lambda_L,\omega,t,-}(B_-) - \tau^{(\mu)}_{\omega,t,-}(B_-)\| = 0 \,. \tag{7.8}$$

Proof: Let $\omega \in \Omega$ be given and $L \in \mathbb{N}$, $t \in \mathbb{R}$ and $\psi \in \mathfrak{h}$ be arbitrary. By Equation (7.7) for any $\Lambda \subset \mathbb{Z}^d$ one obtains

$$\tau^{(\mu)}_{\Lambda,\omega,t,-}(B_-) = U^{(\mu)}_{\Lambda,\omega,-}(t) B_- U^{(\mu)}_{\Lambda,\omega,-}(t)^* = \Gamma_-(U^{(\mu)}_{\Lambda,\omega}(t)) B_- \Gamma_-(U^{(\mu)}_{\Lambda,\omega}(t))^* \,.$$

for any $B_- \in \mathfrak{B}_-$. In addition, one has $\Gamma_-(U) a^*_-(\psi) \Gamma_-(U)^* = a^*_-(U\psi)$ for any unitary operator $U \in \mathscr{U}(\mathfrak{h})$ and any $\psi \in \mathfrak{h}$. We get that for any $L \in \mathbb{N}$ and $\psi \in \mathfrak{h}$

$$\begin{aligned}
\|\tau^{(\mu)}_{\Lambda_L,\omega,t,-}(a^*_-(\psi)) - \tau^{(\mu)}_{\omega,t,-}(a^*_-(\psi))\| &= \|a^*_-(U^{(\mu)}_{\Lambda_L,\omega}(t)\psi) - a^*_-(U^{(\mu)}_{\omega}(t)\psi)\| \\
&= \left\|a^*_-\left(\mathrm{e}^{-\mathrm{i}tH^{(\mu)}_{\Lambda_L,\omega}}\psi\right) - a^*_-\left(\mathrm{e}^{-\mathrm{i}tH^{(\mu)}_{\omega}}\psi\right)\right\| \\
&= \left\|a^*_-\left(\mathrm{e}^{-\mathrm{i}tH^{(\mu)}_{\Lambda_L,\omega}}\psi - \mathrm{e}^{-\mathrm{i}tH^{(\mu)}_{\omega}}\psi\right)\right\| \\
&= \left\|\mathrm{e}^{-\mathrm{i}tH^{(\mu)}_{\Lambda_L,\omega}}\psi - \mathrm{e}^{-\mathrm{i}tH^{(\mu)}_{\omega}}\psi\right\| \,.
\end{aligned}$$

Because $\lim_{L\to\infty} \|H^{(\mu)}_{\Lambda_L,\omega}\psi - H^{(\mu)}_{\omega}\psi\| = 0$ for any $\psi \in \mathfrak{h}$, we have $\lim_{L\to\infty} \left\|\mathrm{e}^{\mathrm{i}tH^{(\mu)}_{\Lambda_L,\omega}}\psi - \mathrm{e}^{\mathrm{i}tH^{(\mu)}_{\omega}}\psi\right\| = 0$ for any $\psi \in \mathfrak{h}$. So we obtain strong convergence of the time evolution automorphisms on $\mathfrak{B}_{c,-}$. Finally, from the fact that $\|\tau^{(\mu)}_{\Lambda_L,\omega,t,-}\| = \|\tau^{(\mu)}_{\omega,t,-}\| = 1$ we get the same holds true for all $B_- \in \mathfrak{B}_-$. ■

Actually, the strong convergence of the time evolution automorphisms as stated in Theorem 7.2 would be enough to conclude the existence of $(\tau^{(\mu)}_{\omega,-}, \beta)$-KMS states for any $\beta \in [0,\infty]$, using the Banach-Alaoglu theorem as in the proof of Theorem 7.1.

But for the non-interacting electron gas one can do better than just stating the existence of KMS states. In addition, one has explicit expressions for the KMS states in terms of their so called two-point functions.

In order to state this expression we introduce the Fermi distribution $F^{(\beta)} : \mathbb{R} \to \mathbb{R}$ at inverse temperature $\beta \in [0,\infty]$ for any $\varepsilon \in \mathbb{R}$ by

$$F^{(\beta)}(\varepsilon) := \begin{cases} 1 & \text{for } \beta = 0 \\ \chi_{]-\infty,0]}(\varepsilon) & \text{for } \beta = \infty \\ (\mathrm{e}^{\beta\varepsilon} + 1)^{-1} & \text{otherwise} \end{cases} \,. \tag{7.9}$$

Theorem 7.3 (*KMS State for Non-Interacting Electrons in a Box*)

For any $L \in \mathbb{N}$ consider the model of the electron gas introduced in Chapter 6 with $\Phi = 0$ and restricted to a box Λ_L using simple or Dirichlet or Neumann boundary conditions. Then, for any fixed realisation $\omega \in \Omega$, $\beta \in [0,\infty]$ and $\mu \in \mathbb{R}$ there exists a unique $(\tau^{(\mu)}_{\Lambda_L,\omega,-}, \beta)$-KMS state $\varrho^{(\beta,\mu)}_{\Lambda_L,\omega,-}$ which is completely determined by its two-point function, i.e. for any $\phi, \psi \in \mathfrak{h}$

$$\varrho^{(\beta,\mu)}_{\Lambda_L,\omega,-}(a^*_-(\psi) a_-(\phi)) = \langle \phi, F^{(\beta)}(H^{(\mu)}_{\Lambda_L,\omega})\psi \rangle \,. \tag{7.10}$$

Proof: First let $\beta \in [0,\infty[$. For non-interacting electron gases we use $H^{(\mu)}_{\Lambda_L,\omega,-} = \mathrm{d}\Gamma_-(H^{(\mu)}_{\Lambda_L,\omega})$ as well as

$$\mathrm{e}^{-\beta \mathrm{d}\Gamma_-(B)} a^*_-(\psi) = a^*_-(\mathrm{e}^{-\beta B}\psi)\mathrm{e}^{-\beta \mathrm{d}\Gamma_-(B)}$$

for any $B \in \mathfrak{B}_c$ and any $\psi \in \mathfrak{h}$. There exists a unique $(\tau^{(\mu)}_{\Lambda_L,\omega,-},\beta)$-KMS state $\varrho^{(\beta,\mu)}_{\Lambda_L,\omega,-}$ defined by Equations (7.1) and (7.2). We calculate

$$\begin{aligned}
&\varrho^{(\beta,\mu)}_{\Lambda_L,\omega,-}\Big(\Big(\prod_{k=1}^{n} a^*_-(\psi_k)\Big)\Big(\prod_{l=1}^{n} a_-(\phi_l)\Big)\Big)\\
&= \mathrm{Tr}\Big(a^*_-(\psi_1)\Big(\prod_{k=2}^{n} a^*_-(\psi_k)\Big)\Big(\prod_{l=1}^{n} a_-(\phi_l)\Big)P^{(\beta,\mu)}_{\Lambda_L,\omega,-}\Big)\\
&= \frac{1}{\mathrm{Tr}\Big(\mathrm{e}^{-\beta \mathrm{d}\Gamma_-(H^{(\mu)}_{\Lambda_L,\omega})}\Big)}\,\mathrm{Tr}\Big(\mathrm{e}^{-\beta \mathrm{d}\Gamma_-(H^{(\mu)}_{\Lambda_L,\omega})} a^*_-(\psi_1)\Big(\prod_{k=2}^{n} a^*_-(\psi_k)\Big)\Big(\prod_{l=1}^{n} a_-(\phi_l)\Big)\Big)\\
&= \frac{1}{\mathrm{Tr}\Big(\mathrm{e}^{-\beta \mathrm{d}\Gamma_-(H^{(\mu)}_{\Lambda_L,\omega})}\Big)}\,\mathrm{Tr}\Big(\mathrm{e}^{-\beta \mathrm{d}\Gamma_-(H^{(\mu)}_{\Lambda_L,\omega})}\Big(\prod_{k=2}^{n} a^*_-(\psi_k)\Big)\Big(\prod_{l=1}^{n} a_-(\phi_l)\Big)\, a^*_-\Big(\mathrm{e}^{-\beta H^{(\mu)}_{\Lambda_L,\omega}}\psi_1\Big)\Big)\\
&= \varrho^{(\beta,\mu)}_{\Lambda_L,\omega,-}\Big(\Big(\prod_{k=2}^{n} a^*_-(\psi_k)\Big)\Big(\prod_{l=1}^{n} a_-(\phi_l)\Big)\, a^*\Big(\mathrm{e}^{-\beta H^{(\mu)}_{\Lambda_L,\omega}}\psi_1\Big)\Big)
\end{aligned}$$

for any multiplet $\phi_1,...,\phi_n,\psi_1,...,\psi_n \in \mathfrak{h}$, where $n \in \mathbb{N}$. We use the CAR in Equations (B.71)-(B.73) to anti-commute the creation operator $a^*\Big(\mathrm{e}^{-\beta H^{(\mu)}_{\Lambda_L,\omega}}\psi_1\Big)$ on the right hand side through the product of creation and annihilation operators to its left. In particular, for $n = 1$ this yields

$$\varrho^{(\beta,\mu)}_{\Lambda_L,\omega,-}\Big(a^*_-\Big(\Big(1+\mathrm{e}^{-\beta H^{(\mu)}_{\Lambda_L,\omega}}\Big)\psi_1\Big)a_-(\phi_1)\Big) = \langle \phi_1, \mathrm{e}^{-\beta H^{(\mu)}_{\Lambda_L,\omega}}\psi_1\rangle\ .$$

Replacing $\phi := \phi_1$ and $\psi := \Big(1+\mathrm{e}^{-\beta H^{(\mu)}_{\Lambda_L,\omega}}\Big)\psi_1$ we get the following expression for the two-point function

$$\varrho^{(\beta,\mu)}_{\Lambda_L,\omega,-}(a^*_-(\psi)a_-(\phi)) = \langle \phi, F^{(\beta)}(H^{(\mu)}_{\Lambda_L,\omega})\psi\rangle\ .$$

In general, for higher products, i.e. for $n \geq 2$, from successive anti-commutation we obtain

$$\begin{aligned}
&\varrho^{(\beta,\mu)}_{\Lambda_L,\omega,-}\Big(a^*_-\Big(\Big(1+\mathrm{e}^{-\beta H^{(\mu)}_{\Lambda_L,\omega}}\Big)\psi_1\Big)\Big(\prod_{k=2}^{n} a^*_-(\psi_k)\Big)\Big(\prod_{l=1}^{n} a_-(\phi_l)\Big)\Big)\\
&= \sum_{j=1}^{n}(-1)^{n-j}\langle \phi_j, \mathrm{e}^{-\beta H^{(\mu)}_{\Lambda_L,\omega}}\psi_1\rangle\, \varrho^{(\beta,\mu)}_{\Lambda_L,\omega,-}\Big(\Big(\prod_{k=2}^{n} a^*_-(\psi_k)\Big)\Big(\prod_{\substack{l=1,\\ l\neq j}}^{n} a_-(\phi_l)\Big)\Big)\ . \qquad (7.11)
\end{aligned}$$

A similar replacement in Equation (7.11) leads to the reduction formula for the $(\tau^{(\mu)}_{\Lambda_L,\omega,-},\beta)$-KMS state

$$\begin{aligned}
&\varrho^{(\beta,\mu)}_{\Lambda_L,\omega,-}\Big(\Big(\prod_{k=1}^{n} a^*_-(\psi_k)\Big)\Big(\prod_{l=1}^{n} a_-(\phi_l)\Big)\Big)\\
&= \sum_{j=1}^{n}(-1)^{n-j}\varrho^{(\beta,\mu)}_{\Lambda_L,\omega,-}(a^*_-(\psi_1)a_-(\phi_j))\, \varrho^{(\beta,\mu)}_{\Lambda_L,\omega,-}\Big(\Big(\prod_{k=2}^{n} a^*_-(\psi_k)\Big)\Big(\prod_{\substack{l=1,\\ l\neq j}}^{n} a_-(\phi_l)\Big)\Big)\ .
\end{aligned}$$

Using a basis of eigenvectors of the number operator to calculate the trace, one directly obtains that $\varrho^{(\beta,\mu)}_{\Lambda_L,\omega,-}\Big(\Big(\prod_{k=1}^{n} a^*_-(\psi_k)\Big)\Big(\prod_{l=1}^{m} a_-(\phi_l)\Big)\Big) = 0$ whenever $n,m \in \mathbb{N}$ with $n \neq m$ and $\phi_1,...,\phi_m,\psi_1,...,\psi_n \in \mathfrak{h}$ arbitrary. Since $\varrho^{(\beta,\mu)}_{\Lambda_L,\omega,-}$ is a continuous linear functional on $\mathfrak{B}_-$, which is the closure of finite linear combinations of products of annihilation and creation operators, by a recursive use of the reduction formula one concludes that $\varrho^{(\beta,\mu)}_{\Lambda_L,\omega,-}$ is completely determined by its two-point function.

Next, we consider the case $\beta = \infty$. Using Theorem 4.5 for a sequence of $(\tau^{(\mu)}_{\Lambda_L,\omega,-},\beta_n)$-KMS states, where $(\beta_n)_{n\in\mathbb{N}}$ is a sequence in $[0,\infty[$ with $\lim_{n\to\infty}\beta_n = \beta$. Since $\lim_{n\to\infty} F^{(\beta_n)}(\varepsilon) = \chi_{]-\infty,0]}(\varepsilon) = F^{(\beta)}(\varepsilon)$ for any $\varepsilon\in\mathbb{R}$, one also has $\lim_{n\to\infty}\langle\phi, F^{(\beta_n)}(H^{(\mu)}_{\Lambda_L,\omega}),\psi\rangle = \langle\phi, F^{(\beta)}(H^{(\mu)}_{\Lambda_L,\omega}),\psi\rangle$. From this and the fact, that the time evolution automorphism is the same for all states of the sequence, by Theorem 4.5 one concludes that the sequence of $(\tau^{(\mu)}_{\Lambda_L,\omega,-},\beta_n)$-KMS states has a weak*- limit point $\varrho^{(\beta,\mu)}_{\Lambda_L,\omega,-}$ which is a $(\tau^{(\mu)}_{\Lambda_L,\omega,-},\beta)$-KMS state and is determined by its two-point function $\varrho^{(\beta,\mu)}_{\Lambda_L,\omega,-}(a^*_-(\psi)a_-(\phi)) = \langle\phi, F^{(\beta)}(H^{(\mu)}_{\Lambda_L,\omega})\psi\rangle$. ■

Theorem 7.4 (*KMS States for Non-interacting Electrons*)

Consider the model of a non-interacting electron gas introduced in Chapter 6, i.e. $\Phi = 0$. Then, for any fixed realisation $\omega\in\Omega$, $\beta\in[0,\infty]$ and $\mu\in\mathbb{R}$ there is a unique $(\tau^{(\mu)}_{\omega,-},\beta)$-KMS state $\varrho^{(\beta,\mu)}_{\omega,-}$ which is determined by its two-point function, i.e. for any $\phi,\psi\in\mathfrak{h}$ we have

$$\varrho^{(\beta,\mu)}_{\omega,-}(a^*_-(\psi)a_-(\phi)) = \langle\phi, F^{(\beta)}(H^{(\mu)}_{\omega})\psi\rangle\ . \tag{7.12}$$

Proof: Let $\omega\in\Omega$ be given. For any $\psi\in\mathfrak{h}$ one has that $\lim_{L\to\infty}\|H^{(\mu)}_{\Lambda_L,\omega}\psi - H^{(\mu)}_{\omega}\psi\| = 0$. First let $\beta\in[0,\infty[$. Then, since $F^{(\beta)}$ is a bounded continuous function, one also has

$$\varrho^{(\beta,\mu)}_{\omega,-}(a^*_-(\psi)a_-(\phi)) := \lim_{L\to\infty}\varrho^{(\beta,\mu)}_{\Lambda_L,\omega,-}(a^*_-(\psi)a_-(\phi)) = \lim_{L\to\infty}\langle\phi, F^{(\beta)}(H^{(\mu)}_{\Lambda_L,\omega})\psi\rangle = \langle\phi, F^{(\beta)}(H^{(\mu)}_{\omega})\psi\rangle\ .$$

From this one concludes that the sequence $(\varrho^{(\beta,\mu)}_{\Lambda_L,\omega,-})_{L\in\mathbb{N}}$ of $(\tau^{(\mu)}_{\Lambda_L,\omega,-},\beta)$-KMS states has a weak*-limit $\varrho^{(\beta,\mu)}_{\omega,-}$ which due to Theorem 7.2 is a $(\tau^{(\mu)}_{\omega,-},\beta)$-KMS state and on the other hand is completely determined by its two-point function given in Equation (7.12). Since there is no need to pass to subsequences of the sequence of $(\tau^{(\mu)}_{\Lambda_L,\omega,-},\beta)$-KMS states, we have that $\varrho^{(\beta,\mu)}_{\omega,-}$ is unique.

For $\beta=\infty$ one proceeds as in the proof of Theorem 7.3, considers a sequence of $(\tau^{(\mu)}_{\omega,-},\beta_n)$-KMS states, where $(\beta_n)_{n\in\mathbb{N}}$ is a sequence in $\mathbb{R}$ with $\lim_{n\to\infty}\beta_n = \beta$. Then, using Theorem 4.5, one concludes that there is a unique $(\tau^{(\mu)}_{\omega,-},\beta)$-KMS state $\varrho^{(\beta,\mu)}_{\omega,-}$ with a two-point function as in Equation (7.12). ■

Covariant KMS States

Assuming that for each realisation of the system there is a unique KMS state, one has that $\varrho^{(\beta,\mu)}_{-} : \Omega\to \mathrm{Sta}(\mathfrak{B}_-)$, $\omega\mapsto\varrho^{(\beta,\mu)}_{\omega,-}$ forms a covariant KMS state. Note that the assumptions of a unique KMS limit state in each realisation is satisfied for the non-interacting electron gas. Typically, systems possess unique phases at high temperatures. Therefore, the following theorem is of use whenever one is interested in a high temperature regime.

Theorem 7.5 (*Covariant KMS States*)

Let $\beta\in[0,\infty]$, $\mu\in\mathbb{R}$ and assume that for almost every $\omega\in\Omega$ and $t\in\mathbb{R}$ the sequence of covariant time evolution automorphisms $(\tau^{(\mu)}_{\Lambda_L,\omega,t,-})_{L\in\mathbb{N}}$ strongly converges to $\tau^{(\mu)}_{\omega,t,-}$, such that there exists a $(\tau^{(\mu)}_{\omega,-},\beta)$-KMS state $\varrho^{(\beta,\mu)}_{\omega,-}$. In addition, assume that $\varrho^{(\beta,\mu)}_{\omega,-}$ is the unique $(\tau^{(\mu)}_{\omega,-},\beta)$-KMS state for almost every $\omega\in\Omega$. Then, $\varrho^{(\beta,\mu)}_{-} : \Omega\to\mathrm{Sta}(\mathfrak{B}_-)$, $\omega\mapsto\varrho^{(\beta,\mu)}_{\omega,-}$ transforms covariantly.

Proof: Let $\beta\in[0,\infty]$, $\omega\in\Omega$ and $(L_n)_{n\in\mathbb{N}}$ be any subsequence of $(L)_{L\in\mathbb{N}}$. Let $(\varrho^{(\beta,\mu)}_{\Lambda_{L_n},\omega,-})_{n\in\mathbb{N}}$ be the corresponding sequence of $(\tau^{(\beta,\mu)}_{\Lambda_{L_n},\omega,-},\beta)$-KMS states defined via the Equations (7.1) and (7.2). Then, due to the Banach-Alaoglu theorem, there exists a subsequence $(L_{n_k})_{k\in\mathbb{N}}$ and a state $\varrho^{(n_k)_{k\in\mathbb{N}}}_{\omega,-}$ such that for any $B_- \in \mathfrak{B}_-$ one has

$$\lim_{k\to\infty}\left|\varrho^{(\beta,\mu)}_{\Lambda_{L_{n_k}},\omega,-}(B_-) - \varrho^{(n_k)_{k\in\mathbb{N}}}_{\omega,-}(B_-)\right| = 0\,.$$

It is essential that the choice of the subsequence $(n_k)_{k\in\mathbb{N}}$, and therefore also the limit state in general, will depend on $\omega \in \Omega$. Due to Theorem 4.5 the state $\varrho^{(n_k)_{k\in\mathbb{N}}}_{\omega,-}$ is a $(\tau^{(\mu)}_{\omega,-},\beta)$-KMS state. But assuming uniqueness of the $(\tau^{(\mu)}_{\omega,-},\beta)$-KMS state, we have that it does not depend on the choice of subsequence, i.e. we have that already $(\varrho^{(\beta,\mu)}_{\Lambda_L,\omega,-})_{L\in\mathbb{N}}$ converges to the unique $(\tau^{(\mu)}_{\omega,-},\beta)$-KMS state $\varrho^{(\beta,\mu)}_{\omega,-} := \varrho^{(n_k)_{k\in\mathbb{N}}}_{\omega,-}$, i.e.

$$\lim_{L\to\infty}|\varrho^{(\beta,\mu)}_{\Lambda_L,\omega,-}(B_-) - \varrho^{(\beta,\mu)}_{\omega,-}(B_-)| = 0$$

for any $B_- \in \mathfrak{B}_-$. The measurability of the mapping $\varrho^{(\beta,\mu)}_{-} : \Omega \to \mathrm{Sta}(\mathfrak{B}_-)$, $\omega \mapsto \varrho^{(\beta,\mu)}_{\omega,-}$ follows from measurability of $\varrho^{(\beta,\mu)}_{\Lambda_L,-} : \Omega \to \mathrm{Sta}(\mathfrak{B}_-)$, $\omega \mapsto \varrho^{(\beta,\mu)}_{\Lambda_L,\omega,-}$ for each $L \in \mathbb{N}$ and weak-* convergence. The covariance follows from an application of Theorem 5.6. ■

7.2. Construction of Time Dependent States

Now we construct the state of the electron gas in the general situation, where the state is time dependent due to the presence of an electric field. Given a volume $\Lambda \subset \mathbb{Z}^d$, a realisation $\omega \in \Omega$ and a $(\tau^{(\mu)}_{\Lambda,\omega,-},\beta)$-KMS state $\varrho^{(\beta,\mu)}_{\Lambda,\omega,-}$ one can construct another state via

$$\rho^{(E,\beta,\mu)}_{\Lambda,\omega,t,r,-} := \varrho^{(\beta,\mu)}_{\Lambda,\omega,-} \circ (\tau^{(E,\mu)}_{\Lambda,\omega,t,r,-} \circ \gamma^{(E)}_{r,-})^{-1} \tag{7.13}$$

for any $t, r \in \mathbb{R}$. The interpretation of this construction is the following. Typically, one will be given a situation, where $r \ll t$ and the electric field is switched on adiabatically. Then, $|E(r)| \ll |E(t)|$ and the state $\rho^{(E,\beta,\mu)}_{\Lambda,\omega,t,r,-}$ describes an electron gas, which at time r was in thermal equilibrium at inverse temperature β, already considering the presence of a small electric field. Then, this state is evolved to time t, when the electric field is stronger. If the following limit exists for all $\omega \in \Omega$, we define another state via

$$\rho^{(E,\beta,\mu)}_{\Lambda,\omega,t,-}(B_-) := \lim_{r\to-\infty}\rho^{(E,\beta,\mu)}_{\Lambda,\omega,t,r,-}(B_-) \tag{7.14}$$

for all $B_- \in \mathfrak{B}_-$. This state describes a system, that was in equilibrium in the infinite past, when in any case no electric field was present. If the electric field is switched on in the finite past, the limit in Equation (7.14) exists. More precisely, assuming that no electric field is present for $r \le s$, where $s \in \mathbb{R}$ is a fixed starting time, one has $F^{(E)}(r) := \int_{-\infty}^{r} E(q)\,\mathrm{d}q = 0$ for all $r \le s$. This causes simplifications in the automorphisms on the right hand side of Equation (7.13) that hold for any $r \le s$ and lead to the existence of the limit in Equation (7.14)

$$\begin{aligned}\rho^{(E,\beta,\mu)}_{\Lambda,\omega,t,r,-} &= \varrho^{(\beta,\mu)}_{\Lambda,\omega,-} \circ (\tau^{(E,\mu)}_{\Lambda,\omega,t,r,-} \circ \gamma^{(E)}_{r,-})^{-1} = \varrho^{(\beta,\mu)}_{\Lambda,\omega,-} \circ (\tau^{(E,\mu)}_{\Lambda,\omega,t,s,-} \circ \tau^{(E,\mu)}_{\Lambda,\omega,s,r,-} \circ \gamma^{(E)}_{r,-})^{-1}\\ &= \varrho^{(\beta,\mu)}_{\Lambda,\omega,-} \circ (\tau^{(E,\mu)}_{\Lambda,\omega,t,s,-} \circ \tau^{(\mu)}_{\Lambda,\omega,s-r,-})^{-1} = \varrho^{(\beta,\mu)}_{\Lambda,\omega,-} \circ \tau^{(\mu)}_{\Lambda,\omega,r-s,-} \circ \tau^{(E,\mu)}_{\Lambda,\omega,s,t,-}\\ &= \varrho^{(\beta,\mu)}_{\Lambda,\omega,-} \circ \tau^{(E,\mu)}_{\Lambda,\omega,s,t,-} = \rho^{(E,\beta,\mu)}_{\Lambda,\omega,t,s,-}\,.\end{aligned}$$

For the case that $\Lambda = \mathbb{Z}^d$, we have that the mappings $\rho^{(E,\beta,\mu)}_{t,r,-} : \Omega \to \mathrm{Sta}(\mathfrak{B}_-)$, $\omega \mapsto \rho^{(E,\beta,\mu)}_{\omega,t,r,-}$ and, if it exists, $\rho^{(E,\beta,\mu)}_{t,-} : \Omega \to \mathrm{Sta}(\mathfrak{B}_-)$, $\omega \mapsto \rho^{(E,\beta,\mu)}_{\omega,t,-}$ are covariant states, for any $t, r \in \mathbb{R}$ whenever the time evolution $\tau^{(E,\beta,\mu)}_{t,r,-}$ is a covariant automorphism and $\varrho^{(\beta,\mu)}_{-}$ is a covariant KMS state.

Non-Interacting Case

Analysing the situation for non-interacting electron gases one may use the advantage of having explicit expressions for the time dependent state in Equation (7.13). This is why we focus on this case again. The simplifications mentioned above are, for example, reflected in the following formula

$$U^{(E,\mu)}_{\Lambda,\omega,-}(t,r) = \Gamma_-(U^{(E,\mu)}_{\Lambda,\omega}(t,r)) \tag{7.15}$$

for any subset $\Lambda \subset \mathbb{Z}^d$, realisation $\omega \in \Omega$ and times $t, r \in \mathbb{R}$. For the time evolution automorphisms one obtains

$$\tau^{(E,\mu)}_{\Lambda,\omega,t,r,-}(a^*_-(\psi)) = a^*_-(U^{(E,\mu)}_{\Lambda,\omega}(t,r)\psi) \tag{7.16}$$

for any $\psi \in \mathfrak{h}$. In general, we can use the following formula for products of creation and annihilation operators

$$\begin{aligned}
&(\tau^{(E,\mu)}_{\Lambda,\omega,t,r,-} \circ \gamma^{(E)}_{r,-})^{-1}\Big(\Big(\prod_{k=1}^{m} a^*_-(\psi_k)\Big)\Big(\prod_{l=1}^{n} a_-(\phi_l)\Big)\Big) \\
&= \Big(\prod_{k=1}^{m} a^*_-(G^{(E)}(r)^* U^{(E,\mu)}_{\Lambda,\omega}(r,t)\psi_k)\Big)\Big(\prod_{l=1}^{n} a_-(G^{(E)}(r)^* U^{(E,\mu)}_{\Lambda,\omega}(r,t)\phi_l)\Big)\,,
\end{aligned} \tag{7.17}$$

where $m, n \in \mathbb{N}$ and $\psi_1, ..., \psi_m, \phi_1, ..., \phi_n \in \mathfrak{h}$. Applying the KMS state $\varrho^{(\beta,\mu)}_{\Lambda,\omega,-}$ on both sides of the above equation, where either $\Lambda = \Lambda_L$ for some $L \in \mathbb{N}$ or $\Lambda = \mathbb{Z}^d$. Considering the reduction formula (7.11) for the KMS state leads to the result that the time dependent state is completely determined by its two-point function. Precisely, for the case $n = m$ one obtains

$$\begin{aligned}
&\rho^{(E,\beta,\mu)}_{\Lambda,\omega,t,r,-}\Big(\Big(\prod_{k=1}^{n} a^*_-(\psi_k)\Big)\Big(\prod_{l=1}^{n} a_-(\phi_l)\Big)\Big) \\
&= \sum_{j=1}^{n} (-1)^{n-j} \rho^{(E,\beta,\mu)}_{\Lambda,\omega,t,r,-}(a^*_-(\psi_1)a_-(\phi_j))\, \rho^{(E,\beta,\mu)}_{\Lambda,\omega,t,r,-}\Big(\Big(\prod_{k=2}^{n} a^*_-(\psi_k)\Big)\Big(\prod_{\substack{l=1,\\ l\neq j}}^{n} a_-(\phi_l)\Big)\Big)\,.
\end{aligned} \tag{7.18}$$

For $n \neq m$ both sides vanish. In order to express the two-point function one can define an effective density matrix by

$$P^{(E,\beta,\mu)}_{\Lambda,\omega}(t,r) := \tau^{(E)}_{\Lambda,\omega,t,r}(F^{(\beta)}(H^{(E,\mu)}_{\Lambda,\omega}(r))) \tag{7.19}$$

for any $\omega \in \Omega$ and $t, r \in \mathbb{R}$. One obtains

$$\begin{aligned}
\rho^{(E,\beta,\mu)}_{\Lambda,\omega,t,r,-}(a^*_-(\psi)a_-(\phi)) &= \varrho^{(\beta,\mu)}_{\Lambda,\omega,-}(a^*_-(G^{(E)}(r)^* U^{(E,\mu)}_{\Lambda,\omega}(r,t)\psi)a_-(G^{(E)}(r)^* U^{(E,\mu)}_{\Lambda,\omega}(r,t)\phi)) \\
&= \langle G^{(E)}(r)^* U^{(E,\mu)}_{\Lambda,\omega}(r,t)\phi, F^{(\beta)}(H^{(\mu)}_{\Lambda,\omega}) G^{(E)}(r)^* U^{(E,\mu)}_{\Lambda,\omega}(r,t)\psi\rangle \\
&= \langle \phi, \tau^{(E)}_{\Lambda,\omega,t,r}(\gamma^{(E)}_r(F^{(\beta)}(H^{(\mu)}_{\Lambda,\omega})))\psi\rangle \\
&= \langle \phi, \tau^{(E)}_{\Lambda,\omega,t,r}(F^{(\beta)}(\gamma^{(E)}_r(H^{(\mu)}_{\Lambda,\omega})))\psi\rangle \\
&= \langle \phi, \tau^{(E)}_{\Lambda,\omega,t,r}(F^{(\beta)}(H^{(E,\mu)}_{\Lambda,\omega}(r)))\psi\rangle \\
&= \langle \phi, P^{(E,\beta,\mu)}_{\Lambda,\omega}(t,r)\psi\rangle\,.
\end{aligned} \tag{7.20}$$

Note that the density matrix satisfies the so called von Neumann equation, i.e. for any $t, r \in \mathbb{R}$

$$\begin{cases} \mathrm{i}\partial_t P^{(E,\beta,\mu)}_{\Lambda,\omega}(t,r) = [H^{(E,\mu)}_{\Lambda,\omega}(t), P^{(E,\beta,\mu)}_{\Lambda,\omega}(t,r)] \\ P^{(E,\beta,\mu)}_{\Lambda,\omega}(r,r) = F^{(\beta)}(H^{(E,\mu)}_{\Lambda,\omega}(r)) \end{cases} . \tag{7.21}$$

Finally, for any operator of finite support $B \in \mathfrak{B}_c$ we have that $\mathrm{d}\Gamma_-(B)$ is of finite support, so one can apply the state of the system to it. Then, using Equation (B.75) for any $\omega \in \Omega$ and $t, r \in \mathbb{R}$ one obtains

$$\begin{aligned} \rho^{(E,\beta,\mu)}_{\Lambda,\omega,t,r,-}(\mathrm{d}\Gamma_-(B)) &= \varrho^{(\beta,\mu)}_{\Lambda,\omega,-}\Big(\sum_{x\in\mathbb{Z}^d} a^*_-(B\delta_x)a_-(\delta_x)\Big) = \sum_{x\in\mathbb{Z}^d} \varrho^{(\beta,\mu)}_{\Lambda,\omega,-}\Big(a^*_-(B\delta_x)a_-(\delta_x)\Big) \\ &= \sum_{x\in\mathbb{Z}^d} \langle \delta_x, P^{(E,\beta,\mu)}_{\Lambda,\omega}(t,r)B\delta_x\rangle = \mathrm{Tr}\big(P^{(E,\beta,\mu)}_{\Lambda,\omega}(t,r)B\big) . \end{aligned} \tag{7.22}$$

8 Current Density and Conductivity

To a man standing on the shore, time passes quicker than to a man on a boat, especially, if the man on the boat is with his wife.

(Woody Allen)

Having defined the current density operator and given the state of the electron gas, we are able to define the current density as the quantum mechanical expectation value of the current density operator with respect to the state of the electron gas. The result is a quantity, that still depends on time and position of the measurement as well as on the concrete realisation of the random system.

Then, in view of our final goal, which is to find a Kubo formula for the conductivity of an extended electron gas, we need the spatial mean of the current density over all possible positions of measurement in a fixed realisation. As a consequence of Birkhoff's theorem, for ergodic systems one finds that this spatial average almost surely exists and is independent of the realisation. This we will achieve in Theorem 8.5.

Also in this chapter we will define the so called linear response current and the conductivity. Roughly speaking this is done by differentiating the spatially averaged current density with respect to the strength of the external electric field at zero field strength. The existence of the latter quantity for an extended non-interacting electron gas is subject to Chapter 9.

8.1. Current Density

We consider the model of an electron gas introduced in Chapter 6. In this situation, the current density is the quantum mechanical expectation value of the measurement implemented by the current density operator (6.89) with respect to the state of the system constructed in Chapter 7.

Definition 8.1 (*Current Density*)

For $\Lambda \subset \mathbb{Z}^d$, $\omega \in \Omega$ and $t, r \in \mathbb{R}$ and $y \in \mathbb{Z}^d$ the *current density* $j_{\Lambda,\omega,r}(t, y; E, \beta, \mu)$ is the quantum mechanical expectation value of the current density operator $J^{(E)}_{\Lambda,\omega,-}(t, y)$ with respect to the state $\rho^{(E,\beta,\mu)}_{\Lambda,\omega,t,r,-}$ introduced in Equation (7.14). For each $k \in \{1, ..., d\}$ its components are given by

$$j_{\Lambda,\omega,k,r}(t, y; E, \beta, \mu) := \rho^{(E,\beta,\mu)}_{\Lambda,\omega,t,r,-}(J^{(E)}_{\Lambda,\omega,k,-}(t, y)) , \tag{8.1}$$

$$j_{\Lambda,\omega}(t, y; E, \beta, \mu) := \lim_{r\to-\infty} j_{\Lambda,\omega,r}(t, y; E, \beta, \mu) . \tag{8.2}$$

Note that for $\omega \in \Omega$, $t \in \mathbb{R}$ and $y \in \mathbb{Z}^d$ the limit in Equation (8.2) exists whenever the limit state $\rho^{(E,\beta,\mu)}_{\Lambda,\omega,t,-}$ in Equation (7.13) exists. For example, this will be the case, if $\Lambda \subset \mathbb{Z}^d$ is finite.

We concentrate on the case $\Lambda = \mathbb{Z}^d$, where the current density satisfies the following transformation law, which we use to prove the existence of spatial averages.

Theorem 8.2 (*Transformation Law of the Current Density*)

For almost every $\omega \in \Omega$, any $t, r \in \mathbb{R}$ and $y, a \in \mathbb{Z}^d$ the current density satisfies the following transformation law

$$j_{\omega,r}(t, y; E,\beta,\mu) = j_{\phi_a(\omega),r}(t, y + a; E,\beta,\mu) , \tag{8.3}$$

$$j_{\omega}(t, y; E,\beta,\mu) = j_{\phi_a(\omega)}(t, y + a; E,\beta,\mu) . \tag{8.4}$$

Proof: Because of the fact that $\rho^{(E,\beta,\mu)}_{t,r,-} : \Omega \to \mathrm{Sta}(\mathfrak{B}_-),\ \omega \mapsto \rho^{(E,\beta,\mu)}_{\omega,t,r,-}$ is a covariant state for any $t, r \in \mathbb{R}$ and due to the transformation law for the current density operator given in Equation (6.91), for any $k \in \{1, ..., d\}$, $y, a \in \mathbb{Z}^d$ and almost every $\omega \in \Omega$ we have

$$\begin{aligned} j_{\omega,k,r}(t, y; E,\beta,\mu) &= \rho^{(E,\beta,\mu)}_{\omega,t,r,-}(J^{(E)}_{\omega,k,-}(t, y)) \\ &= \rho^{(E,\beta,\mu)}_{\omega,t,r,-}(\varphi_{-a}(\varphi_a(J^{(E)}_{\omega,k,-}(t, y)))) \\ &= \rho^{(E,\beta,\mu)}_{\phi_a(\omega),t,r,-}(J^{(E)}_{\phi_a(\omega),k,-}(t, y + a)) \\ &= j_{\phi_a(\omega),k,r}(t, y + a; E,\beta,\mu) . \end{aligned}$$

This proves Equation (8.3). Taking the limit $r \to -\infty$ on both sides of (8.3) leads to Equation (8.4). ■

8.2. Mean Current Density

In this paragraph we define the average current density in two different situations of the system introduced in Chapter 6 described by states as constructed in Chapter 7. In the first case, where the system is restricted to a finite volume $\Lambda \subset \mathbb{Z}^d$, the average current density still depends on the realisation of the system.

Definition 8.3 (*Mean Current Density for Finite Systems*)

For a finite subset $\Lambda \subset \mathbb{Z}^d$, $\omega \in \Omega$ and $t, r \in \mathbb{R}$ we define the *mean current density* as the spatial average of the current density as in Definition 8.1, i.e.

$$j_{\Lambda,\omega,r}(t; E,\beta,\mu) := \frac{1}{|\Lambda|} \sum_{y \in \Lambda} j_{\Lambda,\omega,r}(t, y; E,\beta,\mu) , \tag{8.5}$$

$$j_{\Lambda,\omega}(t; E,\beta,\mu) := \lim_{r \to -\infty} j_{\Lambda,\omega,r}(t; E,\beta,\mu) . \tag{8.6}$$

Next, we consider th case $\Lambda = \mathbb{Z}^d$, where again, the label Λ is suppressed in the notation. Note that in this case the average current density by definition does not depend on the realisation of the system.

Definition 8.4 (*Mean Current Density for Extended Systems*)

For an electron gas in $\mathbb{Z}^d$ and $t, r \in \mathbb{R}$ we define the *mean current density* by taking the expectation value of the random variable $j_r(t, 0; E,\beta,\mu) : \Omega \to \mathbb{R}^d,\ \omega \mapsto j_{\omega,r}(t, 0; E,\beta,\mu)$

$$j_r(t; E,\beta,\mu) := \mathbb{E}[j_r(t, 0; E,\beta,\mu)] , \tag{8.7}$$

$$j(t; E,\beta,\mu) := \lim_{r \to -\infty} j_r(t; E,\beta,\mu) . \tag{8.8}$$

Of course, there is a relation between the Equations (8.5) and (8.7). The latter is just the former in the limit of infinite volume. This is made precise by the following theorem.

Theorem 8.5 (*Limit of Infinite Volume*)

For $L \in \mathbb{N}$ let Λ_L be a subset of $\mathbb{Z}^d$ inside a closed cube of side length $(2L+1)$ that is centred at $0 \in \mathbb{Z}^d$. Then, for almost every $\omega \in \Omega$ and all $t, r \in \mathbb{R}$ the following limit exists

$$j_r(t; E, \beta, \mu) = \lim_{L\to\infty} j_{\Lambda_L,\omega,r}(t; E, \beta, \mu) = \lim_{L\to\infty} \frac{1}{|\Lambda_L|} \sum_{y\in\Lambda_L} j_{\omega,r}(t, y; E, \beta, \mu) \, . \tag{8.9}$$

Proof: Let $t, r \in \mathbb{R}$ be arbitrary. From the transformation law of the current density (8.3) and an application of Birkhoff's ergodic theorem one gets that for almost every $\omega \in \Omega$ the following limit exists

$$\begin{aligned} j_r(t; E, \beta, \mu) &= \mathbb{E}[j_r(t, 0; E, \beta, \mu)] \\ &\overset{a.s.}{=} \lim_{L\to\infty} \frac{1}{|\Lambda_L|} \sum_{y\in\Lambda_L} j_{\phi_{-y}(\omega),r}(t, 0; E, \beta, \mu) \\ &= \lim_{L\to\infty} \frac{1}{|\Lambda_L|} \sum_{y\in\Lambda_L} j_{\omega,r}(t, y; E, \beta, \mu) \, . \end{aligned}$$

■

For the case of a non-interacting electron gas, one can calculate more explicit expressions for the quantity defined in Equation (8.7) and also prove existence of the limit in Equation (8.8). In particular, Equation (8.8) is in agreement with the definition of the current density in (BGKS05, KLM07, KM08). We present this result in the subsequent chapter, using the theory of spaces of covariant operators as achieved in (BGKS05). We postpone this discussion for the reason of first defining the so called linear response current and the conductivity.

8.3. Linear Response Current

Our goal in this section is to give a precise meaning to the term conductivity for the discrete system introduced in Chapter 6. A physicists common understanding considers conductivity as a constant that depends on the material of a given sample as well as on its temperature. But it does not depend on the size of the sample. For a lead of copper the information that should enter a formula for the conductivity is the material, i.e. the lead is a certain alloy. But the electrical conductivity should neither depend on the cross section nor on the length of the lead. This is why, from now on we concentrate on the case of an infinite system. This is a way of gauging the material dependent constant conductivity to a standard volume, namely the infinite volume $\Lambda = \mathbb{Z}^d$. Such a procedure is justified by the fact, that in typical experiments the samples of materials are infinitely large having microscopic scales in view. Suppose that we are given an electric field $E \in \mathcal{E}(\mathbb{R}, \mathbb{R}^d)$. Then, for any $\lambda \in \mathbb{R}$ we define $E_\lambda := \lambda\, E \in \mathcal{E}(\mathbb{R}, \mathbb{R}^d)$ and consider the averaged current density induced by the external electric field E_λ.

Definition 8.6 (*Linear Response Current*)

For $E \in \mathcal{E}(\mathbb{R}, \mathbb{R}^d)$, $t, \mu \in \mathbb{R}$ and $\beta \in [0, \infty]$ we consider the current density $j(t; E_\lambda, \beta, \mu)$. If the mapping $\mathbb{R} \to \mathbb{R}^d, \lambda \mapsto j(t; E_\lambda, \beta, \mu)$ is differentiable at 0, the *linear response current* $j_{\mathrm{res}}(t; E, \beta, \mu)$ is defined as

$$j_{\mathrm{res}}(t; E, \beta, \mu) := \partial_\lambda\, j(t; E_\lambda, \beta, \mu)|_{\lambda=0} \, . \tag{8.10}$$

8.4. DC Conductivity

We define the direct current conductivity. Therefore, we consider homogeneous fields which are switched on adiabatically with adiabatic parameter $\eta \in]0, \infty[$. More concretely, for any $E \in \mathbb{R}^d$ we define the electric field $E_\eta^{\mathrm{DC}} \in \mathcal{E}(\mathbb{R}, \mathbb{R}^d)$ for all $t \in \mathbb{R}$ via

$$E_\eta^{\mathrm{DC}}(t) := E\, \mathrm{e}^{\eta t} .$$

Definition 8.7 (*DC Conductivity at Adiabatic Switching*)

Assume that at inverse temperature $\beta \in [0, \infty]$ and chemical potential $\mu \in \mathbb{R}$ the linear response current in Definition 8.6 exists for any $E \in \mathcal{E}(\mathbb{R}, \mathbb{R}^d)$ at time $0 \in \mathbb{R}$. Then, the *direct current conductivity at adiabatic switching* $\eta \in]0, \infty[$ is the tensor $\sigma^{\mathrm{DC}}(\eta, \beta, \mu) \in M_d(\mathbb{C})$ such that for all $E \in \mathbb{R}^d$ the following identity holds

$$j_{\mathrm{res}}(0; E_\eta^{\mathrm{DC}}, \beta, \mu) =: \sigma^{\mathrm{DC}}(\eta, \beta, \mu)(E) . \tag{8.11}$$

Definition 8.8 (*DC Conductivity*)

Assume that at time $0 \in \mathbb{R}$, inverse temperature $\beta \in [0, \infty]$ and chemical potential $\mu \in \mathbb{R}$ the linear response current in Definition 8.6 exists for any $E \in \mathcal{E}(\mathbb{R}, \mathbb{R}^d)$. Then, if the following limit exists for all $E \in \mathbb{R}^d$, the *direct current conductivity* is the tensor $\sigma^{\mathrm{DC}}(\beta, \mu) \in M_d(\mathbb{C})$ such the following identity holds

$$\lim_{\eta \to 0} j_{\mathrm{res}}(0; E_\eta^{\mathrm{DC}}, \beta, \mu) = \lim_{\eta \to 0} \sigma^{\mathrm{DC}}(\eta, \beta, \mu)(E) =: \sigma^{\mathrm{DC}}(\beta, \mu)(E) . \tag{8.12}$$

8.5. AC Conductivity

Analogously, we define the alternating current conductivity. We assume that $E \in \mathcal{E}(\mathbb{R}, \mathbb{R}^d)$ is an inverse Fourier transform, i.e. for $t \in \mathbb{R}$ we assume

$$E(t) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{E}(\nu)\, \mathrm{e}^{\mathrm{i} t \nu}\, \mathrm{d}\nu .$$

Moreover, we assume that $\hat{E} \in L^1(\mathbb{R}, \mathbb{C}^d)$ is continuous and satisfies the condition $\hat{E}(\nu) = \overline{\hat{E}(-\nu)}$ for all $\nu \in \mathbb{R}$. For such electric fields and $\eta \in]0, \infty[$ we define $E_\eta^{AC} \in \mathcal{E}(\mathbb{R}, \mathbb{R}^d)$ by

$$E_\eta^{\mathrm{AC}}(t) := E(t)\, \mathrm{e}^{\eta t} .$$

Definition 8.9 (*AC Conductivity at Adiabatic Switching*)

Assume that at inverse temperature $\beta \in [0, \infty]$ and chemical potential $\mu \in \mathbb{R}$ the linear response current in Definition 8.6 exists for any $\mathcal{E}(\mathbb{R}, \mathbb{R}^d)$ at any time $t \in \mathbb{R}$. If it exists, the *alternating current conductivity at adiabatic switching* $\eta \in]0, \infty[$ is the measurable mapping $\mathbb{R} \to M_d(\mathbb{C})$, $\nu \mapsto \sigma^{\mathrm{AC}}(\nu; \eta, \beta, \mu)$ such that for all $E \in \mathcal{E}(\mathbb{R}, \mathbb{R}^d)$ that satisfy the assumptions above the following identity holds

$$j_{\mathrm{res}}(t; E_\eta^{\mathrm{AC}}, \beta, \mu) =: \frac{\mathrm{e}^{\eta t}}{\sqrt{2\pi}} \int_{\mathbb{R}} \sigma^{\mathrm{AC}}(\nu; \eta, \beta, \mu)(\hat{E}(\nu))\, \mathrm{e}^{\mathrm{i}\nu t}\, \mathrm{d}\nu . \tag{8.13}$$

Definition 8.10 (*AC Conductivity*)

Assume that at inverse temperature $\beta \in [0, \infty]$ and chemical potential $\mu \in \mathbb{R}$ the linear response current in Definition 8.6 exists for any $\mathcal{E}(\mathbb{R}, \mathbb{R}^d)$ at any time $t \in \mathbb{R}$. If it exists, the *alternating current conductivity* is the measurable mapping $\mathbb{R} \to M_d(\mathbb{C}),\ \nu \mapsto \sigma^{\mathrm{AC}}(\nu;\beta,\mu)$ such that for all $E \in \mathcal{E}(\mathbb{R}, \mathbb{R}^d)$ that satisfy the assumptions above the following identity holds

$$\lim_{\eta\to 0} j_{\mathrm{res}}(t; E_\eta^{\mathrm{AC}},\beta,\mu) =: \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \sigma^{\mathrm{AC}}(\nu;\beta,\mu)(\hat{E}(\nu))\, \mathrm{e}^{\mathrm{i}\nu t}\, \mathrm{d}\nu\, . \tag{8.14}$$

Remarks

We like to emphasise the fact that not only the definitions in this chapter but also Theorems 8.2 and 8.5 apply to interacting models of electron gases as introduced in Chapter 6. The only condition that needs to be satisfied is that the gas without electric field has to be described by a covariant KMS state. Of course, this condition is crucial, since for non-trivial interactions we only succeeded in the construction of covariant states in space dimension $d = 1$.
The definition of the linear response current and the definition of the DC conductivity are in agreement with (BGKS05). The assumptions on the electric fields for the definition of the AC conductivity as well as the definition of the AC conductivity itself are in agreement with (KLM07, KM08).

9 Non-Interacting Systems

He had bought a large map representing the sea,
Without the least vestige of land;
And the crew were much pleased when they found it to be
A map they could all understand.

(Lewis Carrol)

In this chapter we will consider a concrete model of an extended electron gas and carry out the procedures, which, only in form of recipes, were described in Chapter 8.

So far, we were able to define the electric current density of interacting ergodic systems influenced by an external electric field. However, we will only be able to prove existence of linear response current and direct current conductivity as well as alternating current conductivity for the special case of a non-interacting electron gas. From thermal considerations for a similar model this is also achieved in (BSPK13b), where not only existence of the objects of interest but also certain properties of the latter are proven.

Up to the point of defining a current density, the most significant constriction is the construction of KMS states, which for the case of a non-trivial interaction we have only succeeded in space dimension $d = 1$. However, given the covariant KMS state which the electron gas was in before an external electric field was switched on, one automatically obtains the covariant state of the system at arbitrary times by an application of the covariant time evolution automorphism.

Then, the existence of the current density is evident from its definition as the quantum mechanical expectation value of the current density operator with respect to the state of the system. Moreover, considering an ergodic electron gas, one gets the existence of the mean current density using the concept of covariant states. This we achieved in Theorem 8.5.

But in view of proving existence of a linear response current, one suffers from the fact, that only in the case of a non-interacting electron gas, the expressions for the state of the system simplify. Therefore, one may derive more concrete expressions for the current density as well as for the mean current. Unfortunately, in order to prove the existence of a linear response current an involved analysis of these expressions seems inevitable.

In more detail, considering the non-interacting electron gas, already in (BGKS05, KM08, KLM07) the differentiation process with respect to the strength of the electric field leading from the mean current density to the linear response current can only be performed, if the state of the system satisfies an additional localisation assumption. Roughly speaking, this localisation assumption is stated on the level of two-point function. As we know from Chapter 7, for the non-interacting electron gas, the two-point function completely determines the state of the system.

So the dilemma is, that for the general case of an interacting electron gas, there are no explicit expressions for the state of the system to carry out the linear response theory. Especially, one lacks a natural generalisation of the localisation criterion, mentioned above, towards interacting systems. Our goal is to carry out linear response theory for the special case of a non-interacting electron gas, but having a more general case in view. Therefore, we will always be worried about stating formulas, that naturally generalise to interacting electron gases, although in certain steps of our procedure we cannot avoid using special consequences from considering a non-interacting electron gas.

Sections 9.2 and 9.3 present the procedures generally described in Sections 8.1 and 8.2 for the special case of a non-interacting electron gas. The main achievement of these sections is to establish manageable formulas for the current density as well as for the mean current density. Already at this point, the latter quantity can be compared to the results of (BGKS05, KM08, KLM07).

Then, in Section 9.4 a formula for the linear response current is derived using results of the linear response theory from (BGKS05).

From the Kubo formula, in Section 9.5 we directly obtain the DC conductivity. In Section 9.6 we discuss concepts for the AC Conductivity.

9.1. General Simplifications

For making life a little easier[1], we sum up the additional structure, which is given considering the case of non-interacting electron gases. For any realisation $\omega \in \Omega$, times $t, r \in \mathbb{R}$, external electric field $E \in \mathcal{E}(\mathbb{R}, \mathbb{R}^d) = \{E \in C(\mathbb{R}, \mathbb{R}^d) : \|\chi_{]-\infty,t]} E\|_1 < \infty, \forall t \in \mathbb{R}\}$, inverse temperature $\beta \in [0, \infty]$ and chemical potential $\mu \in \mathbb{R}$ one has

$$H^{(E,\mu)}_{\omega,-}(t) = \mathrm{d}\Gamma_-(H^{(E,\mu)}_\omega(t)) \,, \tag{9.1}$$

$$U^{(E,\mu)}_{\omega,-}(t,r) = \Gamma_-(U^{(E,\mu)}_\omega(t,r)) \,. \tag{9.2}$$

Using the language of operator algebras, the simplifications above imply, that the following formulas hold for any $\psi \in \mathfrak{h}$

$$\mathcal{H}^{(E,\mu)}_{\omega,t,-}(a^*_-(\psi)) = a^*_-(H^{(E,\mu)}_\omega(t)\psi) \,, \tag{9.3}$$

$$\tau^{(E,\mu)}_{\omega,t,r,-}(a^*_-(\psi)) = a^*_-(U^{(E,\mu)}_\omega(t,r)\psi) \,. \tag{9.4}$$

As a consequence of this structure, the covariant state of the non-interacting electron gas is completely determined in terms of its two-point function. In general one has

$$\rho^{(E,\beta,\mu)}_{\omega,t,r,-}(a^*_-(\psi)a_-(\phi)) = \langle \phi, P^{(E,\beta,\mu)}_\omega(t,r)\psi \rangle \,, \tag{9.5}$$

$$\rho^{(E,\beta,\mu)}_{\omega,t,r,-}(\mathrm{d}\Gamma_-(B)) = \mathrm{Tr}(P^{(E,\beta,\mu)}_\omega(t,r)B) \tag{9.6}$$

for any $\phi, \psi \in \mathfrak{h}$ and $B \in \mathfrak{B}_c$. In these formulas the effective density matrix is given by

$$P^{(E,\beta,\mu)}_\omega(t,r) = \tau^{(E)}_{\omega,t,r}(F^{(\beta)}(H^{(E,\mu)}_\omega(r))) \,, \tag{9.7}$$

where the Fermi distribution appears. The latter is the function which for any $\varepsilon \in \mathbb{R}$ is given by

$$F^{(\beta)}(\varepsilon) = \begin{cases} (\mathrm{e}^{\beta\varepsilon} + 1)^{-1} & \text{for } 0 < \beta < \infty \\ \chi_{]-\infty,0]}(\varepsilon) & \text{for } \beta = \infty \\ 1 & \text{for } \beta = 0 \end{cases} \,. \tag{9.8}$$

[1] We do not want the reader to jump through the previous chapters in order to collect all the important structures for the non-interacting case.

9.2. Current Density

In the following lemma we just prove a more explicit and simple formula for the calculation of the current density of a non-interacting electron gas.

Theorem 9.1

Consider the model of Chapter 6 for the special case of a non-interacting electron gas at temperature $\beta \in [0, \infty]$ and with chemical potential $\mu \in \mathbb{R}$ under the influence of an external electric field $E \in \mathcal{E}(\mathbb{R}, \mathbb{R}^d)$. Then, in any realisation $\omega \in \Omega$, at arbitrary times $t, r \in \mathbb{R}$, position $y \in \mathbb{Z}^d$ and $k \in \{1, ..., d\}$ the current density of the system is given by

$$j_{\omega,k,r}(t, y; E, \beta, \mu) = \langle \delta_y, P_\omega^{(E,\beta,\mu)}(t, r) D_{\omega,k}^{(E)}(t) \delta_y \rangle + \langle \delta_y, D_{\omega,k}^{(E)}(t) P_\omega^{(E,\beta,\mu)}(t, r) \delta_y \rangle . \tag{9.9}$$

Proof: For any $\omega \in \Omega$, $t, r \in \mathbb{R}$, $y \in \mathbb{Z}^d$ and $k \in \{1, ..., d\}$ we use the fact, that $J_{\omega,k,-}^{(E)}(t, y) = \mathrm{d}\Gamma_-(J_{\omega,k}^{(E)}(t, y))$ is a second quantised operator of finite support. So, we can apply Equation (9.6) to obtain

$$\begin{aligned} j_{\omega,k,r}(t, y; E, \beta, \mu) &= \rho_{\omega,t,r,-}^{(E,\beta,\mu)}(J_{\omega,k,-}^{(E)}(t, y)) \\ &= \rho_{\omega,t,r,-}^{(E,\beta,\mu)}(\mathrm{d}\Gamma_-(J_{\omega,k}^{(E)}(t, y))) \\ &= \mathrm{Tr}(P_\omega^{(E,\beta,\mu)}(t, r) J_{\omega,k}^{(E)}(t, y)) \\ &= \mathrm{Tr}(P_\omega^{(E,\beta,\mu)}(t, r) D_{\omega,k}^{(E)}(t) \chi_y) + \mathrm{Tr}(P_\omega^{(E,\beta,\mu)}(t, r) \chi_y D_{\omega,k}^{(E)}(t)) \\ &= \mathrm{Tr}(\chi_y P_\omega^{(E,\beta,\mu)}(t, r) D_{\omega,k}^{(E)}(t) \chi_y) + \mathrm{Tr}(\chi_y D_{\omega,k}^{(E)}(t) P_\omega^{(E,\beta,\mu)}(t, r) \chi_y) \\ &= \langle \delta_y, P_\omega^{(E,\beta,\mu)}(t, r) D_{\omega,k}^{(E)}(t) \delta_y \rangle + \langle \delta_y, D_{\omega,k}^{(E)}(t) P_\omega^{(E,\beta,\mu)}(t, r) \delta_y \rangle . \end{aligned}$$

■

9.3. Mean Current Density

Theorem 9.2

Consider the model of Chapter 6 for the special case of a non-interacting electron gas at temperature $\beta \in [0, \infty]$ and with chemical potential $\mu \in \mathbb{R}$ under the influence of an external electric field $E \in \mathcal{E}(\mathbb{R}, \mathbb{R}^d)$. Then, for any $t, r \in \mathbb{R}$ and $k \in \{1, ..., d\}$ the mean current density of the system is given by

$$j_{k,r}(t; E, \beta, \mu) = 2 \langle\langle P^{(E,\beta,\mu)}(t, r), D_k^{(E)}(t) \rangle\rangle . \tag{9.10}$$

Proof: For any $t, r \in \mathbb{R}$ and any $k \in \{1, ..., d\}$ we simply use Theorem 9.1 and the fact that the mappings $P^{(E,\beta,\mu)}(t, r) : \Omega \to \mathfrak{B},\ \omega \mapsto P_\omega^{(E,\beta,\mu)}(t, r)$ and $D_k^{(E)} : \Omega \to \mathfrak{B},\ \omega \mapsto D_{\omega,k}^{(E)}(t, r)$ are in $\mathcal{K}^2$ to calculate

$$\begin{aligned} j_{k,r}(t; E, \beta, \mu) &= \mathbb{E}[j_{k,r}(t, 0; E, \beta, \mu)] \\ &= \mathbb{E}[\langle \delta_0, P^{(E,\beta,\mu)}(t, r) D_k^{(E)}(t) \delta_0 \rangle + \langle \delta_0, D_k^{(E)}(t) P^{(E,\beta,\mu)}(t, r) \delta_0 \rangle] \\ &= \mathbb{E}[\langle \delta_0, P^{(E,\beta,\mu)}(t, r) D_k^{(E)}(t) \delta_0 \rangle] + \mathbb{E}[\langle \delta_0, D_k^{(E)}(t) P^{(E,\beta,\mu)}(t, r) \delta_0 \rangle] \\ &= \langle\langle P^{(E,\beta,\mu)}(t, r), D_k^{(E)}(t) \rangle\rangle + \langle\langle D_k^{(E)}(t)^\star, P^{(E,\beta,\mu)}(t, r)^\star \rangle\rangle \\ &= 2 \langle\langle P^{(E,\beta,\mu)}(t, r), D_k^{(E)}(t) \rangle\rangle . \end{aligned}$$

■

On the C^*-algebra $\mathfrak{B}_-^\Omega := \mathcal{BM}(\Omega, \mathfrak{B}_-)$ of bounded measurable functions from probability space Ω to $\mathfrak{B}_-$ we consider the states $\Theta_{t,r,-}^{(E,\beta,\mu)} : \mathfrak{B}_-^\Omega \to \mathbb{C}$ and $\Theta_-^{(\beta,\mu)} : \mathfrak{B}_-^\Omega \to \mathbb{C}$ defined by

$$\Theta_{t,r,-}^{(E,\beta,\mu)}(B_-) := \mathbb{E}[\rho_{t,r,-}^{(E,\beta,\mu)}(B_-)] , \tag{9.11}$$

$$\Theta_-^{(\beta,\mu)}(B_-) := \mathbb{E}[\varrho_-^{(\beta,\mu)}(B_-)] \tag{9.12}$$

for $t, r \in \mathbb{R}$ and $B_- \in \mathfrak{B}_-^\Omega$. The C^*-algebra $\mathfrak{B}_-^\Omega$ contains the important subspace $\mathfrak{C}_-^\Omega$, which is defined as the linear span of operators of the form $C_- = a_-^*(C\delta_x)a_-(\delta_x)$ with $C \in \mathcal{K}^\infty$ and $x \in \mathbb{Z}^d$ and the adjoints of these operators. Note that due to Equation (6.90), for all $t \in \mathbb{R}$ and $y \in \mathbb{Z}^d$ one has $J_-^{(E)}(t, y) \in \mathfrak{C}_-^\Omega$, and that the mean current density is given by

$$j_{k,r}(t; E, \beta, \mu) = \Theta_{t,r,-}^{(E,\beta,\mu)}(J_{k,-}^{(E)}(t, 0)) . \tag{9.13}$$

Next, we are interested in taking the limit $r \to -\infty$. This we achieve by differentiating $\Theta_{t,r,-}^{(E,\beta,\mu)}(C_-)$ for $C_- \in \mathfrak{C}_-^\Omega$ with respect to r. In addition, a localisation condition enters (BGKS05). This condition will be part of the assumptions in all subsequent theorems of this chapter.

Assumption

We assume that the system at inverse temperature $\beta \in [0, \infty]$ and chemical potential $\mu \in \mathbb{R}$ initially is in a $(\tau_-^{(\mu)}, \beta)$-KMS state, such that for all $k \in \{1, ..., d\}$

$$\mathcal{X}_k(F^{(\beta)}(H^{(\mu)})) \in \mathcal{K}^2 . \tag{9.14}$$

Obviously, since the Fermi distribution appears, this condition is highly specialised to the case of non-interacting electron gases, where the Fermi distribution determines the whole KMS state. There is no obvious generalisation of (9.14) towards interacting systems. However, in Chapter 10 we present attempts to find such a generalising assumption.

Lemma 9.3

Consider the model of a non-interacting electron gas introduced in Chapter 6 which satisfies (9.14) for inverse temperature $\beta \in [0, \infty]$ and chemical potential $\mu \in \mathbb{R}$. Then, for all $t \in \mathbb{R}$ and $C_- \in \mathfrak{C}_-^\Omega$ the mapping $\mathbb{R} \to \mathbb{C}$, $r \mapsto \Theta_{t,r,-}^{(E,\beta,\mu)}(C_-)$ is differentiable. Moreover, the following limit exists

$$\lim_{r\to-\infty} \Theta_{t,r,-}^{(E,\beta,\mu)}(C_-) = \Theta_{t,t,-}^{(E,\beta,\mu)}(C_-) - \int_{-\infty}^{t} \partial_r \Theta_{t,r,-}^{(E,\beta,\mu)}(C_-)\, \mathrm{d}r . \tag{9.15}$$

Proof : By linearity it is enough to prove the statement for $C_- = a_-^*(C\delta_x)a_-(\delta_x)$ with some $C \in \mathcal{K}^\infty$ and $x \in \mathbb{Z}^d$. First, using Equation (9.6) we find that for any $\omega \in \Omega$

$$\begin{aligned}\rho_{\omega,t,r,-}^{(E,\beta,\mu)}(C_{\omega,-}) &= \rho_{\omega,t,r,-}^{(E,\beta,\mu)}(a_-^*(C_\omega\delta_x)a_-(\delta_x)) \\ &= \langle \delta_x, P_\omega^{(E,\beta,\mu)}(t, r)C_\omega\delta_x\rangle .\end{aligned}$$

Then, taking the expectation value on both sides, we obtain $\Theta_{t,r,-}^{(E,\beta,\mu)}(C_-) = \langle\langle P^{(E,\beta,\mu)}(t, r), C\rangle\rangle$. Because of $\mathcal{X}_k(F^{(\beta)}(H^{(\mu)})) \in \mathcal{K}^2$ and $\mathcal{H}_r^{(E)}(F^{(\beta)}(H^{(E,\mu)}(r))) = 0$, an application of Lemmas 6.6 and 6.16 leads to the result that for any $t \in \mathbb{R}$ the mapping $\mathbb{R} \to \mathcal{K}^2$, $r \mapsto P^{(E,\beta,\mu)}(t, r)$ is differentiable with

$$\begin{aligned}\partial_r P^{(E,\beta,\mu)}(t, r) &= \partial_r[\tau_{t,r}^{(E)}(\gamma_r^{(E)}(F^{(\beta)}(H^{(\mu)})))] \\ &= \tau_{t,r}^{(E)}(\mathcal{H}_r^{(E)}(F^{(\beta)}(H^{(E,\mu)}(r)))) + \tau_{t,r}^{(E)}(\gamma_r^{(E)}(\langle E(r), \mathcal{X}\rangle(F^{(\beta)}(H^{(\mu)})))) \\ &= \tau_{t,r}^{(E)}(\langle E(r), \mathcal{X}\rangle(F^{(\beta)}(H^{(E,\mu)}(r)))) .\end{aligned}$$

It directly follows, that for all $t \in \mathbb{R}$ the mapping $\mathbb{R} \to \mathbb{C}, r \mapsto \Theta^{(E,\beta,\mu)}_{t,r,-}(C_-)$ is differentiable. In particular, for $C_- = a^*_-(C\delta_x)a_-(\delta_x)$ with some $C \in \mathcal{K}^\infty$ and $x \in \mathbb{Z}^d$ the derivative is given by

$$\begin{aligned}\partial_r \Theta^{(E,\beta,\mu)}_{t,r,-}(C_-) &= \partial_r \langle\langle P^{(E,\beta,\mu)}(t,r), C\rangle\rangle \\ &= \langle\langle \partial_r P^{(E,\beta,\mu)}(t,r), C\rangle\rangle \\ &= \langle\langle \tau^{(E)}_{t,r}(\langle E(r), \mathcal{X}\rangle(F^{(\beta)}(H^{(E,\mu)}(r)))), C\rangle\rangle \\ &= \langle\langle \gamma^{(E)}_r(\langle E(r), \mathcal{X}\rangle(F^{(\beta)}(H^{(\mu)}))), \tau^{(E)}_{r,t}(C)\rangle\rangle \ .\end{aligned}$$

Moreover, because of Lemmas 6.5 and 6.15, for any $t \in \mathbb{R}$ the mapping $\mathbb{R} \to \mathbb{C}, r \mapsto \partial_r \Theta^{(E,\beta,\mu)}_{t,r,-}(C_-)$ is continuous. Thus, for $t, r \in \mathbb{R}$ we obtain

$$\Theta^{(E,\beta,\mu)}_{t,r,-}(C_-) = \Theta^{(E,\beta,\mu)}_{t,t,-}(C_-) - \int_r^t \partial_q \Theta^{(E,\beta,\mu)}_{t,q,-}(C_-)\, \mathrm{d}q \ .$$

Next, we take the limit $r \to -\infty$. Again, due to linearity, it is sufficient to consider $C_- = a^*_-(C\delta_x)a_-(\delta_x)$ with some $C \in \mathcal{K}^\infty$ and $x \in \mathbb{Z}^d$. Because of $\mathcal{X}_k(F^{(\beta)}(H^{(\mu)})) \in \mathcal{K}^2$, there is a constant $M > 0$, such that

$$\begin{aligned}|\partial_r \Theta^{(E,\beta,\mu)}_{t,r,-}(C_-)| = |\langle\langle \partial_r P^{(E,\beta,\mu)}(t,r), C\rangle\rangle| &\le |||\partial_r P^{(E,\beta,\mu)}(t,r)|||_2\ |||C|||_2 \\ &\le d\ |E(r)| \max\{\ |||[\mathcal{X}_k(F^{(\beta)}(H^{(\mu)}))|||_2 : k \in \{1, ..., d\}\}\ |||C|||_2 \\ &\le M|E(r)| \ .\end{aligned}$$

Because of $(\chi_{]-\infty,t]}E) \in L^1(\mathbb{R}, \mathbb{R}^d)$ for any $t \in \mathbb{R}$, from dominated convergence theorem we obtain

$$\begin{aligned}\lim_{r\to-\infty} \Theta^{(E,\beta,\mu)}_{t,r,-}(C_-) &= \Theta^{(E,\beta,\mu)}_{t,t,-}(C_-) - \lim_{r\to-\infty} \int_r^t \partial_q \Theta^{(E,\beta,\mu)}_{t,q,-}(C_-)\, \mathrm{d}q \\ &= \Theta^{(E,\beta,\mu)}_{t,t,-}(C_-) - \int_{-\infty}^t \partial_q \Theta^{(E,\beta,\mu)}_{t,q,-}(C_-)\, \mathrm{d}q \ .\end{aligned}$$

■

Theorem 9.4

Consider the model of a non-interacting electron gas introduced in Chapter 6 which satisfies (9.14) for inverse temperature $\beta \in [0, \infty]$ and chemical potential $\mu \in \mathbb{R}$. Then, the current density exists and for any $t \in \mathbb{R}$ and $k \in \{1, ..., d\}$ it is given by

$$j_k(t; E, \beta, \mu) = -\int_{-\infty}^t \partial_r \Theta^{(E,\beta,\mu)}_{t,r,-}(J^{(E)}_{k,-}(t,0))\, \mathrm{d}r \tag{9.16}$$

$$= -2\int_{-\infty}^t \langle\langle\langle E(r), \mathcal{X}\rangle(F^{(\beta)}(H^{(\mu)})), (\tau^{(E)}_{t,r} \circ \gamma^{(E)}_r)^{-1}(D^{(E)}_k(t))\rangle\rangle\, \mathrm{d}r \ . \tag{9.17}$$

Proof: We adopt the current density operator $J^{(E)}_-(t,0)$ for $C_- \in \mathfrak{C}^\Omega_-$ to Equation (9.15). This yields the existence of $j(t; E, \beta, \mu)$ for any $t \in \mathbb{R}$ and proves Equation (9.16), because for any $k \in \{1, ..., d\}$ one has

$$\begin{aligned}\Theta^{(E,\beta,\mu)}_{t,t,-}(J^{(E)}_{k,-}(t,0)) &= \mathbb{E}[\rho^{(E,\beta,\mu)}_{t,t,-}(J^{(E)}_{k,-}(t,0))] \\ &= \mathbb{E}[\varrho^{(\beta,\mu)}_-((\gamma^{(E)}_{t,-})^{-1}(\gamma^{(E)}_{t,-}(J_{k,-}(0)))] \\ &= \mathbb{E}[\varrho^{(\beta,\mu)}_-(J_{k,-}(0))] \\ &= \Theta^{(\beta,\mu)}_-(J_{k,-}(0)) \ , \\ j_k(t; E, \beta, \mu) &= \Theta^{(E,\beta,\mu)}_{t,t,-}(J^{(E)}_{k,-}(t,0)) - \int_{-\infty}^t \partial_r \Theta^{(E,\beta,\mu)}_{t,r,-}(J^{(E)}_{k,-}(t,0))\, \mathrm{d}r \\ &= \Theta^{(\beta,\mu)}_-(J_{k,-}(0)) - \int_{-\infty}^t \partial_r \Theta^{(E,\beta,\mu)}_{t,r,-}(J^{(E)}_{k,-}(t,0))\, \mathrm{d}r \ .\end{aligned}$$

Next, we prove equation (9.17) via the representation of the current density operator given in Equation (6.90) as well as the special form of the two-point function of the non-interacting state. First, we calculate

$$\begin{aligned}\Theta_-^{(\beta,\mu)}(J_{k,-}(0)) &= \mathbb{E}[\varrho_-^{(\beta,\mu)}(J_{k,-}(0))]\\ &= \mathbb{E}[\varrho_-^{(\beta,\mu)}(a_-^*(D_k\delta_0)a_-(\delta_0))] + \mathbb{E}[\varrho_-^{(\beta,\mu)}(a_-^*(\delta_0)a_-(D_k\delta_0))]\\ &= \mathbb{E}[\langle\delta_0, F^{(\beta)}(H^{(\mu)})D_k\delta_0\rangle] + \mathbb{E}[\langle D_k\delta_0, F^{(\beta)}(H^{(\mu)})\delta_0\rangle]\\ &= 2\,\langle\langle F^{(\beta)}(H^{(\mu)}), D_k\rangle\rangle\,.\end{aligned}$$

Since the velocity operator is defined via the commutator of the Schrödinger operator and the position operator, the expression on the right hand side vanishes (BGKS05). Next, again using the representation (6.90) for the current density operator, we prove that the integral on the right hand side of Equation (9.16) yields the right hand side of Equation (9.17). Note that in the proof of Theorem 9.2 we calculated $\Theta_{t,r,-}^{(E,\beta,\mu)}(J_-^{(E)}(t,y)) = 2\,\langle\langle P^{(E,\beta,\mu)}(t,r), D^{(E)}(t)\rangle\rangle$. Finally, one obtains

$$\begin{aligned}\partial_r\Theta_{t,r,-}^{(E,\beta,\mu)}(J_{k,-}^{(E)}(t,0)) &= 2\,\partial_r\langle\langle P^{(E,\beta,\mu)}(t,r), D_k^{(E)}(t)\rangle\rangle\\ &= 2\,\partial_r\langle\langle\tau_{t,r}^{(E)}(\gamma_r^{(E)}(F^{(\beta)}(H^{(\mu)}))), D_k^{(E)}(t)\rangle\rangle\\ &= 2\,\langle\langle\langle E(r), X\rangle(F^{(\beta)}(H^{(\mu)})), (\tau_{t,r}^{(E)}\circ\gamma_r^{(E)})^{-1}(D_k^{(E)}(t))\rangle\rangle\,.\end{aligned}$$

■

9.4. Linear Response Current

In this section we present the Kubo formula for the linear response current for the non-interacting electron gas. We finally achieve the connection of this work to the Kubo formulas presented in (BGKS05). This is accomplished by the following theorem.

Theorem 9.5 (*Kubo Formula for the Linear Response Current I*)

Consider the model of a non-interacting electron gas introduced in Chapter 6 which satisfies (9.14) for inverse temperature $\beta \in [0,\infty]$ and chemical potential $\mu \in \mathbb{R}$. Then, the linear response current exists and for $t \in \mathbb{R}$ and $k \in \{1,...,d\}$ it is given by

$$j_{\mathrm{res},k}(t;E,\beta,\mu) = -2\sum_{l=1}^{d}\int_{-\infty}^{t} E_l(r)\,\langle\langle X_l(F^{(\beta)}(H^{(\mu)})), \tau_{r-t}(D_k)\rangle\rangle\,\mathrm{d}r\,. \tag{9.18}$$

Proof: Let $k \in \{1,...,d\}$. We have $j_k(t;0,\beta,\mu) = \Theta_-^{(\beta,\mu)}(J_{k,-}(0)) = 0$. Thus, for $\lambda \neq 0$ we obtain

$$\begin{aligned}\frac{1}{\lambda}\,(j_k(t;\lambda E,\beta,\mu) - j_k(t;0,\beta,\mu)) &= -\int_{-\infty}^{t}\frac{1}{\lambda}\,\partial_r\Theta_{t,r,-}^{(\lambda E,\beta,\mu)}(J_{k,-}^{(\lambda E)}(t,0))\,\mathrm{d}r\\ &= -2\int_{-\infty}^{t}\langle\langle\gamma_r^{(\lambda E)}(\langle E(r), X\rangle(F^{(\beta)}(H^{(\mu)}))), \tau_{r,t}^{(\lambda E)}(D_k^{(\lambda E)}(t))\rangle\rangle\,\mathrm{d}r\,.\end{aligned}$$

We prove existence of the limit $\lambda \to 0$ via dominated convergence theorem. The integrand on the right hand side has an integrable majorant due to the fact that for all $\lambda \in \mathbb{R}$ and all $k \in \{1,...,d\}$ we have

$$\begin{aligned}&|\langle\langle\gamma_r^{(\lambda E)}(\langle E(r), X\rangle(F^{(\beta)}(H^{(\mu)}))), \tau_{r,t}^{(\lambda E)}(D_k^{(\lambda E)}(t))\rangle\rangle|\\ &\leq |E(r)|\,\max\{|||\gamma_r^{(\lambda E)}(X_l(F^{(\beta)}(H^{(\mu)})))|||_2 : l \in \{1,...,d\}\}\,\max\{|||\tau_{r,t}^{(\lambda E)}(\gamma_t^{(\lambda E)}(D_k))|||_2 : k \in \{1,...,d\}\}\\ &= |E(r)|\,\max\{|||X_l(F^{(\beta)}(H^{(\mu)}))|||_2 : l \in \{1,...,d\}\}\,\max\{|||D_k|||_2 : k \in \{1,...,d\}\}\\ &\leq M\,|E(r)|\end{aligned}$$

for some constant $M > 0$. Moreover, from Lemmas 6.7 and 6.17 we get that for all $t, r \in \mathbb{R}$

$$\lim_{\lambda\to 0}\langle\langle\gamma_r^{(\lambda E)}(\langle E(r),\mathcal{X}\rangle(F^{(\beta)}(H^{(\mu)}))),\tau_{r,t}^{(\lambda E)}(\gamma_t^{(\lambda E)}(D_k))\rangle\rangle = \langle\langle\langle E(r),\mathcal{X}\rangle(F^{(\beta)}(H^{(\mu)})),\tau_{r-t}(D_k)\rangle\rangle\ .$$

Summing up, we get that the linear response current exists and that it is given by the following expression

$$\begin{aligned} j_{\mathrm{res},k}(t;E,\beta,\mu) &= \partial_\lambda j(t;\lambda E,\beta,\mu)|_{\lambda=0} = \lim_{\lambda\to 0}\frac{1}{\lambda}\left(j(t;\lambda E,\beta,\mu) - j(t;0,\beta,\mu)\right) \\ &= -2\lim_{\lambda\to 0}\int_{-\infty}^{t}\langle\langle\gamma_r^{(\lambda E)}(\langle E(r),\mathcal{X}\rangle(F^{(\beta)}(H^{(\mu)})),\tau_{r,t}^{(\lambda E)}(D_k^{(\lambda E)}(r)))\rangle\rangle\,\mathrm{d}r \\ &= -2\int_{-\infty}^{t}\lim_{\lambda\to 0}\langle\langle\gamma_r^{(\lambda E)}(\langle E(r),\mathcal{X}\rangle(F^{(\beta)}(H^{(\mu)}))),\tau_{r,t}^{(\lambda E)}(\gamma_t^{(\lambda E)}(D_k))\rangle\rangle\,\mathrm{d}r \\ &= -2\int_{-\infty}^{t}\langle\langle\langle E(r),\mathcal{X}\rangle(F^{(\beta)}(H^{(\mu)})),\tau_{r-t}(D_k)\rangle\rangle\,\mathrm{d}r \\ &= -2\sum_{l=1}^{d}\int_{-\infty}^{t} E_l(r)\,\langle\langle\mathcal{X}_l(F^{(\beta)}(H^{(\mu)})),\tau_{r-t}(D_k)\rangle\rangle\,\mathrm{d}r\ . \end{aligned}$$

■

Note that the right hand side of (9.18) is exactly the expression that was also obtained as a Kubo formula for the linear response current in (BGKS05). From our point of view, the integrand on the right hand side of (9.18) suffers from the fact, that it contains operators on the one-electron space. It is no expression purely given in terms of Fock space quantities. But of course, the latter would be a desirable feature for the integrand to possess, since we are interested in formulas that easily generalise to, or even better already permit, models of interacting electron gases.

As pointed out several times before, one cannot expect to leave the level of Fock spaces in the description of interacting electron gases, i.e. the expressions of interest do not only feature one-electron quantities. This is why in the following we like to regain Fock space quantities in the integrand of Equation (9.18). A close look on the proofs of Theorems 9.2-9.5 motivates the endeavour to express the integrand as the following expectation value

$$-\sum_{l=1}^{d} E_l(r)\,\langle\langle\mathcal{X}_l(F^{(\beta)}(H^{(\mu)})),\tau_{r-t}(D_k)\rangle\rangle = \sum_{l=1}^{d} E_l(r)\,\mathbb{E}[\varrho_-^{(\beta,\mu)}(\mathcal{X}_{l,-}(\tau_{r-t,-}^{(\mu)}(J_{k,-}(0)))]\ . \tag{9.19}$$

Also a formal calculation motivates the expression on the right hand side of this equation. We try to achieve such a formula in the following.

First, for any $k \in \{1,...,d\}$ and $\phi,\psi \in \mathfrak{h}_c$ we consider the commutator of the position operator with a product of a creation and an annihilation operator. From Lemma B.21 we obtain

$$\begin{aligned} \mathcal{X}_{k,-}(a_-^*(\psi)a_-(\phi)) &= \mathcal{X}_{k,-}(a_-^*(\psi))a_-(\phi) + a_-^*(\psi)\,\mathcal{X}_{k,-}(a_-(\phi)) \\ &= a_-^*(\mathrm{i}X_k\psi)a_-(\phi) + a_-^*(\psi)a_-(\mathrm{i}X_k\phi)\ . \end{aligned}$$

Next, we apply the $(\tau_{\omega,-}^{(\mu)},\beta)$-KMS state $\varrho_{\omega,-}^{(\beta,\mu)}$ of the non-interacting electron gas on both sides. Using the special structure from Equation (9.5) for the states of non-interacting systems we get

$$\begin{aligned} \varrho_{\omega,-}^{(\beta,\mu)}(\mathcal{X}_k(a_-^*(\psi)a_-(\phi))) &= \varrho_{\omega,-}^{(\beta,\mu)}(a_-^*(\mathrm{i}X_k\psi)a_-(\phi)) + \varrho_{\omega,-}^{(\beta,\mu)}(a_-^*(\psi)a_-(\mathrm{i}X_k\phi)) \\ &= \langle\phi, F^{(\beta)}(H_\omega^{(\mu)})(\mathrm{i}X_k\psi)\rangle + \langle(\mathrm{i}X_k\phi), F^{(\beta)}(H_\omega^{(\mu)})\psi\rangle \\ &= \langle\phi,\mathrm{i}[F^{(\beta)}(H_\omega^{(\mu)}),X_k]\psi\rangle \\ &= -\langle\phi,\mathcal{X}_k(F^{(\beta)}(H_\omega^{(\mu)}))\psi\rangle\ . \end{aligned} \tag{9.20}$$

Now, the idea is the following. In a sense, that we still need to specify, we want to extend the functional, which is a composition of the equilibrium state $\varrho_{\omega,-}^{(\beta,\mu)}$ and the commutator with the position operator $\mathcal{X}_{k,-}$. The extension shall be defined on the subspace of operators which includes the time evolved current density operator $\tau_{\omega,t,-}^{(\mu)}(J_{\omega,k,-}(0))$ for all times $t \in \mathbb{R}$.
For the non-interacting model this is achieved in the following way. By formula (6.90) the current density operator is a quadratic expression in terms of creation- and annihilation operators. We have

$$J_{\omega,k,-}(0) = a_-^*(D_{\omega,k}\delta_0)a_-(\delta_0) + a_-^*(\delta_0)a_-(D_{\omega,k}\delta_0) .$$

For non-interacting electron gases, using (9.4), an application of a time evolution automorphism to the current density operator leads to an expression that also is quadratic in creation and annihilation operators. In more detail, one has

$$\tau_{\omega,t,-}^{(\mu)}(J_{\omega,k,-}(0)) = a_-^*(U_\omega^{(\mu)}(t)D_{\omega,k}\delta_0)a_-(U_\omega^{(\mu)}(t)\delta_0) + a_-^*(U_\omega^{(\mu)}(t)\delta_0)a_-(U_\omega^{(\mu)}(t)D_{\omega,k}\delta_0) .$$

Having this in mind, the program outlined above culminates in the desire to extend the sesquilinear forms defined by

$$\Xi_{k,x}^{(\beta,\mu)} : \mathcal{K}_c^\infty \times \mathcal{K}_c^\infty \to \mathbb{C},\ (B, C) \mapsto \mathbb{E}[\varrho_-^{(\beta,\mu)}(\mathcal{X}_{k,-}(a_-^*(C\delta_x)a_-(B\delta_x)))] \tag{9.21}$$

for any $x \in \mathbb{Z}^d$ and $k \in \{1, ..., d\}$, where

$$\mathcal{K}_c^\infty := \{B \in \mathcal{K}^\infty : B_\omega(\mathfrak{h}_c) \subset \mathfrak{h}_c \text{ for almost every } \omega \in \Omega\} . \tag{9.22}$$

Note that for example $\mathrm{id}, H^{(\mu)}, D_k \in \mathcal{K}_c^\infty$ for any $\mu \in \mathbb{R}$ and $k \in \{1, ..., d\}$. Moreover, $\mathcal{K}_c^\infty$ is a subalgebra of $\mathcal{K}^\infty$. But in general, for arbitrary $B \in \mathcal{K}_c^\infty$ one cannot expect to have $U^{(\mu)}(t)B \in \mathcal{K}_c^\infty$. However, one can prove the following lemmas.

Lemma 9.6

Consider the model of a non-interacting electron gas as described in Chapter 6 with any chemical potential $\mu \in \mathbb{R}$. Then, for any $B \in \mathcal{K}_c^\infty$ we have that $U^{(\mu)}(t)B$ is in the closure $\overline{\mathcal{K}_c^\infty}$ of $\mathcal{K}_c^\infty$ with respect to the norm on $\mathcal{K}^\infty$.

Proof: The propagator $U^{(\mu)}(t)$ is an element of $\mathcal{K}^\infty$ and it can be expressed via the exponential series

$$U^{(\mu)}(t) = \mathrm{e}^{-\mathrm{i}tH^{(\mu)}} = \sum_{n=0}^{\infty} \frac{(\mathrm{i}tH^{(\mu)})^n}{n!} .$$

The latter is absolutely convergent with respect to the norm on $\mathcal{K}^\infty$. Since $H^{(\mu)} \in \mathcal{K}_c^\infty$ and since $\mathcal{K}_c^\infty$ is an algebra, for any $N \in \mathbb{N}_0$ one has

$$U_N^{(\mu)}(t) := \sum_{n=0}^{N} \frac{(\mathrm{i}tH^{(\mu)})^n}{n!} \in \mathcal{K}_c^\infty .$$

So $(U_N^{(\mu)}(t)B)_{N\in\mathbb{N}_0}$ is a sequence in $\mathcal{K}_c^\infty$ that converges with respect to the norm on $\mathcal{K}^\infty$ to $U^{(\mu)}(t)B$, due to the fact that

$$0 \le \lim_{N\to\infty} |||U^{(\mu)}(t)B - U_N^{(\mu)}(t)B|||_\infty \le \lim_{N\to\infty} |||U^{(\mu)}(t) - U_N^{(\mu)}(t)|||_\infty\ |||B|||_\infty = 0 .$$

Thus, $U^{(\mu)}(t)B$ is an element of the closure $\overline{\mathcal{K}_c^\infty}$ of $\mathcal{K}_c^\infty$ with respect to the norm on $\mathcal{K}^\infty$. ■

Lemma 9.7

Consider the model of a non-interacting electron gas as described in Chapter 6 at inverse temperature $\beta \in [0, \infty]$ and with chemical potential $\mu \in \mathbb{R}$. Then, for all $k \in \{1, ..., d\}$ and $x \in \mathbb{Z}^d$ one has

$$\Xi_{k,x}^{(\beta,\mu)} = \Xi_{k,0}^{(\beta,\mu)} . \tag{9.23}$$

Assuming that condition (9.14) holds, one may extend $\Xi_k^{(\beta,\mu)} := \Xi_{k,0}^{(\beta,\mu)}$ to a bounded sesquilinear form on $\overline{\mathcal{K}_c^\infty}$.

Proof: Let $B, C \in \mathcal{K}_c^\infty$ be arbitrary. Then, for almost every $\omega \in \Omega$ and all $x \in \mathbb{Z}^d$ from covariance of all operators we get

$$\begin{aligned}
\varrho_{\omega,-}^{(\beta,\mu)}(\mathcal{X}_{k,-}(a_-^*(C_\omega\delta_x)a_-(B_\omega\delta_x))) &= -\langle B_\omega\delta_x, \mathcal{X}_k(F^{(\beta)}(H_\omega^{(\mu)}))C_\omega\delta_x\rangle \\
&= -\langle B_{\phi_{-x}(\omega)}\delta_0, \mathcal{X}_k(F^{(\beta)}(H_{\phi_{-x}(\omega)}^{(\mu)}))C_{\phi_{-x}(\omega)}\delta_0\rangle \\
&= \varrho_{\phi_{-x}(\omega),-}^{(\beta,\mu)}(\mathcal{X}_{k,-}(a_-^*(C_{\phi_{-x}(\omega)}\delta_0)a_-(B_{\phi_{-x}(\omega)}\delta_0))) .
\end{aligned}$$

Taking the expectation value on both sides leads to

$$\begin{aligned}
\Xi_{k,x}^{(\beta,\mu)}(B, C) &= \mathbb{E}[\varrho_-^{(\beta,\mu)}\,(\mathcal{X}_{k,-}\,(a_-^*(B\delta_x)a_-(C\delta_x))))\,] \\
&= \mathbb{E}[\varrho_-^{(\beta,\mu)}\,(\mathcal{X}_{k,-}\,(a_-^*(B\delta_0)a_-(C\delta_0))))\,] \\
&= \Xi_{k,0}^{(\beta,\mu)}(B, C) .
\end{aligned}$$

This proves the first statement. Now assume $\mathcal{X}_k(F^{(\beta)}(H^{(\mu)})) \in \mathcal{K}^2$. The boundedness of $\Xi_k^{(\beta,\mu)}$ then is the result of the following calculation.

$$\begin{aligned}
\Xi_k^{(\beta,\mu)}(B, C) &= \mathbb{E}[\varrho_-^{(\beta,\mu)}(\mathcal{X}_k(a_-^*(B\delta_0)a_-(C\delta_0)))] = -\mathbb{E}[\langle B\delta_0, \mathcal{X}_k(F^{(\beta)}(H^{(\mu)}))C\delta_0\rangle] \\
&= -\langle\langle B, \mathcal{X}_k(F^{(\beta)}(H^{(\mu)}))C\rangle\rangle = -\langle\langle(\mathcal{X}_k(F^{(\beta)}(H^{(\mu)}))C)^\star, B^\star\rangle\rangle \\
&= -\mathbb{E}[\langle(\mathcal{X}_k(F^{(\beta)}(H^{(\mu)}))C)^*\delta_0, B^*\delta_0\rangle] = -\mathbb{E}[\langle C^*\mathcal{X}_k(F^{(\beta)}(H^{(\mu)}))^*\delta_0, B^*\delta_0\rangle] \\
&= -\mathbb{E}[\langle\mathcal{X}_k(F^{(\beta)}(H^{(\mu)}))\delta_0, CB^*\delta_0\rangle] = -\langle\langle\mathcal{X}_k(F^{(\beta)}(H^{(\mu)})), CB^\star\rangle\rangle ,
\end{aligned}$$

so that from Cauchy-Schwarz inequality we get

$$\begin{aligned}
|\Xi_k^{(\beta,\mu)}(B, C)| &\leq |||\, \mathcal{X}_k(F^{(\beta)}(H^{(\mu)}))\, |||_2\; |||CB^*|||_2 \\
&\leq |||\, \mathcal{X}_k(F^{(\beta)}(H^{(\mu)}))\, |||_2\; |||B|||_\infty\; |||C|||_\infty .
\end{aligned}$$

Thus, for any $k \in \{1, ..., d\}$ one can extend $\Xi_k^{(\beta,\mu)}$ uniquely to a sesquilinear form on the closure of $\mathcal{K}_c^\infty$ with respect to $|||\cdot|||_\infty$. We also denote this form by $\Xi_k^{(\beta,\mu)}$. ■

Next, we define the spaces $\mathfrak{S}_-^\Omega$ and $\bar{\mathfrak{S}}_-^\Omega$ as the subspaces of $\mathfrak{B}_-^\Omega$ spanned by linear combinations of operators of the form $a_-^*(C\delta_x)a_-(B\delta_x)$, where $x \in \mathbb{Z}^d$ and $B, C \in \mathcal{K}_c^\infty$ or $B, C \in \overline{\mathcal{K}_c^\infty}$, respectively. For any $k \in \{1, ..., d\}$ we define a functional on $\mathfrak{S}_-^\Omega$ via linear extension of

$$\mathbb{E}[\varrho_-^{(\beta,\mu)}\,(\mathcal{X}_{k,-}\,(a_-^*(C\delta_x)a_-(B\delta_x)))\,] := \Xi_k^{(\beta,\mu)}(B, C) . \tag{9.24}$$

Technically, the left hand side is just notation. But this notation is justified by linearity of $\mathbb{E}$, $\varrho_-^{(\beta,\mu)}$ and $\mathcal{X}_{k,-}$ and the fact that the expression $\mathbb{E}[\varrho_-^{(\beta,\mu)}(\mathcal{X}_{k,-}(a_-^*(C\delta_x)a_-(B\delta_x)))]$ is well-defined for any $B, C \in \mathcal{K}_c^\infty$ and $x \in \mathbb{Z}^d$. In the latter case, the left hand side of (9.24) equals $\Xi_k^{(\beta,\mu)}(B, C)$ as it was shown in Lemma 9.6.

Theorem 9.8 (*Kubo Formula for the Linear Response Current II*)

Consider the model of a non-interacting electron gas introduced in Chapter 6 at inverse temperature $\beta \in [0, \infty]$ and with chemical potential $\mu \in \mathbb{R}$. Then, assuming condition (9.14) is satisfied, for $E \in \mathcal{E}(\mathbb{R}, \mathbb{R}^d)$ the linear response current exists and for any $k \in \{1, ..., d\}$ and $t \in \mathbb{R}$ it is given by the Kubo formula

$$j_{\mathrm{res},k}(t; E, \beta, \mu) = \sum_{l=1}^{d} \int_{-\infty}^{t} E_l(r)\, \mathbb{E}[\varrho_-^{(\beta,\mu)}(\mathcal{X}_{l,-}(\tau_{r-t,-}^{(\mu)}(J_{k,-}(0))))]\, \mathrm{d}r\,. \tag{9.25}$$

Proof: For the integrand in the Kubo formula, we like to emphasise the aspect, that it stems from an abstractly defined linear functional on $\bar{\mathfrak{S}}_-^{\Omega}$ which is applied to a time evolved current density operator. In order to do so, for any $k \in \{1, ..., d\}$ we define the linear functional $\Phi_{k,-}^{(\beta,\mu)} : \bar{\mathfrak{S}}_-^{\Omega} \to \mathbb{C}$ via

$$\Phi_{k,-}^{(\beta,\mu)}(S_-) := \mathbb{E}[\varrho_-^{(\beta,\mu)}(\mathcal{X}_{k,-}(S_-))]$$

for any $S_- \in \mathfrak{S}_-^{\Omega}$. In addition, for any $k \in \{1, ..., d\}$ and $t \in \mathbb{R}$ another linear functional $\Psi_{k,t,-}^{(\beta,\mu)} : \mathfrak{S}_-^{\Omega} \to \mathbb{C}$ is defined via linear extension of

$$\Psi_{k,t,-}^{(\beta,\mu)}(a_-^*(C\delta_x)a_-(B\delta_x)) := -\langle\langle \mathcal{X}_k(F^{(\beta)}(H^{(\mu)})), \tau_t(CB^\star)\rangle\rangle$$

for any $B, C \in \overline{\mathcal{K}_c^\infty}$ and $x \in \mathbb{Z}^d$. Because of covariance of the operators in $\mathcal{K}^\infty$, this is well-defined. We claim that these functionals are connected via the relation

$$\Psi_{k,t,-}^{(\beta,\mu)}(S_-) = \Phi_{k,-}^{(\beta,\mu)}(\tau_{t,-}^{(\mu)}(S_-))$$

for any $k \in \{1, ..., d\}$, $t \in \mathbb{R}$ and $S_- \in \mathfrak{S}_-^{\Omega}$. To prove this relation, by linearity it is sufficient to consider $S_- \in \mathfrak{S}_-^{\Omega}$ of the form $S_- = a_-^*(C\delta_x)a_-(B\delta_x)$ for arbitrary $B, C \in \mathcal{K}_c^\infty$ and $x \in \mathbb{Z}^d$. First, note that for all $t \in \mathbb{R}$ one has

$$\begin{aligned}
\tau_{t,-}^{(\mu)}(S_-) &= \tau_{t,-}^{(\mu)}(a_-^*(C\delta_x)a_-(B\delta_x)) \\
&= \tau_{t,-}^{(\mu)}(a_-^*(C\delta_x))\tau_{t,-}^{(\mu)}a_-(B\delta_x)) \\
&= a_-^*(U^{(\mu)}(t)C\delta_x)a_-(U^{(\mu)}(t)B\delta_x)
\end{aligned}$$

as a result of Lemma 9.6 and non-interacting structure as in Equation (9.4). So, for any $t \in \mathbb{R}$ and $S_- \in \mathfrak{S}_-^{\Omega}$ one has $\tau_{t,-}^{(\mu)}(S_-) \in \bar{\mathfrak{S}}_-^{\Omega}$. Next, again only considering $S_- = a_-^*(C\delta_x)a_-(B\delta_x)$ with $B, C \in \mathcal{K}_c^\infty$, we obtain

$$\begin{aligned}
\Phi_{k,-}^{(\beta,\mu)}(\tau_{t,-}^{(\mu)}(S_-)) &= \Phi_{k,-}^{(\beta,\mu)}(\tau_{t,-}^{(\mu)}(a_-^*(C\delta_x)a_-(B\delta_x))) \\
&= \Phi_{k,-}^{(\beta,\mu)}(a_-^*(U^{(\mu)}(t)C\delta_x)a_-(U^{(\mu)}(t)B\delta_x)) \\
&= \Xi_k^{(\beta,\mu)}(U^{(\mu)}(t)B, U^{(\mu)}(t)C) \\
&= -\langle\langle \mathcal{X}_k(F^{(\beta)}(H^{(\mu)})), U^{(\mu)}(t)CB^*U^{(\mu)}(t)^*\rangle\rangle \\
&= -\langle\langle \mathcal{X}_k(F^{(\beta)}(H^{(\mu)})), \tau_t(CB^*)\rangle\rangle \\
&= \Psi_{k,t,-}^{(\beta,\mu)}(a_-^*(C\delta_x)a_-(B\delta_x)) \\
&= \Psi_{k,t,-}^{(\beta,\mu)}(S_-)
\end{aligned}$$

for any $k \in \{1, ..., d\}$ and $t \in \mathbb{R}$. Obviously, $J_{k,-}(0) = a_-^*(D_k\delta_0)a_-(\delta_0) + a_-^*(\delta_0)a_-(D_k\delta_0) \in \mathfrak{S}_-^{\Omega}$ as well as

$$\begin{aligned}
\Psi_{l,t,-}^{(\beta,\mu)}(J_{k,-}(0)) &= \Psi_{l,t,-}^{(\beta,\mu)}(a_-^*(D_k\delta_0)a_-(\delta_0)) + \Psi_{l,t,-}^{(\beta,\mu)}(a_-^*(\delta_0)a_-(D_k\delta_0)) \\
&= -\langle\langle \mathcal{X}_l(F^{(\beta)}(H^{(\mu)})), \tau_t(D_k)\rangle\rangle - \langle\langle \mathcal{X}_l(F^{(\beta)}(H^{(\mu)})), \tau_t(D_k^\star)\rangle\rangle \\
&= -2\,\langle\langle \mathcal{X}_l(F^{(\beta)}(H^{(\mu)})), \tau_t(D_k)\rangle\rangle
\end{aligned}$$

for any $t \in \mathbb{R}$ and $k, l \in \{1, ..., d\}$. Finally, starting with the Kubo formula in Theorem 9.5 and taking together the above considerations, we obtain the statement of Theorem 9.8 through

$$\begin{aligned} j_{\mathrm{res},k}(t; E, \beta, \mu) &= -2 \sum_{l=1}^{d} \int_{-\infty}^{t} E_l(r) \langle\langle X_l(F^{(\beta)}(H^{(\mu)})), \tau_{r-t}(D_k)\rangle\rangle \, \mathrm{d}r \\ &= \sum_{l=1}^{d} \int_{-\infty}^{t} E_l(r) \, \Psi^{(\beta,\mu)}_{l,r-t,-}(J_{k,-}(0)) \, \mathrm{d}r \\ &= \sum_{l=1}^{d} \int_{-\infty}^{t} E_l(r) \, \Phi^{(\beta,\mu)}_{l,-}(\tau^{(\mu)}_{r-t,-}(J_{k,-}(0))) \, \mathrm{d}r \\ &= \sum_{l=1}^{d} \int_{-\infty}^{t} E_l(r) \, \mathbb{E}[\varrho^{(\beta,\mu)}_{-}(X_{l,-}(\tau^{(\mu)}_{r-t,-}(J_{k,-}(0))))] \, \mathrm{d}r \, . \end{aligned}$$

■

Note that on the right hand side of the Kubo formula (9.25) the integrand is purely constructed from Fock space quantities. Thus, in principle, this Kubo formula could also hold for interacting electron gases. At least, there are direct analogues for all objects appearing, even for a models including interaction. However, one more time it has to be pointed out clearly, that we are not able to perform the analysis in full generality considering interacting models.

9.5. DC Conductivity

With the Kubo formulas for the linear response current we automatically get similar expressions for the DC conductivity at adiabatic switching. For $E \in \mathbb{R}^d$ and $\eta > 0$ one just needs to consider the special case $E^{\mathrm{DC}}_{\eta} \in \mathcal{E}(\mathbb{R}, \mathbb{R}^d)$ for the electric field as described in Section 8.4. Summing up, we obtain the following theorem.

Theorem 9.9 (*DC Conductivity at Adiabatic Switching*)

Consider the model of a non-interacting electron gas as introduced in Chapter 6 at inverse temperature $\beta \in [0, \infty]$ and with chemical potential $\mu \in \mathbb{R}$. Moreover, assume that condition (9.14) holds. Then, the direct current conductivity $\sigma^{\mathrm{DC}}(\eta, \beta, \mu)$ at adiabatic switching $\eta > 0$ exists and for $k, l \in \{1, ..., d\}$ its components are given by

$$\sigma^{\mathrm{DC}}_{k,l}(\eta, \beta, \mu) = \int_{-\infty}^{0} \mathrm{e}^{\eta r} \, \mathbb{E}[\varrho^{(\beta,\mu)}_{-}(X_{l,-}(\tau^{(\mu)}_{r,-}(J_{k,-}(0))))] \, \mathrm{d}r \, . \tag{9.26}$$

Of course, Equation (9.26) is in agreement with the formula for the DC conductivity at adiabatic switching obtained in (BGKS05), because of the way the integrand in Equation (9.26) is defined. For the sake of completeness we state the result. For any $k, l \in 1, ..., d$ and at adiabatic switching $\eta > 0$ one has

$$\sigma^{\mathrm{DC}}_{k,l}(\eta, \beta, \mu) = -2 \int_{-\infty}^{0} \mathrm{e}^{\eta r} \langle\langle X_l(F^{(\beta)}(H^{(\mu)})), \tau_{r-t}(D_k)\rangle\rangle \, \mathrm{d}r \tag{9.27}$$

whenever $\beta \in [0, \infty]$ and $\mu \in \mathbb{R}$ are chosen such that the condition (9.14) holds. Moreover, in (BGKS05) a Kubo-Středa for the so called quantum Hall conductivity σ^{QH} at zero temperature is proven. The latter quantity also possesses an adiabatic limit. To state the result, for $\beta = \infty$ and $\mu \in \mathbb{R}$ we define $P^{(\mu)} : \Omega \to \mathfrak{B}$, $\omega \mapsto F^{(\infty)}(H^{(\mu)}_{\omega}) = \chi_{]-\infty,0]}(H^{(\mu)}_{\omega}) =: P^{(\mu)}_{\omega}$. In addition, the Liouvillian defined by $\mathcal{L} := -\mathrm{i}\mathcal{H}$ is a self adjoint operator on $\mathcal{K}^2$ (BGKS05).

Using this notation, one gets that the quantum Hall conductivity exists, if $\mu \in \mathbb{R}$ is such that the condition (9.14) is satisfied and for $k, l \in \{1, ..., d\}$ and $\eta > 0$ its components are given by (BGKS05)[Theorem 5.11]

$$\sigma^{\mathrm{QH}}_{k,l}(\eta, \mu) := \sigma^{\mathrm{DC}}_{k,l}(\eta, \infty, \mu) = -\Big\langle\Big\langle \mathrm{i}\frac{\mathcal{L}}{\mathcal{L} + \mathrm{i}\eta}([P^{(\mu)}, \mathcal{X}_k(P^{(\mu)})]), \mathcal{X}_l(P^{(\mu)})\Big\rangle\Big\rangle\,, \tag{9.28}$$

$$\sigma^{\mathrm{QH}}_{k,l}(\mu) := \lim_{\eta\to 0} \sigma^{\mathrm{QH}}_{k,l}(\eta, \mu) = -\langle\langle([P^{(\mu)}, \mathcal{X}_k(P^{(\mu)})]), \mathcal{X}_l(P^{(\mu)})\rangle\rangle\,. \tag{9.29}$$

Note that the right hand sides of Equations (9.28) and (9.29) purely contain one particle objects. Thus, they can not be generalised in an obvious way towards interacting electron gases. Such a procedure would require expressions in terms of objects on Fock space and Fermi algebra on the right hand sides of the above equations. Basically, this is the same type of problem that we fought in Section 9.4. One might get the idea to replace $P^{(\mu)}$ by the ground state $\varrho^{(\mu)}_{-}$, since the former one-particle object is the effective implementation of the latter algebraic object for non-interacting electron gases and the latter object has a direct analogue for interacting electron gases. Then, with the more general algebraic concept of $\varrho^{(\mu)}_{-}$ at hand, one would like to mimic the analysis in the proof (BGKS05)[Theorem 5.11] on an algebraic level. But one is faced with the problem that in the proof (BGKS05)[Theorem 5.11] the projection property $(P^{(\mu)})^2 = P^{(\mu)}$ is used excessively and that there is no direct analogue for this property on an algebraic level. Therefore, we have not been able to reformulate Equations (9.28) and (9.29) in terms of Fock space and Fermi algebraic objects, respectively, as we did in Section 9.4 for the linear response current.

9.6. AC Conductivity

One may also obtain an expression for the AC conductivity. In (KLM07, KM08) this is achieved in terms of the so called conductivity measure on $\mathcal{B}(\mathbb{R})$. Suppose the system satisfies Equation (9.14) at inverse temperature $\beta \in [0, \infty]$ and chemical potential $\mu \in \mathbb{R}$. Then, one can define the so called conductivity measure $\Sigma^{(\beta,\mu)} : \mathcal{B}(\mathbb{R}) \to [-\infty, \infty]$ via

$$\Sigma^{(\beta,\mu)}(B) := \pi\, \langle\langle \dot{X}_1, \chi_B(\mathcal{L}) Y^{(\beta,\mu)}\rangle\rangle \tag{9.30}$$

for any Borel set $B \in \mathcal{B}(\mathbb{R})$, where $Y^{(\beta,\mu)} := \mathcal{X}_1(F^{(\beta)}(H^{(\mu)}))$, $\dot{X}_1 := 2D_1$ and $\mathcal{L} = -\mathrm{i}\mathcal{H}$ is the Liouvillian of the system. In (KM08)[Theorem 1] it is proven that the conductivity measure is a finite positive even Borel measure on $\mathbb{R}$.
Then, one may express the AC conductivity via the conductivity measure. Let $E \in \mathcal{E}(\mathbb{R}, \mathbb{R}^d)$ be an electric field that satisfies the assumptions of Section 8.5 and just points in x_1-direction, i.e. $E(t) = (E_1(t), ..., E_d(t))$ and $E_k(t) = 0$ for all $k \geq 2$ and $t \in \mathbb{R}$. Then, for $t \in \mathbb{R}$, at adiabatic switching $\eta > 0$ one has (KLM07)[Theorem 3.4]

$$j_{\mathrm{res},1}(t; E^{\mathrm{AC}}_{\eta}, \beta, \mu) := \frac{\mathrm{e}^{\eta t}}{\sqrt{2\pi}} \int_{\mathbb{R}} \sigma^{\mathrm{AC}}_{1,1}(\nu; \eta, \beta, \mu)\, \hat{E}_1(\nu)\, \mathrm{e}^{\mathrm{i}\nu t}\, \mathrm{d}\nu\,, \tag{9.31}$$

where the AC conductivity is given by the Stieltjes transform of the conductivity measure, i.e.

$$\sigma^{\mathrm{AC}}_{1,1}(\nu; \eta, \beta, \mu) := -\frac{\mathrm{i}}{\pi} \int_{\mathbb{R}} \frac{1}{\lambda + \nu - \mathrm{i}\eta}\, \Sigma^{(\beta,\mu)}(\mathrm{d}\lambda) \tag{9.32}$$

for any $\nu \in \mathbb{R}$. Also, in the situation above one may define the so called in-phase linear response current at adiabatic switching $\eta > 0$ and time $t \in \mathbb{R}$ via

$$j^{\mathrm{in}}_{\mathrm{res},1}(t; E^{\mathrm{AC}}_{\eta}, \beta, \mu) := \frac{\mathrm{e}^{\eta t}}{\sqrt{2\pi}} \int_{\mathbb{R}} \mathrm{Re}(\sigma^{\mathrm{AC}}_{1,1}(\nu; \eta, \beta, \mu))\, \hat{E}_1(\nu)\, \mathrm{e}^{\mathrm{i}\nu t}\, \mathrm{d}\nu\,. \tag{9.33}$$

Then, if $\beta \in [0,\infty]$ and $\mu \in \mathbb{R}$ satisfy (9.14), in (KLM07)[Corollary 3.5] it is shown that the in-phase linear response current possesses an adiabatic limit which is given by

$$j^{\text{in}}_{\text{res},1}(t; E,\beta,\mu) := \lim_{\eta\to 0} j^{\text{in}}_{\text{res},1}(t; E^{\text{AC}}_{\eta},\beta,\mu) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{E}_1(\nu)\, \mathrm{e}^{\mathrm{i}\nu t}\, \Sigma^{(\beta,\mu)}(\mathrm{d}\nu) \,. \tag{9.34}$$

Again, the results above are stated in terms of objects corresponding to an effective one-particle picture. Therefore, one has no obvious generalisation of these results towards the definition of an AC Conductivity for interacting electron gases. This type of problem is well-known from Sections 9.4 and 9.5. Of course, we would like to mimic the analysis of (KLM07, KM08) with algebraic objects. One might get the idea, that one just needs to consider the Liouvillian $\mathcal{L}_- := -\mathrm{i}\mathcal{H}_-$ in places, where in (KLM07, KM08) the one-particle Liouvillian $\mathcal{L} = -\mathrm{i}\mathcal{H}$ was considered. But the way we achieved $\mathcal{L}_-$, it has less structure than $\mathcal{L}$, since $\mathcal{L}$ is a self-adjoint operator on the Hilbert space $\mathcal{K}^2$ (BGKS05), whereas $\mathcal{L}_-$ lacks the framework of a Hilbert space structure. In our algebraic framework $\mathcal{L}_-$ is just an operator acting on the space of measurable maps of type $\Omega \to \mathfrak{B}_{c,-}$, $\omega \mapsto B_{\omega,-}$. But in order to define the conductivity measure, in (KLM07, KM08) the Hilbert space structure of $\mathcal{K}^2$ was used for $\mathcal{L}$ decisively, for example in form of a spectral calculus for bounded measurable functions. Thus, without embedding $\mathcal{L}_-$ in the framework of an adequate Hilbert space structure, we were not able to carry out an analysis analogous to (KLM07, KM08) leading to the definition of a conductivity measure, which purely depends on many-particle objects.

Of course, one may try to embed $\mathcal{L}_-$ in the framework of some Hilbert space by defining an appropriate scalar product. Intuitively, one may get the idea to define a scalar product on some subspace of the space of covariant elements $B_-, C_- : \Omega \to \mathfrak{B}_-$ via

$$\langle\langle B_-, C_-\rangle\rangle_- := \mathbb{E}[\varrho_-(B^*_- C_-)] \,, \tag{9.35}$$

where $\varrho : \Omega \to \mathrm{Sta}(\mathfrak{B}_-)$ is an adequate covariant state[2]. Unfortunately, given a covariant state, it is hard to prove positivity for the sesquilinear form defined in Equation (9.35). At least, we have not been able to do so.

We like to close this Section with a formal calculation and discussion of a promising approach towards formulas for the AC conductivity which may be generalised towards an analysis for interacting electron gases in a natural way.

In order to do so, for any $z \in \mathbb{C}$ we define the function $F_z : \mathbb{R} \to \mathbb{C}, r \mapsto \chi_{]-\infty,0]}(r)\, \mathrm{e}^{zr}$. Note that for $\eta = \mathrm{Re}(z) > 0$ this function is bounded. Moreover, for bounded measurable functions $f : \mathbb{R} \to \mathbb{C}$ we define[3] the mappings $\tau_{f,-} : \Omega \to \mathscr{B}(\mathfrak{B}_-)$, $\omega \mapsto \tau^{(\mu)}_{\omega,f,-}$ via

$$\tau^{(\mu)}_{\omega,f,-} := \int_{\mathbb{R}} f(r)\, \tau^{(\mu)}_{\omega,r,-}\, \mathrm{d}r \,. \tag{9.36}$$

for all $\omega \in \Omega$, where the right hand side exists in the sense of Bochner integrals, since $\|\tau^{(\mu)}_{\omega,r,-}\| = 1$ for all $\omega \in \Omega$ and $\mu, r \in \mathbb{R}$. Note that the mappings $\tau^{(\mu)}_{\omega,f,-} : \mathfrak{B}_- \to \mathfrak{B}_-$ are linear, but in general will not be homomorphisms on $\mathfrak{B}_-$, since they do not preserve the product structure. The reason for this is that $\mathrm{Aut}(\mathfrak{B}_-)$ is a group with respect to the composition of maps. But it is no vector space, so in general we will only have $\tau^{(\mu)}_{\omega,f,-} \in \mathscr{B}(\mathfrak{B}_-)$.

Using this notation, we now may perform the formal calculation mentioned above. We assume that for $\beta \in [0,\infty]$ and $\mu \in \mathbb{R}$ the system satisfies the assumption (9.14). Then, the linear

[2] At least this construction is closely related to the method of constructing a scalar product in the proof of the GNS theorem (BR87, Wer11).

[3] Such definitions are made fore example in (BR97)[Theorem 5.3.15].

response current exists for all $E \in \mathcal{E}(\mathbb{R}, \mathbb{R}^d)$ that satisfy the assumptions in Section 8.5. For all $k \in \{1, ..., d\}$ we calculate formally

$$
\begin{aligned}
& j_{\mathrm{res},k}(t; E_\eta^{(AC)}, \beta, \mu) \\
&= \sum_{l=1}^{d} \int_{-\infty}^{t} E_l(r)\, \mathrm{e}^{\eta r}\, \mathbb{E}[\varrho_-^{(\beta,\mu)}(\mathcal{X}_{l,-}(\tau_{r-t,-}^{(\mu)}(J_{k,-}(0))))]\, \mathrm{d}r \\
&= \sum_{l=1}^{d} \int_{-\infty}^{t} \frac{1}{\sqrt{2\pi}} \Big(\int_{\mathbb{R}} \hat{E}_l(\nu)\, \mathrm{e}^{\mathrm{i}\nu r}\, \mathrm{d}\nu \Big)\, \mathrm{e}^{\eta r}\, \mathbb{E}[\varrho_-^{(\beta,\mu)}(\mathcal{X}_{l,-}(\tau_{r-t,-}^{(\mu)}(J_{k,-}(0))))]\, \mathrm{d}r \\
&= \frac{\mathrm{e}^{\eta t}}{\sqrt{2\pi}} \sum_{l=1}^{d} \int_{\mathbb{R}} \Big(\int_{-\infty}^{t} \mathrm{e}^{\eta(r-t)} \mathrm{e}^{\mathrm{i}\nu(r-t)}\, \mathbb{E}[\varrho_-^{(\beta,\mu)}(\mathcal{X}_{l,-}(\tau_{r-t,-}^{(\mu)}(J_{k,-}(0))))]\, \mathrm{d}r \Big)\, \hat{E}_l(\nu)\, \mathrm{e}^{\mathrm{i}\nu t}\, \mathrm{d}\nu \\
&= \frac{\mathrm{e}^{\eta t}}{\sqrt{2\pi}} \sum_{l=1}^{d} \int_{\mathbb{R}} \Big(\int_{-\infty}^{t} \mathrm{e}^{(\eta+\mathrm{i}\nu)(r-t)}\, \mathbb{E}[\varrho_-^{(\beta,\mu)}(\mathcal{X}_{l,-}(\tau_{r-t,-}^{(\mu)}(J_{k,-}(0))))]\, \mathrm{d}r \Big)\, \hat{E}_l(\nu)\, \mathrm{e}^{\mathrm{i}\nu t}\, \mathrm{d}\nu \\
&= \frac{\mathrm{e}^{\eta t}}{\sqrt{2\pi}} \sum_{l=1}^{d} \int_{\mathbb{R}} \Big(\int_{-\infty}^{0} \mathrm{e}^{(\eta+\mathrm{i}\nu)r}\, \mathbb{E}[\varrho_-^{(\beta,\mu)}(\mathcal{X}_{l,-}(\tau_{r,-}^{(\mu)}(J_{k,-}(0))))]\, \mathrm{d}r \Big)\, \hat{E}_l(\nu)\, \mathrm{e}^{\mathrm{i}\nu t}\, \mathrm{d}\nu \\
&= \frac{\mathrm{e}^{\eta t}}{\sqrt{2\pi}} \sum_{l=1}^{d} \int_{\mathbb{R}} \Big(\int_{\mathbb{R}} F_{\eta+\mathrm{i}\nu}(r)\, \mathbb{E}[\varrho_-^{(\beta,\mu)}(\mathcal{X}_{l,-}(\tau_{r,-}^{(\mu)}(J_{k,-}(0))))]\, \mathrm{d}r \Big)\, \hat{E}_l(\nu)\, \mathrm{e}^{\mathrm{i}\nu t}\, \mathrm{d}\nu \\
&= \frac{\mathrm{e}^{\eta t}}{\sqrt{2\pi}} \int_{\mathbb{R}} \sum_{l=1}^{d} \mathbb{E}[\varrho_-^{(\beta,\mu)}(\mathcal{X}_{l,-}(\tau_{F_{\eta+\mathrm{i}\nu},-}^{(\mu)}(J_{k,-}(0))))]\, \hat{E}_l(\nu)\, \mathrm{e}^{\mathrm{i}\nu t}\, \mathrm{d}\nu \,,
\end{aligned}
$$

From this we may formulate the conjecture, that for $k, l \in \{1, ..., d\}$ the components of the AC conductivity at adiabatic switching $\eta > 0$ are given by

$$\sigma_{k,l}^{\mathrm{AC}}(\nu, \eta, \beta, \mu) = \mathbb{E}[\varrho_-^{(\beta,\mu)}(\mathcal{X}_{l,-}(\tau_{F_{\eta+\mathrm{i}\nu},-}^{(\mu)}(J_{k,-}(0))))] \,, \tag{9.37}$$

where at least for non-interacting electron gases the expression on the right hand side of Equation (9.37) can be defined in a sensible way via

$$\mathbb{E}[\varrho_-^{(\beta,\mu)}(\mathcal{X}_{l,-}(\tau_{F_{\eta+\mathrm{i}\nu},-}^{(\mu)}(J_{k,-}(0))))] := -2\langle\langle \mathcal{X}_l(F^{(\beta)}(H^{(\mu)})), \tau_{F_{\eta+\mathrm{i}\nu}}(J_k(0))\rangle\rangle \,. \tag{9.38}$$

Here, analogously to Equation (9.36), for bounded measurable functions on $f : \mathbb{R} \to \mathbb{C}$ we defined the mapping $\tau_f : \Omega \to \mathscr{B}(\mathfrak{V})$, $\omega \mapsto \tau_{\omega,f}$ by

$$\tau_{\omega,f} := \int_{\mathbb{R}} f(r)\, \tau_{\omega,r}\, \mathrm{d}r \,. \tag{9.39}$$

10 Localisation Criteria

In the beginning the universe was created. This has made a lot of people very angry and been widely regarded as a bad move.

(Douglas Adams)

In order to derive the conductivity tensor in form of a Kubo formula, the linear response theory of Chapter 9 required the electron gas to satisfy the localisation criterion (9.14). This localisation criterion is specific for the case of a non-interacting electron gas, since it is formulated in terms of an effective one-particle picture, which is only accessible for non-interacting systems. So, in order to generalise the linear response theory of Chapter 9 towards interacting quantum gases, the localisation criterion (9.14) needs to be replaced by a criterion, which uses objects, that also exist in the case of interacting systems.

Our main motivation for the current chapter is to present different approaches for such generalisations of the localisation criterion (9.14) in view of a future linear response theory considering interacting electron gases. These new criteria will be called *strong* and *weak localisation criterion*, respectively. They are introduced, in Sections 10.1 and 10.2, respectively. Moreover, we motivate both criteria in Theorems 10.2 and 10.4 by considering the special case of a non-interacting electron gas, which satisfies well known localisation estimates in terms of single-particle quantities (AFHS01, GK03). This shall illustrate that the strong as well as the weak localisation criterion are reasonable assumptions on a system.

However, we are not able to carry out a complete linear response theory which mimics the proceeding of Chapter 9 for the model of an interacting electron gas. Instead, we only focus on a sensible definition of the integrand in the Kubo formula (9.25) for interacting electron gases. The reason for this is that the Kubo formula (9.25) only contains the state $\varrho_-^{(\beta,\mu)}$, the position derivations $\mathcal{X}_{l,-}$, the time evolution $\tau_{t,-}^{(\mu)}$ and the current density operator $J_{k,-}(y)$, which all are objects that in principle are accessible for interacting electron gases. Moreover, at least a formal calculation of the linear response current for interacting electron gases shows that the linear response current has exactly the form given in the Kubo formula (9.25), where $\varrho_-^{(\beta,\mu)}$, $\mathcal{X}_{l,-}$, $\tau_{t,-}^{(\mu)}$ and $J_{k,-}(y)$ are the state, position derivation, time evolution and current density operator of the interacting electron gas, respectively. In fact, this situation motivated the definition of the strong and the weak localisation criterion in the first place.

Assuming that the electron gas satisfies either the strong or the weak localisation criterion, in Section 10.3 we are able to define the so called *linear current*[1] j_{lin} by the right hand side of the Kubo formula (9.25), where $\varrho_-^{(\beta,\mu)}$, $\mathcal{X}_{l,-}$, $\tau_{t,-}^{(\mu)}$ and $J_{k,-}(y)$ are the state, position derivation, time evolution and current density operator of the corresponding interacting electron gas. We conjecture that j_{lin} is the linear response current for interacting electron gases, i.e.

$$j_{\text{lin}} = j_{\text{res}} \,. \tag{10.1}$$

[1] Note, that the linear current has to be distinguished from the linear response current j_{res}.

10.1. Strong Localisation Criterion

In order to state the strong as well as the weak localisation criterion, we will need the particle number operator as introduced in Equation (B.76)

$$N_-(\psi) = a_-^*(\psi)a_-(\psi) \tag{10.2}$$

for arbitrary $\psi \in \mathfrak{h}$. Moreover, we need to define the so called support distance mapping

$$f : \mathfrak{h} \times \mathfrak{h} \to [0, \infty[,\ (\phi, \psi) \mapsto \mathrm{dist}(\mathrm{supp}(\phi), \mathrm{supp}(\psi))\ . \tag{10.3}$$

Definition 10.1 (*Strong Localisation Criterion*)

Consider the model of an interacting electron gas introduced in Chapter 6 with chemical potential $\mu \in \mathbb{R}$. Then, the system is said to satisfy the *strong localisation criterion*, if there are constants $M, \varepsilon > 0$ and $\kappa > d + 1$ such that for any $t \in \mathbb{R}$ and $\phi, \psi \in \mathfrak{h}$ the following estimate holds

$$\mathbb{E}[\|[N_-(\phi), \tau_{t,-}^{(\mu)}(N_-(\psi))]\|] \leq \frac{M\ \|\phi\|^2\ \|\psi\|^2}{(1 + \varepsilon f(\phi, \psi))^\kappa}\ . \tag{10.4}$$

In any case, we have that $\mathbb{E}[\mathrm{i}[N_-(\phi), \tau_{t,-}^{(\mu)}(N_-(\psi))]]$ exists in the sense of Bochner integrals, because of the fact that for any $\omega \in \Omega$ one has

$$\begin{aligned}\|[N_-(\phi), \tau_{\omega,t,-}^{(\mu)}(N_-(\psi))]\| &\leq 2\ \|N_-(\phi)\|\ \|\tau_{\omega,t,-}^{(\mu)}(N_-(\psi))\| \\ &= 2\ \|N_-(\phi)\|\ \|N_-(\psi)\| \\ &= 2\ \|\phi\|^2\ \|\psi\|^2\ .\end{aligned}$$

In order to achieve some intuition for the strong localisation criterion we consider the case, where $\phi = \delta_x$ and $\psi = \delta_y$ for any $x, y \in \mathbb{Z}^d$. Then, $f(\delta_x, \delta_y) = |x - y|$ and the electron number operator $N_-(\delta_x)$ is the observable which counts the number of electrons at position $x \in \mathbb{Z}^d$. In terms of measurements, the norm of the commutator $\|[N_-(\delta_x), \tau_{\omega,t,-}^{(\mu)}(N_-(\delta_y))]\|$ has the following interpretation.

First, at position $x \in \mathbb{Z}^d$ the electron number is measured. Then, during time $t \in \mathbb{R}$ elapses, the electron gas evolves. A second measurement of electron number, this time at position $y \in \mathbb{Z}^d$, is performed. The number $\|[N_-(\delta_x), \tau_{\omega,t,-}^{(\mu)}(N_-(\delta_y))]\|$ then indicates how strongly the later measurement at position y is influenced by the earlier measurement at position x.

So inequality (10.4) states that, independently of the evolution time, having a large distance of x and y, one expects the measurement at position y only to be weakly influenced by the measurement at position $x \in \mathbb{Z}^d$. In other words this means, that independently of the time between the two measurements, during which the system evolves, it is unlikely for an electron at position x to be transported to position y.

Although typically, localisation would be associated with exponential decay in the distance of x and y, we chose the name localisation criterion. As it will turn out, the decay in Equation (10.4) is enough for our purpose, which is to define the term

$$\mathbb{E}[\varrho_-^{(\beta,\mu)}(\mathcal{X}_{l,-}(\tau_{t,-}^{(\mu)}(J_{k,-}(0))))] \tag{10.5}$$

in a sensible way. The justification for the interest in this term is that it will become the integrand in the Kubo-type formula for the definition of the linear current as outlined in the introduction to this chapter.

Note that if a system satisfies the strong localisation criterion for some chemical potential $\nu \in \mathbb{R}$, then it satisfies the strong localisation criterion for any $\mu \in \mathbb{R}$. Because of the fact, that for any $\omega \in \Omega$, $\psi \in \mathfrak{h}$ and $\mu, \nu \in \mathbb{R}$ one has $[N_-, H^{(\mu)}_{\omega,-}] = 0 = [N_-, N_-(\psi)]$, we obtain

$$\begin{aligned}
\tau^{(\mu)}_{\omega,t,-}(N_-(\psi)) &= \mathrm{e}^{-\mathrm{i}tH^{(\mu)}_{\omega,-}} N_-(\psi) \mathrm{e}^{\mathrm{i}tH^{(\mu)}_{\omega,-}} \\
&= \mathrm{e}^{-\mathrm{i}t(H^{(\nu)}_{\omega,-}+(\nu-\mu)N_-)} N_-(\psi) \mathrm{e}^{\mathrm{i}t(H^{(\nu)}_{\omega,-}+(\nu-\mu)N_-)} \\
&= \mathrm{e}^{-\mathrm{i}tH^{(\nu)}_{\omega,-}} \mathrm{e}^{\mathrm{i}t(\mu-\nu)N_-} N_-(\psi) \mathrm{e}^{-\mathrm{i}t(\mu-\nu)N_-} \mathrm{e}^{\mathrm{i}tH^{(\nu)}_{\omega,-}} \\
&= \mathrm{e}^{-\mathrm{i}tH^{(\nu)}_{\omega,-}} N_-(\psi) \mathrm{e}^{\mathrm{i}tH^{(\nu)}_{\omega,-}} \\
&= \tau^{(\nu)}_{\omega,t,-}(N_-(\psi)) \, .
\end{aligned}$$

In the following theorem we prove, that at least for non-interacting electron gases there are certain circumstances of interest, where the system satisfies the strong localisation criterion.

Theorem 10.2

Consider the model of a non-interacting electron gas introduced in Chapter 6 with chemical potential $\mu \in \mathbb{R}$. Assume that there are constants $M', \epsilon' > 0$ and $\kappa' > d+1$ such that

$$\mathbb{E}[|\langle \phi, \mathrm{e}^{-\mathrm{i}tH^{(\mu)}} \psi \rangle|] \leq \frac{M' \, \|\phi\| \, \|\psi\|}{(1 + \varepsilon' f(\phi,\psi))^{\kappa'}} \tag{10.6}$$

holds for every $\phi, \psi \in \mathfrak{h}$ and $t \in \mathbb{R}$. Then, the system satisfies the strong localisation criterion.

Proof: We use the canonical anti-commutation relations (B.71)-(B.73) to simplify the commutator

$$\begin{aligned}
&[N_-(\phi), \tau^{(\mu)}_{\omega,t,-}(N_-(\psi))] \\
&\quad = [a^*_-(\phi)a_-(\phi), \tau^{(\mu)}_{\omega,t,-}(a^*_-(\psi)a_-(\psi))] \\
&\quad = [a^*_-(\phi)a_-(\phi), \tau^{(\mu)}_{\omega,t,-}(a^*_-(\psi))\tau^{(\mu)}_{\omega,t,-}(a_-(\psi))] \\
&\quad = [a^*_-(\phi)a_-(\phi), a^*_-(U^{(\mu)}_\omega(t)\psi)a_-(U^{(\mu)}_\omega(t)\psi)] \\
&\quad = a^*_-(U^{(\mu)}_\omega(t)\psi) \, \{a^*_-(\phi), a_-(U^{(\mu)}_\omega(t)\psi)\} \, a_-(\phi) - a^*_-(\phi) \, \{a_-(\phi), a^*_-(U^{(\mu)}_\omega(t)\psi)\} \, a_-(U^{(\mu)}_\omega(t)\psi)
\end{aligned}$$

for any $\omega \in \Omega$, $\phi, \psi \in \mathfrak{h}$ and $t \in \mathbb{R}$. We used, that for the non-interacting electron gas one has $\{a_-(U^{(\mu)}_\omega(t)\psi), a_-(\phi)\} = 0 = \{a^*_-(U^{(\mu)}_\omega(t)\psi), a^*_-(\phi)\}$. So, one has $[N_-(\phi), \tau^{(\mu)}_{\omega,t,-}(N_-(\psi))] = B_{\omega,-} - B^*_{\omega,-}$, where $B_{\omega,-} := -a^*_-(\phi) \, \{a_-(\phi), a^*_-(U^{(\mu)}_\omega(t)\psi)\} \, a_-(U^{(\mu)}_\omega(t)\psi)$. Now, using the fact that in the non-interacting case one has $\{a_-(\phi), a^*_-(U^{(\mu)}_\omega(t)\psi)\} = \langle \phi, \mathrm{e}^{-\mathrm{i}tH^{(\mu)}_\omega} \psi \rangle$, we obtain

$$\begin{aligned}
\mathbb{E}[\|[N_-(\phi), \tau^{(\mu)}_{t,-}(N_-(\psi))]\|] &= \mathbb{E}[\|B_- - B^*_-\|] \leq 2 \, \mathbb{E}[\|B_-\|] \\
&\leq 2 \, \mathbb{E}[\|a_-(\phi)\| \, \|\{a_-(\phi), a^*_-(U^{(\mu)}(t)\psi)\}\| \, \|a_-(U^{(\mu)}(t)\psi)\|] \\
&= 2 \, \mathbb{E}[\|\phi\| \, |\langle \phi, \mathrm{e}^{-\mathrm{i}tH^{(\mu)}} \psi \rangle| \, \|\psi\|] \\
&= 2 \, \mathbb{E}[|\langle \phi, \mathrm{e}^{-\mathrm{i}tH^{(\mu)}} \psi \rangle|] \, \|\phi\| \, \|\psi\| \\
&\leq \frac{2M' \, \|\phi\|^2 \, \|\psi\|^2}{(1 + \varepsilon' f(\phi,\psi))^{\kappa'}} \, .
\end{aligned}$$

■

The above conditions are satisfied whenever the electron gas is completely localised (AFHS01, GK03). The latter property implies the existence of constants $C, \gamma > 0$ such that for any $\phi, \psi \in \mathfrak{h}$ with $\|\phi\| = \|\psi\| = 1$ the following inequality holds

$$\mathbb{E}[\sup\{|\langle \phi, g(H^{(\mu)})\psi \rangle| : \|g\|_\infty \leq 1\}] \leq C \, \mathrm{e}^{-\gamma f(\phi,\psi)} \, . \tag{10.7}$$

Of course, on is allowed the special choice of $g(\lambda) = \mathrm{e}^{-\mathrm{i}t\lambda}$ which for arbitrary $t \in \mathbb{R}$ and $\phi, \psi \in \mathfrak{h}$ yields the estimate

$$\mathbb{E}[|\langle \phi, \mathrm{e}^{-\mathrm{i}tH^{(\mu)}} \psi \rangle|] \leq C \, \|\phi\| \, \|\psi\| \, \mathrm{e}^{-\gamma f(\phi,\psi)} \, .$$

So, one even has an exponential decay in the distance of the supports. Obviously, in this situation, there are constants $M, \varepsilon \in \mathbb{R}$ and $\kappa > d + 1$, such that Inequality (10.6) is satisfied.

10.2. Weak Localisation Criterion

Definition 10.3 (*Weak Localisation Criterion*)

Consider the model of an interacting electron gas introduced in Chapter 6 with chemical potential $\mu \in \mathbb{R}$ in a covariant KMS state $\varrho_-^{(\beta,\mu)} : \Omega \to \mathrm{Sta}(\mathfrak{B}_-)$, $\omega \mapsto \varrho_{\omega,-}^{(\beta,\mu)}$ at inverse temperature $\beta \in [0, \infty]$. Then, the system is said to satisfy the *weak localisation criterion*, if there are constants $M, \varepsilon > 0$ and $\kappa > d + 1$ such that for any $t \in \mathbb{R}$ and $\phi, \psi \in \mathfrak{h}$ the following estimate holds

$$\mathbb{E}[|\varrho_-^{(\beta,\mu)}([N_-(\phi), \tau_{t,-}^{(\mu)}(N_-(\psi))])|] \leq \frac{M \, \|\phi\|^2 \, \|\psi\|^2}{(1 + \varepsilon f(\phi, \psi))^\kappa} \, . \tag{10.8}$$

Clearly, whenever an electron gas satisfies the strong localisation criterion it automatically satisfies the weak localisation criterion at any temperature and any chemical potential. This can be seen from

$$\begin{aligned}\mathbb{E}[|\varrho_-^{(\beta,\mu)}([N_-(\phi), \tau_{t,-}^{(\mu)}(N_-(\psi))])|] &\leq \mathbb{E}[\|\varrho_-^{(\beta,\mu)}\| \, \|[N_-(\phi), \tau_{t,-}^{(\mu)}(N_-(\psi))]\|] \\ &= \mathbb{E}[\|[N_-(\phi), \tau_{t,-}^{(\mu)}(N_-(\psi))]\|] \, ,\end{aligned}$$

which holds for any values of $\beta \in [0, \infty]$, $\mu \in \mathbb{R}$ and $t \in \mathbb{R}$. The following theorem is the analogue to Theorem 10.2 for the weak localisation criterion.

Theorem 10.4

Consider the model of a non-interacting electron gas introduced in Chapter 6 with chemical potential $\mu \in \mathbb{R}$ in its unique covariant ground state $\varrho_-^{(\mu)} : \Omega \to \mathrm{Sta}(\mathfrak{B}_-)$, $\omega \mapsto \varrho_{\omega,-}^{(\mu)}$. Assume that there are constants $M', \epsilon' > 0$ and $\kappa' > d + 1$ such that

$$\mathbb{E}[|\langle \phi, \chi_{]-\infty,0]}(H^{(\mu)}) \mathrm{e}^{-\mathrm{i}tH^{(\mu)}} \psi \rangle|] \leq \frac{M' \, \|\phi\| \, \|\psi\|}{(1 + \varepsilon' f(\phi, \psi))^{\kappa'}} \tag{10.9}$$

holds for every $\phi, \psi \in \mathfrak{h}$ and $t \in \mathbb{R}$. Then, the system satisfies the weak localisation criterion.

Proof: In the case of a non-interacting electron gas, using the canonical anti-commutation relations (B.71) - (B.73), one obtains that for every $\omega \in \Omega$, $t \in \mathbb{R}$ and $\phi, \psi \in \mathfrak{h}$

$$\begin{aligned}&\varrho_{\omega,-}^{(\mu)}([N_-(\phi), \tau_{\omega,t,-}^{(\mu)}(N_-(\psi))]) \\ &\quad = \varrho_{\omega,-}^{(\mu)}(a_-^*(\phi)a_-(\phi)\tau_{\omega,t,-}^{(\mu)}(a_-^*(\psi)a_-(\psi))) - \varrho_{\omega,-}^{(\mu)}(\tau_{\omega,t,-}^{(\mu)}(a_-^*(\psi)a_-(\psi))a_-^*(\phi)a_-(\phi)) \\ &\quad = \varrho_{\omega,-}^{(\mu)}(a_-^*(\phi)a_-(\phi)a_-^*(U_\omega^{(\mu)}(t)\psi)a_-(U_\omega^{(\mu)}(t)\psi)) - \varrho_{\omega,-}^{(\mu)}(a_-^*(U_\omega^{(\mu)}(t)\psi)a_-(U_\omega^{(\mu)}(t)\psi)a_-^*(\phi)a_-(\phi))) \\ &\quad = \langle \phi, U_\omega^{(\mu)}(t)\psi \rangle \, \varrho_{\omega,-}^{(\mu)}(a_-^*(\phi)a_-(U_\omega^{(\mu)}(t)\psi)) - \langle U_\omega^{(\mu)}(t)\psi, \phi \rangle \, \varrho_{\omega,-}^{(\mu)}(a_-^*(U_\omega^{(\mu)}(t)\psi)a_-(\phi))\end{aligned}$$

Note that the equation above is of the form $\varrho_{\omega,-}^{(\mu)}([N_-(\phi), \tau_{\omega,t,-}^{(\mu)}(N_-(\psi))]) = b_\omega - \overline{b_\omega}$, where we defined $b_\omega := \langle \phi, U_\omega^{(\mu)}(t)\psi \rangle \, \varrho_{\omega,-}^{(\mu)}(a_-^*(\phi)a_-(U_\omega^{(\mu)}(t)\psi))$.

Finally, from the fact that one has $\varrho^{(\mu)}_{\omega,-}(a^*_-(U^{(\mu)}_\omega(t)\psi)a_-(\phi)) = \langle\phi, \chi_{]-\infty,0]}(H^{(\mu)}_\omega)\mathrm{e}^{-\mathrm{i}tH^{(\mu)}_\omega}\psi\rangle$ for the two-point function one obtains

$$\begin{aligned}
\mathbb{E}[|\varrho^{(\mu)}_-([N_-(\phi),\tau^{(\mu)}_{t,-}(N_-(\psi))])|] &= \mathbb{E}[|b-\bar{b}|] \leq 2\,\mathbb{E}[|b|] \\
&= 2\,\mathbb{E}[|\langle\phi, U^{(\mu)}(t)\psi\rangle|\,|\varrho^{(\mu)}_-(a^*_-(\phi)a_-(U^{(\mu)}(t)\psi))|] \\
&\leq 2\,\mathbb{E}[\|\phi\|\,\|\psi\|\,|\langle\phi,\chi_{]-\infty,0]}(H^{(\mu)})\mathrm{e}^{-\mathrm{i}tH^{(\mu)}}\psi\rangle|] \\
&\leq 2\,\mathbb{E}[|\langle\phi,\chi_{]-\infty,0]}(H^{(\mu)})\mathrm{e}^{-\mathrm{i}tH^{(\mu)}}\psi\rangle|]\,\|\phi\|\,\|\psi\| \\
&\leq \frac{2M'\,\|\phi\|^2\,\|\psi\|^2}{(1+\varepsilon' f(\phi,\psi))^{\kappa'}}\,. \qquad \blacksquare
\end{aligned}$$

The above conditions are satisfied whenever the electron gas is in a region of localisation for the chemical potential $\mu \in \mathbb{R}$ (AFHS01, GK03). The latter property implies the existence of constants $C, \gamma > 0$ such that for any $\phi, \psi \in \mathfrak{h}$ with $\|\phi\| = \|\psi\| = 1$ the following inequality holds

$$\mathbb{E}[\sup\{|\langle\phi,\chi_{]-\infty,0]}(H^{(\mu)})g(H^{(\mu)})\psi\rangle| : \|g\|_\infty \leq 1\}] \leq C\,\mathrm{e}^{-\gamma f(\phi,\psi)}\,. \tag{10.10}$$

10.3. Linear Current

As outlined above, the main motivation for the strong and the weak localisation criterion is to define a quantity called linear current via the right hand side of a Kubo-type formula as it is given in Equation (9.25) but with the corresponding objects for interacting electron gases in the integrand, i.e. we are interested in a sensible definition of the term

$$\mathbb{E}[\varrho^{(\beta,\mu)}_-(\mathcal{X}_{l,-}(\tau^{(\mu)}_{t,-}(J_{k,-}(0))))] \tag{10.11}$$

for interacting electron gases. The weak localisation criterion, and therefore, since it is an even more restrictive assumption, also the strong localisation criterion will enable us to do so. This is the statement of the subsequent theorem. Accordingly, we assume that the electron gas at inverse temperature $\beta \in [0,\infty]$ and with chemical potential $\mu \in \mathbb{R}$ at least satisfies the weak localisation criterion. In a first step, for any $l \in \{1,...,d\}$ and $t \in \mathbb{R}$ we define

$$\mathbb{E}[\lambda\,\varrho^{(\beta,\mu)}_-(\mathcal{X}_l(\tau^{(\mu)}_{t,-}(N_-(\psi))))] := \mathrm{i}\sum_{x\in\mathbb{Z}^d} x_l\,\mathbb{E}[\lambda\,\varrho^{(\beta,\mu)}_-([N_-(\delta_x),\tau^{(\mu)}_{t,-}(N_-(\psi))])]\,, \tag{10.12}$$

where $\psi \in \mathfrak{h}_c$ and $\lambda : \Omega \to \mathbb{C}$ is an essentially bounded measurable mapping. The series on the right hand side converges, since it is an absolutely convergent series in $\mathbb{C}$ for the fact that one has the estimate

$$\begin{aligned}
\left|\mathbb{E}[\lambda\,\varrho^{(\beta,\mu)}_-([N_-(\delta_x),\tau^{(\mu)}_{t,-}(N_-(\psi))])]\right| &\leq \|\lambda\|_\infty\,\mathbb{E}[|\varrho^{(\beta,\mu)}_-([N_-(\delta_x),\tau^{(\mu)}_{t,-}(N_-(\psi))])|] \\
&\leq \frac{M'\,\|\lambda\|_\infty\,\|\psi\|}{(1+\epsilon'|x-y|)^{\kappa'}}
\end{aligned} \tag{10.13}$$

which holds for any $t \in \mathbb{R}$ and $y \in \mathrm{supp}(\psi)$ with a certain set of constants $M', \epsilon' > 0$ and $\kappa' > d+1$, because of the weak localisation criterion. Then, in a second step one can define $\mathbb{E}[\varrho^{(\beta,\mu)}_-(\mathcal{X}_l(\tau^{(\mu)}_{t,-}(B_-)))]$ via linear extension for measurable mappings $\mathfrak{B}_- : \Omega \to \mathfrak{B}_-$, $\omega \mapsto B_{\omega,-}$, where for almost every $\omega \in \Omega$ one has

$$B_{\omega,-} = \sum_{n\in\mathcal{N}} \lambda_{n,\omega}\,N_-(\psi_n) \tag{10.14}$$

with a finite Index $\mathcal{N}$, bounded mappings $\lambda_n : \Omega \to \mathbb{C},\ \omega \mapsto \lambda_{n,\omega}$ and vectors $\psi_n \in \mathfrak{h}_c$ for all $n \in \mathcal{N}$. Given this situation for any $l \in \{1, ..., d\}$ and $t \in \mathbb{R}$ one has

$$\mathbb{E}[\varrho_-^{(\beta,\mu)}(\mathcal{X}_l(\tau_{t,-}^{(\mu)}(B_-)))] = \sum_{n\in\mathcal{N}} \mathbb{E}[\lambda_n\, \varrho_-^{(\beta,\mu)}(\mathcal{X}_l(\tau_{t,-}^{(\mu)}(N_-(\psi_n))))]\ . \tag{10.15}$$

Theorem 10.5 (*Linear Current*)

Consider the model for an interacting electron gas as introduced in Chapter 6 at inverse temperature $\beta \in [0, \infty]$, with chemical potential $\mu \in \mathbb{R}$ and with electric field $E \in \mathcal{E}(\mathbb{R}, \mathbb{R}^d)$, which satisfies the weak localisation criterion (10.8). Then, for any $t \in \mathbb{R}$ the *linear current* $j_{\text{lin}}(t; E, \beta, \mu) := (j_{\text{lin},1}(t; E, \beta, \mu), ..., j_{\text{lin},d}(t; E, \beta, \mu))$ is well-defined for any $k \in \{1, ..., d\}$ by

$$j_{\text{lin},k}(t; E, \beta, \mu) := \sum_{l=1}^{d} \int_{-\infty}^{t} E_l(r)\ \mathbb{E}[\varrho_-^{(\beta,\mu)}(\mathcal{X}_{l,-}(\tau_{r-t,-}^{(\mu)}(J_{k,-}(0))))]\ \mathrm{d}r\ . \tag{10.16}$$

Proof: In a first step we prove that for any $k \in \{1, ..., d\}$ and $y \in \mathbb{Z}^d$ the components of the current density operator $J_{k,-}(y) : \Omega \to \mathfrak{B}_-,\ \omega \mapsto J_{\omega,k,-}(y)$ can be represented as a finite sum of particle number operators as in Equation (10.14). Since in each realisation $\omega \in \Omega$, at each position $y \in \mathbb{Z}^d$ and for each $k \in \{1, ..., d\}$ the self-adjoint operator $J_{\omega,k}(y)$ has finite support and finite rank, it possesses only finitely many non-zero eigenvalues $\lambda_{k,y,n,\omega} \in [-4d, 4d]$, so $n \in \mathcal{N}$, where $\mathcal{N}$ is finite. Corresponding to these non-zero eigenvalues there are orthonormal eigenvectors $\psi_{k,y,n,\omega} \in \mathfrak{h}_c$, which have support in a finite set Λ that only depends on $y \in \mathbb{Z}^d$. In more detail, using the notation of Chapter 7, for any $y \in \mathbb{Z}^d$, $\omega \in \Omega$ and $k \in \{1, ..., d\}$ we may choose the cube $\Lambda := \Lambda_3 + y$. Therefore, one has $|\mathcal{N}| \le 5^d$. Due to Equation (B.75) for any $y \in \mathbb{Z}^d$, $\omega \in \Omega$ and $k \in \{1, ..., d\}$ one obtains

$$\begin{aligned} J_{\omega,k,-}(y) &= \sum_{n\in\mathcal{N}} a_-^*(J_{\omega,k}(y)\psi_{k,y,n,\omega})a_-(\psi_{k,y,n,\omega}) \\ &= \sum_{n\in\mathcal{N}} \lambda_{k,y,n,\omega}\ a_-^*(\psi_{k,y,n,\omega})a_-(\psi_{k,y,n,\omega}) \\ &= \sum_{n\in\mathcal{N}} \sum_{x\in\Lambda} \lambda_{k,y,n,\omega}\ \psi_{k,y,n,\omega}(x)\ N_-(\delta_x)\ . \end{aligned}$$

Redefinitions of $\mathcal{N}$ and the eigenvalues $\lambda_{k,y,n,\omega}$ yield that $J_{k,-}(y)$ can be represented as in Equation (10.14). Then for any $k, l \in \{1, ..., d\}$, $t \in \mathbb{R}$ the expression

$$\mathbb{E}[\varrho_-^{(\beta,\mu)}(\mathcal{X}_{l,-}(\tau_{t,-}^{(\mu)}(J_{k,-}(0))))] \tag{10.17}$$

is well-defined in terms of Equation (10.15). Moreover, from (10.13) we get that (10.17) is uniformly bounded in $t \in \mathbb{R}$. Since $E \in \mathcal{E}(\mathbb{R}, \mathbb{R}^d)$, the existence of the integral on the right hand side in (10.16) follows immediately. ■

Of course, we assume that, being able to carry out linear response theory for models of interacting electron gases, one would obtain an expression for the linear response current which is identical with the linear current of the system. In other words we conjecture that, if a system satisfies the weak localisation criterion, the identity

$$j_{\text{res}}(t; E, \beta, \mu) = j_{\text{lin}}(t; E, \beta, \mu) \tag{10.18}$$

holds. Unfortunately, we have not been able to carry out a linear response theory for interacting electron gases based on the assumption that the electron gas satisfies the weak localisation criterion in order to prove Conjecture (10.18). But at least, we can prove equality of linear current and linear response current in the case of a non-interacting electron gas. This is achieved in the following theorem.

Theorem 10.6 (*Linear Current and Linear Response Current*)

Consider the model of a non-interacting electron gas as introduced in Chapter 6 with chemical potential $\mu \in \mathbb{R}$ in its covariant KMS state at inverse temperature $\beta \in [0, \infty]$. In addition, assume that there exist constants $C, \gamma > 0$, such that for all $\phi, \phi \in \mathfrak{h}$ with $\|\phi\| = \|\psi\| \leq 1$ the following estimate holds

$$\mathbb{E}[\sup\{|\langle \phi, g(H^{(\mu)})\psi\rangle|^2 : \|g\|_\infty \leq 1\}] \leq C\, \mathrm{e}^{-\gamma f(\phi,\psi)} . \tag{10.19}$$

Then, the linear current as well as the linear response current exist. Moreover, both currents are identical, i.e. for any $t \in \mathbb{R}$ and $E \in \mathcal{E}(\mathbb{R}, \mathbb{R}^d)$ one has

$$j_{\mathrm{res}}(t; E, \beta, \mu) = j_{\mathrm{lin}}(t; E, \beta, \mu) . \tag{10.20}$$

Proof: Let $\beta \in [0, \infty]$ and $\mu \in \mathbb{R}$ be arbitrary. The existence of the linear current is evident, since (10.19) implies weak localisation at any temperature and chemical potential by Theorem 10.4. Similarly, since (10.19) implies $\mathbb{E}[\|X_l g(H^{(\mu)})\delta_0\|^2] < \infty$ as well as $\mathcal{X}_l(g(H^{(\mu)})) \in \mathcal{K}^2$ for all $l \in \{1, ..., d\}$ and bounded measurable functions $g : \mathbb{R} \to \mathbb{C}$ (BGKS05)[Assumption 5.1], we get the existence of the linear response current by choosing $g = F^{(\beta)}$. Note that, even for non-interacting electron gases, Equation (10.20) is non-trivial, since the term $\mathbb{E}[\varrho_-^{(\beta,\mu)}(\mathcal{X}_{l,-}(\tau_{t,-}^{(\mu)}(J_{k,-}(0))))]$ in the integral of the Kubo formula (9.25) and in the integral of the Kubo-type formula (10.16) is defined in Chapter 9 and the present Chapter in two different ways, respectively. Thus, we prove, that both definitions agree. We start with the definition of $\mathbb{E}[\varrho_-^{(\beta,\mu)}(\mathcal{X}_{l,-}(\tau_{t,-}^{(\mu)}(J_{k,-}(0))))]$ due to Theorem 10.5. Using Equation (6.90), for any $t \in \mathbb{R}$ and $k, l \in \{1, ..., d\}$ we have

$$\begin{aligned}\mathbb{E}[\varrho_-^{(\beta,\mu)}(\mathcal{X}_{l,-}(\tau_{t,-}^{(\mu)}(J_{k,-}(0))))] &= \sum_{x\in\mathbb{Z}^d} x_l\, \mathbb{E}[\varrho_-^{(\beta,\mu)}(\mathrm{i}[N_-(\delta_x), \tau_{t,-}^{(\mu)}(J_{k,-}(0))])] \\ = \sum_{x\in\mathbb{Z}^d} x_l\, \underbrace{\mathbb{E}[\varrho_-^{(\beta,\mu)}(\mathrm{i}[N_-(\delta_x), \tau_{t,-}^{(\mu)}(a_-^*(D_k\delta_0)a_-(\delta_0))])]}_{=:T_1(x)} &+ x_l\, \underbrace{\mathbb{E}[\varrho_-^{(\beta,\mu)}(\mathrm{i}[N_-(\delta_x), \tau_{t,-}^{(\mu)}(a_-^*(\delta_0)a_-(D_k\delta_0))])]}_{=:T_2(x)} .\end{aligned}$$

Note that for any $x \in \mathbb{Z}^d$ one has $N_-(\delta_x) = \mathrm{d}\Gamma_-(P_x)$, where $P_x : \mathfrak{h} \to \mathfrak{h}$, $\psi \mapsto \langle \delta_x, \psi\rangle\, \delta_x$ is the projection onto the space spanned by δ_x. Next, the specific structure of the non-interacting electron gas enters, i.e. we use Equations (9.1) - (9.8) and (B.67). We obtain

$$\begin{aligned}T_1(x) &= \mathrm{i}\, \mathbb{E}[\varrho_-^{(\beta,\mu)}([N_-(\delta_x), \tau_{t,-}^{(\mu)}(a_-^*(D_k\delta_0)a_-(\delta_0))])] \\ &= \mathrm{i}\, \mathbb{E}[\varrho_-^{(\beta,\mu)}([\mathrm{d}\Gamma_-(P_x), a_-^*(U^{(\mu)}(t)D_k\delta_0)a_-(U^{(\mu)}(t)\delta_0)])] \\ &= \mathrm{i}\, \mathbb{E}[\varrho_-^{(\beta,\mu)}(a_-^*(P_xU^{(\mu)}(t)D_k\delta_0)a_-(U^{(\mu)}(t)\delta_0)) - \varrho_-^{(\beta,\mu)}(a_-^*(U^{(\mu)}(t)D_k\delta_0)a_-(P_xU^{(\mu)}(t)\delta_0))] \\ &= \mathrm{i}\, \mathbb{E}[\langle U^{(\mu)}(t)\delta_0, F^{(\beta)}(H^{(\mu)})P_xU^{(\mu)}(t)D_k\delta_0\rangle - \langle P_xU^{(\mu)}(t)\delta_0, F^{(\beta)}(H^{(\mu)})U^{(\mu)}(t)D_k\delta_0\rangle] \\ &= \mathrm{i}\, \mathbb{E}[\langle P_xF^{(\beta)}(H^{(\mu)})U^{(\mu)}(t)\delta_0, U^{(\mu)}(t)D_k\delta_0\rangle - \langle F^{(\beta)}(H^{(\mu)})P_xU^{(\mu)}(t)\delta_0, U^{(\mu)}(t)D_k\delta_0\rangle] \\ &= -\mathbb{E}[\langle \mathrm{i}[P_x, F^{(\beta)}(H^{(\mu)})]U^{(\mu)}(t)\delta_0, U^{(\mu)}(t)D_k\delta_0\rangle]\end{aligned} \tag{10.21}$$

for all $k \in 1, ..., d$, $t \in \mathbb{R}$ and $x \in \mathbb{Z}^d$. Moreover, one obtains

$$\begin{aligned}\sum_{x\in\mathbb{Z}^d} x_l\, T_1(x) &= -\sum_{x\in\mathbb{Z}^d} x_l\, \mathbb{E}[\langle \mathrm{i}[P_x, F^{(\beta)}(H^{(\mu)})]U^{(\mu)}(t)\delta_0, U^{(\mu)}(t)D_k\delta_0\rangle] \\ &\overset{(*)}{=} -\mathbb{E}[\langle \mathrm{i}[X_l, F^{(\beta)}(H^{(\mu)})]U^{(\mu)}(t)\delta_0, U^{(\mu)}(t)D_k\delta_0\rangle] \\ &= -\mathbb{E}[\langle \mathcal{X}_l(F^{(\beta)}(H^{(\mu)}))U^{(\mu)}(t)\delta_0, U^{(\mu)}(t)D_k\delta_0\rangle] \\ &= -\mathbb{E}[\langle U^{(\mu)}(-t)\mathcal{X}_l(F^{(\beta)}(H^{(\mu)}))U^{(\mu)}(-t)^*\delta_0, D_k\delta_0\rangle] \\ &= -\langle\langle \tau_{-t}(\mathcal{X}_l(F^{(\beta)}(H^{(\mu)}))), D_k\rangle\rangle \\ &= -\langle\langle \mathcal{X}_l(F^{(\beta)}(H^{(\mu)})), \tau_t(D_k)\rangle\rangle ,\end{aligned} \tag{10.22}$$

where $(*)$ is a crucial step in the calculation above, since it uses that for all $k, l \in \{1, ..., d\}$ and $t \in \mathbb{R}$

$$\lim_{L\to\infty} \mathbb{E}\Big[\Big\langle\Big([X_l, F^{(\beta)}(H^{(\mu)})] - \sum_{x\in\Lambda_L} x_l\, [P_x, F^{(\beta)}(H^{(\mu)})]\Big)U^{(\mu)}(t)\delta_0, U^{(\mu)}(t)D_k\delta_0\Big\rangle\Big] = 0\,. \tag{10.23}$$

We will justify Equation (10.23) at the end of the proof. Analogously to the calculations (10.21) and (10.22), for $T_2(x)$ one obtains

$$T_2(x) = -\mathbb{E}[\langle U^{(\mu)}(t)D_k\delta_0, \mathrm{i}[P_x, F^{(\beta)}(H^{(\mu)})]U^{(\mu)}(t)\delta_0\rangle]\,, \tag{10.24}$$

$$\begin{aligned}\sum_{x\in\mathbb{Z}^d} x_l\, T_2(x) &= -\langle\langle \tau_t(D_k), \mathcal{X}_l(F^{(\beta)}(H^{(\mu)}))\rangle\rangle \\ &= -\langle\langle \mathcal{X}_l(F^{(\beta)}(H^{(\mu)}))^\star, \tau_t(D_k)^\star\rangle\rangle \\ &= -\langle\langle \mathcal{X}_l(F^{(\beta)}(H^{(\mu)})), \tau_t(D_k)\rangle\rangle\,. \end{aligned} \tag{10.25}$$

So overall, for any $k, l \in \{1, ..., d\}$ and $t \in \mathbb{R}$ the calculations (10.22) and (10.25) yield

$$\mathbb{E}[\varrho_-^{(\beta,\mu)}(\mathcal{X}_{l,-}(\tau_{t,-}^{(\mu)}(J_{k,-}(0))))] = \sum_{x\in\mathbb{Z}^d} x_l\, (T_1(x) + T_2(x)) = -2\,\langle\langle \mathcal{X}_l(F^{(\beta)}(H^{(\mu)})), \tau_t(D_k)\rangle\rangle\,. \tag{10.26}$$

Thus, the integrand in the Kubo-type formula (10.16) is identical to the integrand in the Kubo formula (9.18). But the latter is also the integrand in (9.25) due to Theorem 9.8. So indeed, the linear current (10.16) and the linear response current (9.25) are identical.

We are just left to prove (10.23). Since $\mathbb{E}[\|X_l g(H^{(\mu)})\delta_0\|^2] < \infty$ for all $l \in \{1, ..., d\}$ and all bounded measurable functions $g : \mathbb{R} \to \mathbb{C}$, due to (BGKS05)[Assumption 5.1] with $g = F^{(\beta)}$ in (10.23) we may decompose the commutator $[X_l, F^{(\beta)}(H^{(\mu)})]$. We obtain that it is sufficient to prove

$$\lim_{L\to\infty} \mathbb{E}\Big[\Big\langle\Big(X_l F^{(\beta)}(H^{(\mu)}) - \sum_{x\in\Lambda_L} x_l\, P_x F^{(\beta)}(H^{(\mu)})\Big)U^{(\mu)}(t)\delta_0, U^{(\mu)}(t)D_k\delta_0\Big\rangle\Big] = 0\,, \tag{10.27}$$

$$\lim_{L\to\infty} \mathbb{E}\Big[\Big\langle\Big(X_l - \sum_{x\in\Lambda_L} x_l\, P_x\Big)U^{(\mu)}(t)\delta_0, F^{(\beta)}(H^{(\mu)})U^{(\mu)}(t)D_k\delta_0\Big\rangle\Big] = 0\,. \tag{10.28}$$

Since for all $t \in \mathbb{R}$ and $\omega \in \Omega$ one has $U_\omega^{(\mu)}(t) = \mathrm{e}^{-\mathrm{i}tH_\omega^{(\mu)}}$, a repeated application of the Cauchy-Schwarz inequality, first to the scalar product in the expectation values in Equations (10.27) and (10.28), then to the expectation values themselves, yields that it is sufficient to prove

$$\lim_{L\to\infty} \mathbb{E}\Big[\Big\|\Big(X_l - \sum_{x\in\Lambda_L} x_l\, P_x\Big)g(H^{(\mu)})\psi\Big\|^2\Big] = 0 \tag{10.29}$$

for all $l \in \{1, ..., d\}$, all bounded measurable functions $g : \mathbb{R} \to \mathbb{C}$ with $\|g\|_\infty \le 1$ and all $\psi \in \mathfrak{h}_c$. Since $\mathbb{E}[\|X_l g(H^{(\mu)})\delta_0\|^2] < \infty$, we obtain $\mathbb{E}[\|(X_l - \sum_{x\in\Lambda_L} x_l\, P_x)g(H_\omega^{(\mu)})\psi\|^2] < \infty$. Using Parseval's equality, for all $L \in \mathbb{N}$, $l \in \{1, ..., d\}$ and almost every $\omega \in \Omega$ we obtain

$$\begin{aligned} 0 \le \Big\|\Big(X_l - \sum_{x\in\Lambda_L} x_l\, P_x\Big)g(H_\omega^{(\mu)})\psi\Big\|^2 &= \sum_{x\in\mathbb{Z}^d} |x_l(1 - 1_{\Lambda_L}(x))(g(H_\omega^{(\mu)})\psi)(x)|^2 = \sum_{x\in\Lambda_L^c} x_l^2\, |\langle\delta_x, g(H_\omega^{(\mu)})\psi\rangle|^2 \\ &\le \sum_{x\in\mathbb{Z}^d} x_l^2\, |\langle\delta_x, g(H_\omega^{(\mu)})\psi\rangle|^2 = \|X_l g(H_\omega^{(\mu)})\delta_0\|^2 < \infty \end{aligned}$$

In particular, this implies $\lim_{L\to\infty} \sum_{x\in\Lambda_L^c} x_l^2\, |\langle\delta_x, g(H_\omega^{(\mu)})\psi\rangle|^2 = 0$ for almost every $\omega \in \Omega$, all $l \in \{1, ..., d\}$ and all bounded measurable functions $g : \mathbb{R} \to \mathbb{C}$. Moreover, using Fubini's theorem we obtain

$$0 \le \mathbb{E}\Big[\sum_{x\in\Lambda_L^c} x_l^2\, |\langle\delta_x, g(H^{(\mu)})\psi\rangle|^2\Big] = \sum_{x\in\Lambda_L^c} x_l^2\, \mathbb{E}[|\langle\delta_x, g(H^{(\mu)})\psi\rangle|^2] < \sum_{x\in\mathbb{Z}^d} x_l^2\, \mathbb{E}[|\langle\delta_x, g(H^{(\mu)})\psi\rangle|^2] < \infty\,,$$

where in the last step (10.19) is used. An application of the dominated convergence theorem yields

$$\begin{aligned} \lim_{L\to\infty} \mathbb{E}\Big[\Big\|\Big(X_l - \sum_{x\in\Lambda_L} x_l\, P_x\Big)g(H^{(\mu)})\psi\Big\|^2\Big] &= \lim_{L\to\infty} \sum_{x\in\Lambda_L^c} x_l^2\, \mathbb{E}[|\langle\delta_x, g(H^{(\mu)})\psi\rangle|^2] \\ &= \mathbb{E}\Big[\lim_{L\to\infty} \sum_{x\in\Lambda_L^c} x_l^2\, |\langle\delta_x, g(H^{(\mu)})\psi\rangle|^2\Big] = 0 \end{aligned}$$

■

10.4. Remarks

From the considerations above, one might get the impression, that in view of a localisation criterion on Fock space, an interesting quantity to look at is the product of a creation operator $a_-^*(\delta_x)$ and a time evolved annihilation operator $a_-(\delta_y)$ at positions $x, y \in \mathbb{Z}^d$. One could expect, that the norm of this quantity decreases in the distance of $x, y \in \mathbb{Z}^d$. But in fact, it does not. At least, this does not hold for non-interacting electron gases, the most simple case. This it is shown in the following lemma.

Lemma 10.7

Consider the non-interacting electron gas as given by the model of Chapter 6. Then, for any realisation $\omega \in \Omega$, $t \in \mathbb{R}$ and $\phi, \psi \in \mathfrak{h}$ one has

$$\|a_-^*(\phi)\tau_{\omega,t,-}^{(\mu)}(a_-(\psi))\| = \|\phi\| \, \|\psi\| \,. \tag{10.30}$$

Proof: For $\phi = 0$ or $\psi = 0$ Equation (10.30) is trivially satisfied. So, we consider $\phi \neq 0 \neq \psi$. On the one hand, one has the estimate

$$\begin{aligned}
\|a_-^*(\phi)\tau_{\omega,t,-}^{(\mu)}(a_-(\psi))\| &\leq \|a_-^*(\phi)\| \, \|\tau_{\omega,t,-}^{(\mu)}(a_-(\psi))\| \\
&= \|a_-^*(\phi)\| \, \|a_-(\psi)\| \\
&= \|\phi\| \, \|\psi\| \,,
\end{aligned}$$

which holds for arbitrary $\omega \in \Omega$ and $t \in \mathbb{R}$. On the other hand, using $\tau_{\omega,t,-}^{(\mu)}(a_-(\psi)) = a_-(U_\omega^{(\mu)}(t)\psi)$ for non-interacting electron gases, one obtains the estimate

$$\begin{aligned}
\|a_-^*(\phi)\tau_{\omega,t,-}^{(\mu)}(a_-(\psi))\| &= \sup\{\langle \eta, a_-^*(\phi)\tau_{\omega,t,-}^{(\mu)}(a_-(\psi))\xi\rangle : \|\eta\| = \|\xi\| = 1\} \\
&= \sup\{\langle \eta, a_-^*(\phi)a_-(U_\omega^{(\mu)}(t)\psi)\xi\rangle : \|\eta\| = \|\xi\| = 1\} \\
&= \sup\{\langle a_-(\phi)\eta, a_-(U_\omega^{(\mu)}(t)\psi)\xi\rangle : \|\eta\| = \|\xi\| = 1\} \\
&\geq \frac{1}{\|\phi\| \, \|\psi\|} \langle a_-(\phi)\phi, a_-(U_\omega^{(\mu)}(t)\psi)U_\omega^{(\mu)}(t)\psi\rangle \\
&= \frac{1}{\|\phi\| \, \|\psi\|} \|U_\omega^{(\mu)}(t)\psi\|^2 \, \|\phi\|^2 \\
&= \|\phi\| \, \|\psi\| \,.
\end{aligned}$$

■

As a direct consequence of this lemma, for arbitrary times $t \in \mathbb{R}$ and points $x, y \in \mathbb{Z}^d$ one obtains that the equation

$$\mathbb{E}[\|a_-^*(\delta_x)\tau_{t,-}^{(\mu)}(a_-(\delta_y))\|] = \|\delta_x\| \, \|\delta_y\| = 1 \tag{10.31}$$

holds, illustrating that the quantity on the right hand side is not a candidate for a localisation criterion on Fock space. So, it is inevitable to at least consider an anti-commutator of a creation operator at position $y \in \mathbb{Z}^d$ with a time evolved annihilation operator at position $x \in \mathbb{Z}^d$. But only in the case of the strong and the weak localisation criterion, respectively, dealing with number operators one is naturally given an interpretation in terms of measurements, as it was presented in the discussion subsequent to Definition 10.1.

The strong localisation criterion is deeply related to the well-known Lieb-Robinson bounds in the analysis of quantum spin systems[2]. These estimates first appeared in the article (LR72)

[2] A nice overview on Lieb-Robinson bound is given in (NS10).

by the eponymous authors. Roughly speaking, considering quantum spin systems with finite range interaction the authors have shown exponential decay in the distance of the supports of two local operators. Such operators span the C^*-algebra $\mathfrak{A}$. We state the central result of (LR72), partially using our own notation.

Theorem 10.8

For each finite range interaction Φ there exists a finite group velocity v_Φ and a strictly positive increasing function g such that for all $v > v_\Phi$ and all strictly local $A, B \in \mathfrak{A}$

$$\lim_{\substack{|t|\to\infty,\\ |x|>v|t|}} \mathrm{e}^{g(v)|t|} \, \|[A, \tau_t(\varphi_x(B))]\| = 0 \,. \tag{10.32}$$

Here, the system is supposed to be deterministic. But of course, it is natural to ask for analogues to Theorem 10.8 for disordered Systems. This was considered in (NSS12) proving zero velocity Lieb-Robinson bounds. One could try to analyse systems that are explicitly dependent on time. Roughly speaking, in this situation, one has to replace the time translation automorphisms $\{\tau_t : t \in \mathbb{R}\}$ by the less accessible $\{\tau_{t,r}^{(E)} : t, r \in \mathbb{R}\}$. Recently, this was considered in (KGE13). Note that in the criteria mentioned above we considered zero velocity Lieb-Robinson bounds for a special type of operators, namely the particle number operators. In contrast to this the class of strictly local operators A and B considered in (LR72) is more general. In particular, the latter are particle number preserving. Therefore, they are not affected by the chemical potential $\mu \in \mathbb{R}$ in the strong localisation criterion, whereas there is some influence of the chemical potential $\mu \in \mathbb{R}$ in the weak localisation criterion, because the state $\varrho_-^{(\beta,\mu)}$ enters.

Outlook

"Siehst du, Momo", sagte er dann zum Beispiel, "es ist so: Manchmal hat man eine sehr lange Straße vor sich. Man denkt, die ist so schrecklich lang; das kann man niemals schaffen, denkt man." Er blickte eine Weile schweigend vor sich hin, dann fuhr er fort: "Und dann fängt man an, sich zu beeilen. Und man eilt sich immer mehr. Jedesmal, wenn man aufblickt, sieht man, daß es gar nicht weniger wird, was noch vor einem liegt. Und man strengt sich noch mehr an, man kriegt es mit der Angst, und zum Schluß ist man ganz außer Puste und kann nicht mehr. Und die Straße liegt immer noch vor einem. So darf man es nicht machen." Er dachte einige Zeit nach. Dann sprach er weiter: "Man darf nie an die ganze Straße auf einmal denken, verstehst du? Man muß nur an den nächsten Schritt denken, an den nächsten Atemzug, an den nächsten Besenstrich. Und immer wieder nur an den nächsten." Wieder hielt er inne und überlegte, ehe er hinzufügte: "Dann macht es Freude; das ist wichtig, dann macht man seine Sache gut. Und so soll es sein."

(Michael Ende)

We like to close this thesis with some comments and outlooks, trying to motivate future work on related topics. It is the hope of the author to have illustrated transparently the general procedures, starting from the formalism for the description of many-particle physics and ending up with a definition for the electrical conductivity of random ergodic media. In addition, concepts such as covariant states or the current density operator should have been established as the natural objects of interest, having a description of interacting quantum many-particle systems in view. Finally, the relation of the new, operator algebraic approach to the well-known approaches in (BGKS05, KM08, KLM07), as it was subject of the previous chapter, should have brought new insights to the formulas appearing in latter works. However, there are some natural questions to pose and some interesting gaps to close.

Since the underlying work only concentrates on the description of discrete quantum many-particle systems, a natural request is to transfer the operator algebraic approach to an analogous description of continuum quantum many-particle systems. Again, the situation should be that way, that at least for the special case of a non-interacting electron gas, the analysis can be carried out up to the point, where a Kubo formula for the linear response current is obtained. In addition, such a Kubo formula should be in agreement with the corresponding one in (BGKS05). Some of the necessary steps can be transferred very easily. For example, the Schrödinger operator on Fock space, as well as its unitary propagator and therefore the time evolution automorphisms are constructed in an analogous way for a continuum model of a non-interacting electron gas. Also a KMS state for a non-interacting continuum model can be obtained using completely the same methods that we presented in Chapter 7 for a non-interacting discrete model. Even the way this KMS state is determined by its two-point function equals the situation for the discrete model. But there are other concepts, which should be more difficult to transfer, such as the current density operator. For the discrete model, this is a bounded self-adjoint operator, only having a finite support. Defining an analogous observable for the case of a continuum electron gas, featuring the nice attributes of being bounded, self-adjoint and of having compact support, whatever the latter property means, is a non-trivial problem. To the author of this thesis it seems natural to try to achieve such a concept in terms of operator-valued distributions.

But already within the context of discrete systems, interesting problems arise. Clearly, one would be interested in having a more powerful machinery to construct KMS states. For example, it would be a great achievement to prove existence of KMS states in more general situations, such as for interacting systems in arbitrary space dimension and maybe with a more general type of interaction. The construction principle we present in the underlying thesis, just yields a proof of existence of such states, for interacting systems even with the restriction to one space dimension.

Other interesting topics, related to the previous one, are phase transitions and non-uniqueness of phases for random systems as well as the effects of these on the state of the system. More precisely, the states of all possible realisations of the random system should form a covariant state. Therefore, it seems desirable to have a general construction principle, which dictates how to choose the KMS state of a random system in each single realisation, such that considering all realisations as a whole one obtains a covariant KMS state, even if in some realisations one is faced with the problem of non-unique phases.

Having a linear response theory in view, one needs to have more explicit expressions for the state of an interacting electron gas. The pure knowledge of its existence does not seem to be sufficient. Also, one will need to find a replacement for the localisation criterion used in Section 9.4, or, more precisely, a generalisation of it, which has the necessary consequences to carry out linear response theory in the general case of an interacting electron gas. Definitely, to cover interacting electron gases, such a criterion must purely include Fock space quantities. In Chapter 10 we presented some approaches towards such a criterion. However, the Swiss Army Knife of localisation criteria is still not established.

Of course, all the problems presented above are of interest for continuum quantum models of electron gases in random media as well.

Dank

Fear is part of people's life. Some of them don't know how to face it, others, where I include myself, learn coexisting with it or face it, not as a negative thing, but like a autoprotection sensation.

(Ayrton Senna)

Eine Promotion, mag sie in ihren wesentlichen Punkten noch so sehr dem Geiste einer Person entsprungen sein, kann niemals unabhängig von der individuellen Vorgeschichte und des Umfeldes der Person sowie von der wissenschaftlichen Geschichte im Allgemeinen entstehen. Da die wissenschaftliche Geschichte bereits zu Beginn dieser Arbeit zu Genüge ins Blickfeld gerückt wurde, ist es mir an dieser Stelle eine kleine Selbstverständlichkeit und zugleich große Ehre, der Aufgabe nachzukommen, einmal all die Personen ins Blickfeld zu rücken, die das Zustandekommen dieser Arbeit, direkt oder indirekt, ermöglicht haben, und ihnen meinen Dank auszusprechen.

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Die Zeit einer Promotion ist immer mit einer Reihe von Höhen und Tiefen verbunden und mag den Betroffenen, öfter als ihm selbst lieb ist, an besagte Grenzen führen. Grenzen zu erfahren jedoch nicht zu überschreiten, bedarf es des privaten Rückhalts und der Ablenkung vom Berg der Probleme, der sich zuvor aufgebaut hat. Für diesen privaten Ausgleich von den Belastungen des Arbeitsalltags sorgte mein Freundeskreis, dessen Opfer meiner Launen sich der Bedeutsamkeit des Anteils, den sie an der vorliegenden Arbeit tragen, vielleicht nie im vollen Umfang bewusst waren. Mein Dank ist ihnen dafür umso sicherer.

A Particle Density

On a given day, a given circumstance, you think you have a limit. And you then go for this limit and you touch this limit, and you think: "Okay, this is the limit." As soon as you touch this limit, something happens and you suddenly can go a little bit further. With your mind power, your determination, your instinct, and the experience as well, you can fly very high.

(Ayrton Senna)

Finally, we remark, that there are other interesting quantities of interacting electron gases one might focus on. For example, a very simple but nevertheless interesting quantity is the electron density, which we will briefly focus on in this chapter. We consider an interacting electron gas in an ergodic solid state such as described in Chapters 6 and 7. We consider the particle number operator at position $x \in \mathbb{Z}^d$ as defined in Equation (B.76)

$$N_-(x) := N_-(\delta_x) = a_-^*(\delta_x) a_-(\delta_x) \, . \tag{A.1}$$

This operator measures the number of electrons at position $x \in \mathbb{Z}^d$. Analogously, given a finite subset $\Lambda \subset \mathbb{Z}^d$, the operator $N_-(\Lambda) := \sum_{x \in \mathbb{Z}^d} N_-(x)$ measures the number of electrons inside the volume Λ. Note that one has

$$\varphi_{a,-}(a_-^*(\phi)) = \Gamma_-(T(a)) a_-^*(\phi) \Gamma_-(T(a))^* = a_-^*(T(a)\phi)$$

for all $\phi \in \mathfrak{h}$. Since $T(a)\delta_x = \delta_{x+a}$ for all $x, a \in \mathbb{Z}^d$, this leads to the following transformation law for the particle number operator

$$\begin{aligned} \varphi_{a,-}(N_-(x)) &= \varphi_{a,-}(a_-^*(\delta_x) a_-(\delta_x)) = \varphi_{a,-}(a_-^*(\delta_x)) \varphi_{a,-}(a_-(\delta_x)) \\ &= a_-^*(T(a)\delta_x) a_-(T(a)\delta_x) = a_-^*(\delta_{x+a}) a_-(\delta_{x+a}) = N_-(x+a) \, . \end{aligned} \tag{A.2}$$

Definition A.1 (*Particle Number and Particle Density*)

Consider an extended electron gas in a covariant state $\rho_- : \Omega \to \mathrm{Sta}(\mathfrak{B}_-)$, $\omega \mapsto \rho_{\omega,-}$, such as introduced in Chapters 6 and 7. Then, for each realisation $\omega \in \Omega$ of the system the *particle number* $n_\omega(x)$ at any position $x \in \mathbb{Z}^d$ is defined as

$$n_\omega(x) := \rho_{\omega,-}(N_-(x)) \, . \tag{A.3}$$

In addition, in the situation above, we define the *particle density* of the covariant state ρ_- as the expectation value of the random variable $n(0) : \Omega \to \mathbb{R}$, $\omega \mapsto n_\omega(0)$

$$n := \mathbb{E}[n(0)] \, . \tag{A.4}$$

Because of the transformation law for covariant states in Equation (5.8) and the transformation law for the number operator in Equation (A.2), we get that for almost every $\omega \in \Omega$ and any $x, a \in \mathbb{Z}^d$ the particle number satisfies the following transformation law

$$\begin{aligned} n_{\phi_a(\omega)}(x+a) &= \rho_{\phi_a(\omega),-}(N_-(x+a)) \\ &= \rho_{\phi_a(\omega),-}(\varphi_{a,-}(N_-(x))) \\ &= \rho_{\omega,-}(N_-(x)) \\ &= n_\omega(x) . \end{aligned} \tag{A.5}$$

Note that by definition the particle density is a non-random constant. The following self-averaging property justifies the name particle density for this constant.

Theorem A.2

Consider an extended electron gas in a covariant state, such as in Definition A.1. In addition, for any $L \in \mathbb{N}$, let Λ_L be the set of vertices of $\mathbb{Z}^d$ in a closed cube of side length $2L+1$ that is centred at $0 \in \mathbb{Z}^d$. Then, for almost every $\omega \in \Omega$ the following formula holds

$$n = \lim_{L\to\infty} \frac{1}{|\Lambda_L|} \sum_{x\in\Lambda_L} n_\omega(x) . \tag{A.6}$$

Proof: We use the transformation law for the particle number given in Equation (A.5) and apply Birkhoff's theorem. From this we obtain, that for almost every $\omega \in \Omega$

$$\begin{aligned} n &= \mathbb{E}[n(0)] \\ &\overset{\text{a.s.}}{=} \lim_{L\to\infty} \frac{1}{|\Lambda_L|} \sum_{x\in\Lambda_L} n_{\phi_{-x}(\omega)}(0) \\ &= \lim_{L\to\infty} \frac{1}{|\Lambda_L|} \sum_{x\in\Lambda_L} n_\omega(x) . \end{aligned}$$

■

For the special case of a non-interacting electron gas, there is an interesting connection between particle density and the integrated density of states. Precisely, for a non-interacting electron gas, at any value of the chemical potential $\mu \in \mathbb{R}$, there is a unique covariant ground state $\varrho_-^{(\mu)}$, i.e. for any $\omega \in \Omega$ the state $\varrho_{\omega,-}^{(\mu)}$ is a $\tau_{\omega,-}^{(\mu)}$ ground state. This state is completely determined by its two-point function, which is $\varrho_{\omega,-}^{(\mu)}(a_-^*(\psi)a_-(\phi)) = \langle \phi, \chi_{]-\infty,0]}(H_\omega^{(\mu)})\psi\rangle$ for any $\omega \in \Omega$ and $\phi, \psi \in \mathfrak{h}$. This yields

$$\begin{aligned} n &= \mathbb{E}[n(0)] \\ &= \mathbb{E}[\varrho_-^{(\mu)}(N_-(0))] \\ &= \mathbb{E}[\varrho_-^{(\mu)}(a_-^*(\delta_0)a_-(\delta_0))] \\ &= \mathbb{E}\left[\langle \delta_0, \chi_{]-\infty,0]}(H^{(\mu)})\delta_0\rangle\right] \\ &= \mathbb{E}\left[\langle \delta_0, \chi_{]-\infty,\mu]}(H^{(0)})\delta_0\rangle\right] . \end{aligned} \tag{A.7}$$

The expression on the right hand side of Equation (A.7) is the well-known integrated density of states with chemical potential $\mu \in \mathbb{R}$. In this context, maybe it is more common to rename the chemical potential by Fermi energy.

B Many-Particle Formalism

Es kann niemals zwei oder mehrere äquivalente Elektronen im Atom geben, für welche in starken Feldern die Werte aller Quantenzahlen übereinstimmen.

(Wolfgang Pauli)

As it was motivated in Chapter 1, the conductivity tensor of a given solid state is a quantity that linearly relates the strength of an electric field outside the solid state to the current density of an electron gas inside of the latter. In order to define this quantity rigorously as well as in a physically sensible way, we have to use of the mathematical formalism setting the basement of the physics of many-particle systems, i.e. we consider electron gases as a particular kind of quantum mechanical many-particle system.

As postulated by physics, quantum many-particle systems correspond to Hilbert spaces in a certain way. The mathematical challenge is to specify these Hilbert spaces. Our answer to this request comes in two parts.

In a first step, in Section B.1 we consider a Hilbert space that corresponds to a single particle and that is naturally given. From this we construct Hilbert spaces that correspond to N-particle systems. These spaces are used to describe quantum systems of fixed particle number.

In a second step, we consider all N-particle spaces to define the so called Fock space in Section B.2. This space is used to describe a quantum system of arbitrary particle number.

Since, more restrictively, the systems one is typically interested in, either consist of identical fermions, which are particles of half-integer spin, or of identical bosons, which are particles of integer spin, by the rules of quantum statistics, they are described not only in terms of N-particle spaces or in Fock spaces but also in terms of certain subspaces, which are obtained by additional symmetry requirements and which we refer to as fermionic and bosonic subspaces, respectively. We develop the concept of fermionic and bosonic subspaces in parallel to the N-particle spaces and to Fock space as well.

As outlined before, the many-particle Hilbert spaces constructed in this chapter are built from just one Hilbert space, which is related to a single particle. So, it is self-evident to ask for a natural way to construct operators on the former spaces being given some operator on the latter. The answer to this is what in physics literature is referred to as second quantisation[1] of observables. We will achieve this constructions in parallel to the constructions of the Hilbert spaces.

In addition, on Fock spaces another type of operators, namely so called creation and annihilation operators, are of certain interest. Especially in the fermionic case, where these operators are bounded, they span a C^*-algebra known as Fermi algebra which is essential for the underlying work. Section B.2.4 focuses on that topic.

[1] We refer the readers who are interested in that topic to (BR97) or (RS72) for nice introductions and to (Ber66, Coo51, Seg56a, Seg56b) for more information.

B.1. Formalism for Fixed Number of Particles

B.1.1. N-Particle Spaces

We start with a separable Hilbert space $\mathfrak{h}$, that in terms of physics corresponds to a single particle such as one electron. In the generic case, we consider $\mathfrak{h} = \ell^2(\mathbb{Z}^d)$ for some $d \in \mathbb{N}$, but for the following this would be an unnecessary restriction. Moreover, we assume that the set $\mathcal{B} = \{\psi_n : n \in \mathcal{N}\}$ forms an orthonormal basis of $\mathfrak{h}$, where $\mathcal{N}$ is an at most countable set. For $N \in \mathbb{N}$ we define so called N-particle spaces are defined as

$$\mathfrak{F}_N(\mathfrak{h}) := \bigotimes_{r=1}^{N} \mathfrak{h} \,. \tag{B.1}$$

Moreover, for multi-indices $\mathbf{n} = (n_1, ..., n_N) \in \mathcal{N}^N$ we define

$$\psi_{\mathbf{n}} := \bigotimes_{r=1}^{N} \psi_{n_r} \,. \tag{B.2}$$

The set $\mathcal{B}_N := \{\psi_{\mathbf{n}} : \mathbf{n} \in \mathcal{N}^N\}$ then forms an orthonormal basis of $\mathfrak{F}_N(\mathfrak{h})$. The group $\mathcal{S}_N$ containing all permutations of the set $\{1, ..., N\}$ has a natural right action on $\mathcal{N}^N$ such that for $\pi \in \mathcal{S}_N$ the multiindex $\mathbf{n} \in \mathcal{N}^N$ is mapped to the multiindex $\mathbf{n}_\pi := (n_{\pi(1)}, ..., n_{\pi(N)})$. This induces a group $\mathcal{G}_N$ of unitary operators G_π. The latter are defined via linear extension of their action on vectors of $\mathcal{B}_N$ which is given by

$$G_\pi \psi_{\mathbf{n}} := \psi_{\mathbf{n}_\pi} \,. \tag{B.3}$$

Lemma B.1

G_π is independent of the choice of basis $\mathcal{B}_N$. The mapping $\mathcal{S}_N \to \mathscr{U}(\mathfrak{F}_N(\mathfrak{h}))$, $\pi \mapsto G_\pi$ forms a unitary representation of $\mathcal{S}_N$ on $\mathfrak{F}_N(\mathfrak{h})$.

Proof: Given any set of vectors $\phi_k \in \mathfrak{h}$ with $k \in \{1, ..., N\}$ we can construct the vectors $\phi := \bigotimes_{k=1}^N \phi_k$ and $\phi_\pi := \bigotimes_{k=1}^N \phi_{\pi(k)}$. Note that for any vector $\psi_{\mathbf{n}} \in \mathcal{B}_N$ we have $(\psi_{\mathbf{n}})_\pi = \psi_{\mathbf{n}_\pi} = G_\pi \psi_{\mathbf{n}}$. We get

$$\begin{aligned}\langle \phi, \psi_{\mathbf{n}} \rangle &= \Big\langle \bigotimes_{r=1}^{N} \phi_r, \bigotimes_{s=1}^{N} \psi_{n_s} \Big\rangle = \prod_{r=1}^{N} \langle \phi_r, \psi_{n_r} \rangle \\ &= \prod_{r=1}^{N} \langle \phi_{\pi(r)}, \psi_{n_{\pi(r)}} \rangle = \Big\langle \bigotimes_{r=1}^{N} \phi_{\pi(r)}, \bigotimes_{s=1}^{N} \psi_{n_{\pi(s)}} \Big\rangle = \langle \phi_\pi, \psi_{\mathbf{n}_\pi} \rangle \,.\end{aligned}$$

This result enables us calculate $G_\pi \phi$ using the fact that $\mathcal{B}_N$ is an orthonormal basis of $\mathfrak{F}_N(\mathfrak{h})$.

$$\begin{aligned}G_\pi \phi &= G_\pi \sum_{\mathbf{n} \in \mathcal{N}^N} \langle \phi, \psi_{\mathbf{n}} \rangle \psi_{\mathbf{n}} = \sum_{\mathbf{n} \in \mathcal{N}^N} \langle \phi, \psi_{\mathbf{n}} \rangle G_\pi \psi_{\mathbf{n}} \\ &= \sum_{\mathbf{n} \in \mathcal{N}^N} \langle \phi_\pi, \psi_{\mathbf{n}_\pi} \rangle \psi_{\mathbf{n}_\pi} = \sum_{\mathbf{n} \in \mathcal{N}^N} \langle \phi_\pi, \psi_{\mathbf{n}} \rangle \psi_{\mathbf{n}} = \phi_\pi\end{aligned}$$

Now let $\mathcal{B}' := \{\psi'_n : n \in \mathbb{N}\}$ be another orthonormal basis of $\mathfrak{h}$. Then, another orthonormal basis $\mathcal{B}'_N$ of $\mathfrak{F}_N(\mathfrak{h})$ and maps G'_π are induced. We have $G'_\pi \psi'_{\mathbf{n}} = \psi'_{\mathbf{n}_\pi} = (\psi'_{\mathbf{n}})_\pi = G_\pi \psi'_{\mathbf{n}}$ for any vector $\psi'_{\mathbf{n}} \in \mathcal{B}'_N$. Since G_π and G'_π are linear mappings on $\mathfrak{F}_N(\mathfrak{h})$ that are identical on the orthonormal basis $\mathcal{B}'_N$ of $\mathfrak{F}_N(\mathfrak{h})$, they are identical on the full Hilbert space $\mathfrak{F}_N(\mathfrak{h})$. This proves independence of G_π on the choice of basis $\mathcal{B}_N$.

Next let $\pi, \sigma \in \mathcal{S}_N$ be arbitrary. Because $G_\sigma G_\pi \psi_{\mathbf{n}} = G_{\sigma\pi} \psi_{\mathbf{n}}$ for arbitrary $\psi_{\mathbf{n}} \in \mathcal{B}_N$ the mapping $\mathcal{S}_N \to \mathscr{U}(\mathfrak{F}_N(\mathfrak{h}))$, $\pi \mapsto G_\pi$ forms a unitary representation of $\mathcal{S}_N$ on $\mathfrak{F}_N(\mathfrak{h})$. ∎

By $\mathfrak{G}_N$ we denote the algebra spanned by the group of operators $\mathcal{G}_N$. For any $G \in \mathfrak{G}_N$ we define the subspace

$$\mathfrak{F}_G(\mathfrak{h}) := G(\mathfrak{F}_N(\mathfrak{h})) . \tag{B.4}$$

Only if G has closed image $\mathfrak{F}_G(\mathfrak{h})$ is a Hilbert space. In particular, we have $\mathfrak{F}_{G_\pi}(\mathfrak{h}) = \mathfrak{F}_N(\mathfrak{h})$ for any $\pi \in \mathcal{S}_N$. There are two elements of special physical interest in $\mathfrak{G}_N$ that have closed image and are given by

$$S_{N,-} := \frac{1}{N!} \sum_{\pi\in\mathcal{S}_N} \operatorname{sgn}(\pi) G_\pi , \tag{B.5}$$

$$S_{N,+} := \frac{1}{N!} \sum_{\pi\in\mathcal{S}_N} G_\pi . \tag{B.6}$$

Lemma B.2 (*Fermionic and Bosonic Subspaces*)

The mappings $S_{N,-}$ and $S_{N,+}$ are orthogonal projections on subspaces of $\mathfrak{F}_N(\mathfrak{h})$. Moreover, the subspaces $\mathfrak{F}_{N,-}(\mathfrak{h}) := \mathfrak{F}_{S_{N,-}}(\mathfrak{h})$ and $\mathfrak{F}_{N,+}(\mathfrak{h}) := \mathfrak{F}_{S_{N,+}}(\mathfrak{h})$ of $\mathfrak{F}_N(\mathfrak{h})$ are Hilbert spaces.

Proof : First we prove the statement for $S_{N,-}$. We use the facts that $G_\sigma G_\pi = G_{\pi\sigma}$ and $G_\pi^* = G_\pi^{-1} = G_{\pi^{-1}}$ as well as $\operatorname{sgn}(\sigma)\operatorname{sgn}(\pi) = \operatorname{sgn}(\pi\sigma)$ and $\operatorname{sgn}(\pi) = \operatorname{sgn}(\pi^{-1})$, so

$$\begin{aligned} S_{N,-}^2 &= \Big(\frac{1}{N!} \sum_{\pi\in\mathcal{S}_N} \operatorname{sgn}(\pi) G_\pi\Big)^2 = \frac{1}{(N!)^2} \sum_{\sigma,\pi\in\mathcal{S}_N}^{N} \operatorname{sgn}(\sigma)\operatorname{sgn}(\pi) G_\sigma G_\pi \\ &= \frac{1}{(N!)^2} \sum_{\sigma,\pi\in\mathcal{S}_N}^{N} \operatorname{sgn}(\pi\sigma) G_{\pi\sigma} = \frac{1}{N!} \sum_{\pi\in\mathcal{S}_N}^{N} \operatorname{sgn}(\pi) G_\pi = S_{N,-} \end{aligned}$$

and

$$\begin{aligned} S_{N,-}^* &= \frac{1}{N!} \sum_{\pi\in\mathcal{S}_N} \operatorname{sgn}(\pi) G_\pi^* = \frac{1}{N!} \sum_{\pi\in\mathcal{S}_N} \operatorname{sgn}(\pi) G_{\pi^{-1}} \\ &= \frac{1}{N!} \sum_{\pi\in\mathcal{S}_N} \operatorname{sgn}(\pi^{-1}) G_{\pi^{-1}} = \frac{1}{N!} \sum_{\pi\in\mathcal{S}_N} \operatorname{sgn}(\pi) G_\pi = S_{N,-} . \end{aligned}$$

In the bosonic case we have analogously

$$\begin{aligned} S_{N,+}^2 &= \Big(\frac{1}{N!} \sum_{\pi\in\mathcal{S}_N} G_\pi\Big)^2 = \frac{1}{(N!)^2} \sum_{\sigma,\pi\in\mathcal{S}_N}^{N} G_\sigma G_\pi \\ &= \frac{1}{(N!)^2} \sum_{\sigma,\pi\in\mathcal{S}_N}^{N} G_{\pi\sigma} = \frac{1}{N!} \sum_{\pi\in\mathcal{S}_N}^{N} G_\pi = S_{N,+} . \end{aligned}$$

and

$$\begin{aligned} S_{N,+}^* &= \frac{1}{N!} \sum_{\pi\in\mathcal{S}_N} G_\pi^* = \frac{1}{N!} \sum_{\pi\in\mathcal{S}_N} G_{\pi^{-1}} \\ &= \frac{1}{N!} \sum_{\pi\in\mathcal{S}_N} G_\pi = S_{N,+} . \end{aligned}$$

$S_{N,-}$ an $S_{N,+}$ are orthogonal projections. This implies that their images $\mathfrak{F}_{N,-}(\mathfrak{h})$ and $\mathfrak{F}_{N,+}(\mathfrak{h})$ are closed subspaces of $\mathfrak{F}_N(\mathfrak{h})$, so they are Hilbert spaces. ■

Our next goal is to construct bases of these spaces. Because $\mathcal{B}_N$ is an orthonormal basis of $\mathfrak{F}_N(\mathfrak{h})$ the linear spans of the sets $S_{N,-}(\mathcal{B}_N)$ and $S_{N,+}(\mathcal{B}_N)$ are $\mathfrak{F}_{N,-}(\mathfrak{h})$ and $\mathfrak{F}_{N,+}(\mathfrak{h})$, respectively. But in general the elements of these sets neither have to be orthonormal nor they have to be linearly independent. We consider the scalar product of the projections of vectors $\psi_{\mathbf{m}}, \psi_{\mathbf{n}} \in \mathcal{B}_N$ onto $\mathfrak{F}_{N,-}(\mathfrak{h})$.

$$\begin{aligned}
\langle S_{N,-}\psi_{\mathbf{m}}, S_{N,-}\psi_{\mathbf{n}}\rangle &= \left\langle \frac{1}{N!}\sum_{\sigma\in\mathcal{S}_N} \mathrm{sgn}(\sigma) G_\sigma \psi_{\mathbf{m}}, \frac{1}{N!}\sum_{\pi\in\mathfrak{S}_N} \mathrm{sgn}(\pi) G_\pi \psi_{\mathbf{n}}\right\rangle \\
&= \frac{1}{(N!)^2}\sum_{\sigma,\pi\in\mathcal{S}_N} \mathrm{sgn}(\sigma)\mathrm{sgn}(\pi)\,\langle G_\sigma\psi_{\mathbf{m}}, G_\pi\psi_{\mathbf{n}}\rangle \\
&= \frac{1}{(N!)^2}\sum_{\sigma,\pi\in\mathcal{S}_N} \mathrm{sgn}(\sigma\pi)\langle \psi_{\mathbf{m}_\sigma}, \psi_{\mathbf{n}_\pi}\rangle \\
&= \frac{1}{(N!)^2}\sum_{\sigma,\pi\in\mathcal{S}_N} \mathrm{sgn}(\sigma\pi)\left\langle \bigotimes_{r=1}^{N} \psi_{m_{\sigma(r)}}, \bigotimes_{s=1}^{N} \psi_{n_{\pi(s)}}\right\rangle \\
&= \frac{1}{(N!)^2}\sum_{\sigma,\pi\in\mathcal{S}_N} \mathrm{sgn}(\sigma\pi) \prod_{r=1}^{N}\langle \psi_{m_{\sigma(r)}}, \psi_{n_{\pi(r)}}\rangle \\
&= \frac{1}{(N!)^2}\sum_{\sigma,\pi\in\mathcal{S}_N} \mathrm{sgn}(\pi\sigma^{-1}) \prod_{r=1}^{N}\langle \psi_{m_r}, \psi_{n_{\pi(\sigma^{-1}(r))}}\rangle \\
&= \frac{1}{N!}\sum_{\pi\in\mathcal{S}_N} \mathrm{sgn}(\pi) \prod_{r=1}^{N}\langle \psi_{m_r}, \psi_{n_{\pi(r)}}\rangle \\
&= \frac{1}{N!}\det(C(\mathbf{m},\mathbf{n})) \qquad \text{(B.7)}
\end{aligned}$$

To simplify notation we introduced the correlation matrix defined by $C(\mathbf{m},\mathbf{n})_{rs} := \langle\psi_{m_r}, \psi_{n_s}\rangle$. Moreover, for a better understanding of the scalar product we introduce the occupation number function m on $\mathcal{N}\times\mathcal{N}^N$ that counts the multiplicity of the value $k \in \mathcal{N}$ appearing as a component of the multiindex $\mathbf{n}$, i.e. $\mathrm{m}(k,\mathbf{n}) = |\{r : n_r = k\}|$. Using this function one can define equivalence classes on the set of multiindices of length N by $\mathbf{m} \sim \mathbf{n}$ if and only if $\mathrm{m}(k,\mathbf{m}) = \mathrm{m}(k,\mathbf{n})$ for all $k \in \mathcal{N}$. We write $[\mathbf{n}]$ for the equivalence class of $\mathbf{n}$. By definition of the equivalence relation there is a unique function $\tilde{\mathrm{m}}$ defined on $\mathcal{N} \times (\mathcal{N}^N/\sim)$ satisfying $\mathrm{m}(k,\mathbf{n}) = \tilde{\mathrm{m}}(k,[\mathbf{n}])$ for all $(k,\mathbf{n}) \in \mathcal{N}\times\mathcal{N}^N$. Note that for arbitrary $\pi \in \mathcal{S}_N$ we have $[\mathbf{n}_\pi] = [\mathbf{n}]$ and, moreover, $[\mathbf{n}] = \{\mathbf{n}_\pi | \, \pi \in \mathcal{S}_N\}$. From Equation (B.7) one can directly read off the following facts.

- If $[\mathbf{m}] \neq [\mathbf{n}]$ the scalar product on the left hand side is zero because for all permutations $\pi \in \mathcal{S}_N$ the product in the second last line includes factors that are zero.
- If $\mathrm{m}(k,\mathbf{m}) > 1$ or $\mathrm{m}(k,\mathbf{n}) > 1$ for some $k \in \mathcal{N}$ the scalar product on the left hand side is zero because $C(\mathbf{m},\mathbf{n})$ has at least two identical lines or rows, respectively. Thus, the determinant on the right hand side vanishes.
- If $\mathrm{m}(k,\mathbf{n}) \leq 1$ for all $k \in \mathcal{N}$ we have $\langle S_{N,-}\psi_{\mathbf{n}_\pi}, S_{N,-}\psi_{\mathbf{n}}\rangle = \frac{\mathrm{sgn}(\pi)}{N!}$ for any $\pi \in \mathcal{S}_N$.

From these facts we conclude that a basis of $\mathfrak{F}_{N,-}(\mathfrak{h})$ can be constructed by choosing one representative multiindex $\mathbf{n}$ in each equivalence class $[\mathbf{n}]$ that satisfies $\tilde{\mathrm{m}}(k,[\mathbf{n}]) \leq 1$ for all $k \in \mathcal{N}$. Then, the set of vectors $S_{N,-}\psi_{\mathbf{n}}$ corresponding to these multiindices is an orthogonal basis of $\mathfrak{F}_{N,-}(\mathfrak{h})$. Since by the third fact these vectors may depend by a factor (-1) on the choice of the representing multiindex, we fix the latter to be the unique one of increasingly ordered [2] components. There is a one to one correspondence between these multiindices and the finite subsets $\{\mathbf{n}\}$ of $\mathcal{N}$ of order N. The set of these subsets we denote by $\mathcal{P}_{N,-}(\mathcal{N})$. Using our choice of representative as well as the correspondence mentioned above we define

$$\psi_{\{\mathbf{n}\},-} := \sqrt{N!}\, S_{N,-}\psi_{\mathbf{n}} \,. \tag{B.8}$$

From the considerations above we get that $\mathcal{B}_{N,-} := \{\psi_{\{\mathbf{n}\},-} : \{\mathbf{n}\} \in \mathcal{P}_{N,-}(\mathcal{N})\}$ forms an orthonormal basis of $\mathfrak{F}_{N,-}(\mathfrak{h})$.

Now we turn to the bosonic case. Analogously to the fermionic case, we consider the scalar product of the projections of vectors $\psi_{\mathbf{m}}, \psi_{\mathbf{n}} \in \mathcal{B}_N$ onto $\mathfrak{F}_{N,+}(\mathfrak{h})$. To simplify notation we introduce a generalised Kronecker δ on $M \times M$, where M is some arbitrary set, by setting δ equal to one on the diagonal and zero otherwise.

$$\begin{aligned}
\langle S_{N,+}\psi_{\mathbf{m}}, S_{N,+}\psi_{\mathbf{n}}\rangle &= \left\langle \frac{1}{N!}\sum_{\sigma\in\mathcal{S}_N} G_\sigma\psi_{\mathbf{m}}, \frac{1}{N!}\sum_{\pi\in\mathcal{S}_N} G_\pi\psi_{\mathbf{n}}\right\rangle \\
&= \frac{1}{(N!)^2}\sum_{\sigma,\pi\in\mathcal{S}_N} \langle G_\sigma\psi_{\mathbf{m}}, G_\pi\psi_{\mathbf{n}}\rangle \\
&= \frac{1}{(N!)^2}\sum_{\sigma,\pi\in\mathcal{S}_N} \langle \psi_{\mathbf{m}_\sigma}, \psi_{\mathbf{n}_\pi}\rangle \\
&= \frac{1}{(N!)^2}\sum_{\sigma,\pi\in\mathcal{S}_N} \left\langle \bigotimes_{r=1}^{N}\psi_{m_{\sigma(r)}}, \bigotimes_{s=1}^{N}\psi_{n_{\pi(s)}}\right\rangle \\
&= \frac{1}{(N!)^2}\sum_{\sigma,\pi\in\mathcal{S}_N} \prod_{r=1}^{N}\langle \psi_{m_{\sigma(r)}}, \psi_{n_{\pi(r)}}\rangle \\
&= \frac{1}{(N!)^2}\sum_{\sigma,\pi\in\mathcal{S}_N} \prod_{r=1}^{N}\langle \psi_{m_r}, \psi_{n_{\pi(\sigma^{-1}(r))}}\rangle \\
&= \frac{1}{N!}\sum_{\pi\in\mathcal{S}_N} \prod_{r=1}^{N}\langle \psi_{m_r}, \psi_{n_{\pi(r)}}\rangle \\
&= \frac{1}{N!}\delta([\mathbf{m}],[\mathbf{n}])\prod_{k\in\mathcal{N}} \tilde{\mathrm{m}}(k,[\mathbf{n}])!
\end{aligned} \tag{B.9}$$

So the scalar product on the left hand side is completely determined by the equivalence classes of the multiindices $\mathbf{m}$ and $\mathbf{n}$ and it vanishes as $[\mathbf{m}] \neq [\mathbf{n}]$. Analogously to the fermionic case, in each equivalence class $[\mathbf{n}] \in (\mathcal{N}^N/\sim)$, we choose the representative $\mathbf{n}$ whose components are increasingly ordered and define

$$\psi_{[\mathbf{n}],+} := \sqrt{\frac{N!}{\prod_{k\in\mathbb{N}} \mathrm{m}(k,\mathbf{n})!}}\, S_{N,+}\psi_{\mathbf{n}} \,. \tag{B.10}$$

From the considerations above we get that $\mathcal{B}_{N,+} := \{\psi_{[\mathbf{n}],+} : [\mathbf{n}] \in (\mathcal{N}^N/\sim)\}$ forms an orthonormal basis of $\mathfrak{F}_{N,+}(\mathfrak{h})$.

[2] We assume that $\mathcal{N}$ is given with some natural counting that induces an ordering.

B.1.2. Operators on N-Particle Spaces

By constructing the N-particle spaces from a given one-particle space the request for natural constructions of operators on the former spaces given an operator on the latter space arises. We will challenge this request in the following by introducing two particular but natural constructions which at first sight do not seem related. But as it will turn out at the end of this section the two different constructions are connected. The first and more simple construction is the N-fold tensor product of a given operator on one-particle space. The second construction is lifting a given one-particle operator to N-particle space by multiplying it with unities and summation over all possible positions of the one-particle operator within the resulting product operators. Both constructions are natural in a way that they act symmetrically on each factor of N-particle spaces. As a consequence of this symmetry the restrictions of the resulting operators to G-subspaces can be seen as operators on the G-spaces in their own right.

First Construction

Given some densely defined operator A on $\mathfrak{h}$ with domain $D(A)$ for any $N \in \mathbb{N}$ and $k \in \{1, ..., N\}$ we construct densely defined operators $A_{N,k}$ with domains $D(A_{N,k}) = \mathfrak{h}\otimes...\otimes\mathfrak{h}\otimes D(A)\otimes\mathfrak{h}\otimes...\otimes\mathfrak{h}$, where $D(A)$ only appears in the k-th factor of the tensor product, and

$$A_{N,k} := \bigotimes_{l=1}^{N} A^{\delta_{k,l}} \tag{B.11}$$

with $A^0 :=$ id and $A^1 := A$. If A is a bounded operator, we have $\|A_{N,k}\| = \|A\|$ for any $N \in \mathbb{N}$ and $k \in \{1, ..., N\}$. The operators $A_{N,k}$ are closeable, if A is closeable, and their closures are self-adjoint, if A is self-adjoint (RS72). In these situations, by $A_{N,k}$ we automatically denote the closures. Finally, if A is a self-adjoint operator, for any bounded Borel function f on the real line we have

$$f(A_{N,k}) = f(A)_{N,k} \ . \tag{B.12}$$

Second Construction

For any $N \in \mathbb{N}$, taking the product over $k \in \{1, ..., N\}$ of the operators $A_{N,k}$ in Equation (B.11), we construct an operator $\Gamma_N(A)$ on $\mathfrak{F}_N(\mathfrak{h})$ with domain $D(\Gamma_N(A)) = \bigotimes_{k=1}^{N} D(A)$

$$\Gamma_N(A) := \prod_{k=1}^{N} A_{N,k} = \bigotimes_{k=1}^{N} A \ . \tag{B.13}$$

Again, if $\Gamma_N(A)$ is closeable, we automatically denote its closure by $\Gamma_N(A)$. If A is closeable or self-adjoint, then the same holds true for $\Gamma_N(A)$.

Lemma B.3 (*Symmetry*)

Let A be a densely defined operator on $\mathfrak{h}$ and $G \in \mathfrak{G}_N$. Then, $G(D(\Gamma_N(A))) \subseteq D(\Gamma_N(A))$. Moreover, G is a bounded operator on $D(\Gamma_N(A))$ with respect to the graph norm of $\Gamma_N(A)$, the space $G(D(\Gamma_N(A)))$ is a dense subspace of $\mathfrak{F}_G(\mathfrak{h})$ and for any $\phi \in D(\Gamma_N(A))$ we have

$$G\Gamma_N(A)\phi = \Gamma_N(A)G\phi \ . \tag{B.14}$$

Proof: First we prove that for arbitrary $G_\pi \in \mathcal{G}_N$ the operator $\Gamma_N(A)G_\pi$ is defined on $D(\Gamma_N(A))$ and is identical to $G_\pi\Gamma_N(A)$. Then, since the elements of $\mathcal{G}_N$ span the algebra $\mathfrak{G}_N$, by linearity of $\Gamma_N(A)$ the statement of the lemma follows. For $\phi_1, ..., \phi_N \in D(A)$ arbitrary let $\phi := \bigotimes_{r=1}^N \phi_r \in D(\Gamma_N(A))$ such that $G_\pi\phi = \bigotimes_{k=1}^N \phi_{\pi(k)} \in D(\Gamma_N(A))$. Since vectors of the type of ϕ span $D(\Gamma_N(A))$ and since $G_{\pi^{-1}}$ is the inverse of G_π, it follows that $G_\pi(D(\Gamma_N(A))) = D(\Gamma_N(A))$ so that $\Gamma_N(A)G_\pi$ and $G_\pi\Gamma_N(A)$ are both densely defined operators on $D(\Gamma_N(A))$. By linearity of these operators it is sufficient to show that they agree on vectors of type of ϕ.

$$\Gamma_N(A)G_\pi\phi = \Big(\bigotimes_{k=1}^N A\Big)\Big(\bigotimes_{r=1}^N \phi_{\pi(r)}\Big) = \bigotimes_{k=1}^N A\phi_{\pi(k)} = G_\pi\Gamma_N(A)\phi$$

Thus, for general $G \in \mathfrak{G}_N$ we have $G(D(\Gamma_N(A))) \subseteq D(\Gamma_N(A))$ and for any $\phi \in D(\Gamma_N(A))$ we obtain

$$\begin{aligned} ||G\phi||^2_{\Gamma_N(A)} &= ||G\phi||^2 + ||\Gamma_N(A)G\phi||^2 = ||G\phi||^2 + ||G\Gamma_N(A)\phi||^2 \\ &\leq ||G||^2\,(||\phi||^2 + ||\Gamma_N(A)\phi||^2) = ||G||^2\,||\phi||^2_{\Gamma_N(A)} . \end{aligned}$$

This proves that G is a bounded linear operator on $D(\Gamma_N(A))$ with respect to the graph norm of $\Gamma_N(A)$. Finally, for any $\psi \in \mathfrak{F}_G(\mathfrak{h})$ we can find a $\phi \in \mathfrak{F}_N(\mathfrak{h})$ such that $G\phi = \psi$. Then, since $D(\Gamma_N(A))$ is dense in $\mathfrak{F}_N(\mathfrak{h})$, we can choose a sequence $(\phi_n)_{n\in\mathbb{N}}$ in $D(\Gamma_N(A))$ that converges to ϕ and by boundedness of G we get for $(\psi_n)_{n\in\mathbb{N}} := (G\phi_n)_{n\in\mathbb{N}}$ which is a sequence in $G(D(\Gamma_N(A)))$ that it converges to ψ, because

$$||\psi - \psi_n|| = ||G\phi - G\phi_n|| = ||G(\phi - \phi_n)|| \leq |G||\,||\phi - \phi_n|| .$$

■

So if $G \in \mathfrak{G}_N$ has closed image, then $\mathfrak{F}_G(\mathfrak{h})$ is a Hilbert space and by Lemma B.3 the restriction

$$\Gamma_G(A) := \Gamma_N(A)|_{G(D(\Gamma_N(A)))} \tag{B.15}$$

is a densely defined operator on $\mathfrak{F}_G(\mathfrak{h})$ in its own right. To simplify notation we also define

$$\Gamma_{N,-}(A) := \Gamma_{S_{N,-}}(A) , \tag{B.16}$$

$$\Gamma_{N,+}(A) := \Gamma_{S_{N,+}}(A) . \tag{B.17}$$

If $\Gamma_G(A)$ is closeable, we also denote its closure by $\Gamma_G(A)$. Analogously, if $\Gamma_{N,-}(A)$ or $\Gamma_{N,+}(A)$ are closeable, we also use the notations $\Gamma_{N,-}(A)$ and $\Gamma_{N,+}(A)$ for the closures, respectively.

Lemma B.4 (*Products*)

Let A and B be two densely defined operators on $\mathfrak{h}$ such that AB is densely defined. Then, for any $G \in \mathfrak{G}_N$ and any $\phi \in D(\Gamma_G(AB))$ we have

$$\Gamma_G(AB)\phi = \Gamma_G(A)\Gamma_G(B)\phi . \tag{B.18}$$

Proof: For $\phi_1, ..., \phi_N \in D(AB)$ arbitrary we have that $\phi := \bigotimes_{r=1}^N \phi_r \in D(\Gamma_N(AB))$ and it follows that $\Gamma_N(B)\phi = \Big(\bigotimes_{k=1}^N B\Big)\Big(\bigotimes_{r=1}^N \phi_r\Big) = \bigotimes_{k=1}^N B\phi_k \in \bigotimes_{k=1}^N D(A) = D(\Gamma_N(A))$, such that

$$\begin{aligned} \Gamma_N(A)\Gamma_N(B)\phi &= \Big(\bigotimes_{k=1}^N A\Big)\Big(\bigotimes_{l=1}^N B\Big)\Big(\bigotimes_{r=1}^N \phi_r\Big) = \Big(\bigotimes_{k=1}^N A\Big)\Big(\bigotimes_{l=1}^N B\phi_l\Big) \\ &= \Big(\bigotimes_{k=1}^N AB\phi_k\Big) = \Big(\bigotimes_{k=1}^N AB\Big)\Big(\bigotimes_{r=1}^N \phi_r\Big) = \Gamma_N(AB)\phi . \end{aligned}$$

By linearity the above equality holds for all $\phi \in D(\Gamma_N(AB))$. Then, restriction to $\phi \in G(D(\Gamma_N(AB)))$ proves the statement of the lemma. ■

Lemma B.5 (*Adjoints*)

Let A be a densely defined operator on $\mathfrak{h}$ with densely defined adjoint. For any $G \in \mathfrak{G}_N$ we have $D(\Gamma_G(A^*)) \subseteq D(\Gamma_G(A)^*)$ and for all $\phi \in D(\Gamma_G(A^*))$

$$\Gamma_G(A)^*\phi = \Gamma_G(A^*)\phi \, . \tag{B.19}$$

Proof: For any $\phi_1, ..., \phi_N \in D(A^*)$ and any $\psi_1, ..., \psi_N \in D(A)$ we have $\phi := \bigotimes_{r=1}^N \phi_r \in D(\Gamma_N(A^*))$ and $\psi := \bigotimes_{s=1}^N \psi_s \in D(\Gamma_N(A))$. We obtain

$$\begin{aligned}
\langle \Gamma_N(A^*)\phi, \psi\rangle &= \Big\langle \Big(\bigotimes_{k=1}^N A^*\Big)\Big(\bigotimes_{r=1}^N \phi_r\Big), \bigotimes_{s=1}^N \psi_s \Big\rangle = \Big\langle \bigotimes_{k=1}^N A^*\phi_k, \bigotimes_{s=1}^N \psi_s \Big\rangle \\
&= \prod_{k=1}^N \langle A^*\phi_k, \psi_k\rangle = \prod_{k=1}^N \langle \phi_k, A\psi_k\rangle = \Big\langle \bigotimes_{r=1}^N \phi_r, \bigotimes_{l=1}^N A\psi_l \Big\rangle \\
&= \Big\langle \bigotimes_{r=1}^N \phi_r, \Big(\bigotimes_{l=1}^N A\Big)\Big(\bigotimes_{s=1}^N \psi_s\Big)\Big\rangle = \langle \phi, \Gamma_N(A)\psi\rangle \, .
\end{aligned}$$

By linearity the above equality holds for all $\phi \in D(\Gamma_N(A^*))$ and $\psi \in D(\Gamma_N(A))$. Then, restriction to $\phi \in D(\Gamma_G(A^*))$ and $\psi \in D(\Gamma_G(A))$ proves the statement of the lemma. ■

In the following we assume that $A \in \mathcal{B}(\mathfrak{h})$ is a bounded operator. Then, also $\Gamma_N(A)$ is a bounded operator with norm

$$\|\Gamma_N(A)\| = \Big\|\bigotimes_{k=1}^N A\Big\| = \prod_{k=1}^N \|A\| = \|A\|^N \, . \tag{B.20}$$

Moreover, from Lemma B.3 by boundedness of all operators involved we obtain that for any $A \in \mathscr{B}(\mathfrak{h})$ the operator $\Gamma_N(A)$ commutes with any $G \in \mathfrak{G}_N$, i.e. we have

$$[\Gamma_N(A), G] = 0 \, . \tag{B.21}$$

From this result we get that for any $G \in \mathfrak{G}_N$ with closed image the operator $\Gamma_G(A) = \Gamma_N(A)|_{\mathfrak{F}_G(\mathfrak{h})}$ is a bounded operator on the Hilbert space $\mathfrak{F}_G(\mathfrak{h})$. Because $\Gamma_G(A)$ is a restriction of $\Gamma_N(A)$, by Equation (B.20) we always have $\|\Gamma_G(A)\| \leq \|A\|^N$.

Lemma B.6 (*Homomorphism*)

For any $G \in \mathfrak{G}_N$ the map $\Gamma_G : \mathscr{B}(\mathfrak{h}) \to \mathscr{B}(\mathfrak{F}_G(\mathfrak{h}))$, $A \mapsto \Gamma_G(A)$ is a *-homomorphism of semigroups, i.e. for any $A, B \in \mathscr{B}(\mathfrak{h})$

$$\Gamma_G(AB) = \Gamma_G(A)\Gamma_G(B) \, , \tag{B.22}$$

$$\Gamma_G(A^*) = \Gamma_G(A)^* \, . \tag{B.23}$$

Moreover, the mappings $\Gamma_G : \mathscr{B}_{\text{inv}}(\mathfrak{h}) \to \mathscr{B}_{\text{inv}}(\mathfrak{F}_G(\mathfrak{h}))$ and $\Gamma_G : \mathscr{U}(\mathfrak{h}) \to \mathscr{U}(\mathfrak{F}_G(\mathfrak{h}))$ are *-homomorphisms of *-groups.

Proof: The first statement of Lemma B.6 directly follows from the Lemmas B.4 and B.5 by continuity of all operators. Now let $A \in \mathscr{B}_{\text{inv}}(\mathfrak{h})$ and $U \in \mathscr{U}(\mathfrak{h})$ be arbitrary. Because of $\Gamma_G(\text{id}_{\mathfrak{h}}) = \text{id}_{\mathfrak{F}_G}(\mathfrak{h})$, we have that $\Gamma_G(A^{-1}) = \Gamma_G(A)^{-1}$ which proves that Γ_G maps $\mathscr{B}_{\text{inv}}(\mathfrak{h})$ to $\mathscr{B}_{\text{inv}}(\mathfrak{F}_G(\mathfrak{h}))$. Finally, we have $\Gamma_G(U)^* = \Gamma_G(U^*) = \Gamma_G(U^{-1}) = \Gamma_G(U)^{-1}$ which proves that Γ_G maps $\mathscr{U}(\mathfrak{h})$ to $\mathscr{U}(\mathfrak{F}_G(\mathfrak{h}))$. ■

Third Construction

For any $N \in \mathbb{N}$, taking the sum over $k \in \{1, ..., N\}$ of the operators $A_{N,k}$ in Equation (B.11), we construct an operator $\mathrm{d}\Gamma_N(A)$ on $\mathfrak{F}_N(\mathfrak{h})$ with domain $D(\Gamma_N(A)) = \bigotimes_{k=1}^N D(A)$ by

$$\mathrm{d}\Gamma_N(A) := \sum_{k=1}^N A_{N,k} \, . \tag{B.24}$$

If $\mathrm{d}\Gamma_N(A)$ is closeable, we automatically denote the closures by $\mathrm{d}\Gamma_N(A)$. If A is closeable or self-adjoint, then the same holds true for $\mathrm{d}\Gamma_N(A)$.

Lemma B.7 (*Symmetry*)

Let A be a densely defined operator on $\mathfrak{h}$. Then, $G(D(\mathrm{d}\Gamma_N(A))) \subseteq D(\mathrm{d}\Gamma_N(A))$ for any $G \in \mathfrak{G}_N$ and $G(D(\mathrm{d}\Gamma_N(A)))$ is a dense subspace of $\mathfrak{F}_G(\mathfrak{h})$. Moreover, G is a bounded operator on $D(\mathrm{d}\Gamma_N(A))$ with respect to the graph norm of $\mathrm{d}\Gamma_N(A)$ and for any $\phi \in D(\mathrm{d}\Gamma_N(A))$ we have

$$G\mathrm{d}\Gamma_N(A)\phi = \mathrm{d}\Gamma_N(A)G\phi \, . \tag{B.25}$$

Proof: For $k \in \{1, ..., N\}$ and $\phi_1, ..., \phi_N \in D(A)$ arbitrary let $\phi := \bigotimes_{r=1}^N \phi_r \in D(\mathrm{d}\Gamma_N(A))$ such that $G_\pi\phi = \bigotimes_{k=1}^N \phi_{\pi(k)} \in D(\mathrm{d}\Gamma_N(A))$. Since linear combinations of vectors of the type of ϕ span $D(\mathrm{d}\Gamma_N(A))$ and since $G_{\pi^{-1}}$ is the inverse of G_π, it follows that $G_\pi(D(\mathrm{d}\Gamma_N(A))) = D(\mathrm{d}\Gamma_N(A))$, so that $\mathrm{d}\Gamma_N(A)G_\pi$ and $G_\pi\mathrm{d}\Gamma_N(A)$ are both densely defined operators on $D(\mathrm{d}\Gamma_N(A))$. By linearity of these operators it is sufficient to show that they agree on vectors of type of ϕ.

$$\begin{aligned} A_{N,k}G_\pi\phi &= \Big(\bigotimes_{l=1}^N A^{\delta_{kl}}\Big)\Big(\bigotimes_{r=1}^N \phi_{\pi(r)}\Big) = \bigotimes_{l=1}^N A^{\delta_{kl}}\phi_{\pi(l)} \\ &= \bigotimes_{l=1}^N A^{\delta_{\pi(k)\pi(l)}}\phi_{\pi(l)} = G_\pi A_{N,\pi(k)}\phi \, . \end{aligned}$$

Then, by linearity the equality holds for all $\phi \in D(\mathrm{d}\Gamma_N(A))$ and

$$\begin{aligned} \mathrm{d}\Gamma_N(A)G_\pi\phi &= \sum_{k=1}^N A_{N,k}G_\pi\phi = \sum_{k=1}^N G_\pi A_{N,\pi(k)}\phi \\ &= G_\pi \sum_{k=1}^N A_{N,\pi(k)}\phi = G_\pi \sum_{k=1}^N A_{N,k}\phi = G_\pi\mathrm{d}\Gamma_N(A)\phi \, . \end{aligned}$$

Once again by linearity we get $G(D(\mathrm{d}\Gamma_N(A))) \subset D(\mathrm{d}\Gamma_N(A))$ and Equation (B.25) for $G \in \mathfrak{G}_N$ arbitrary. Moreover, using this result for any $\phi \in D(\mathrm{d}\Gamma_N(A))$ we obtain

$$\begin{aligned} \|G\phi\|^2_{\mathrm{d}\Gamma_N(A)} &= \|G\phi\|^2 + \|\mathrm{d}\Gamma_N(A)G\phi\|^2 = \|G\phi\|^2 + \|G\mathrm{d}\Gamma_N(A)\phi\|^2 \\ &\leq \|G\|^2 \left(\|\phi\|^2 + \|\mathrm{d}\Gamma_N(A)\phi\|^2\right) = \|G\|^2 \, \|\phi\|^2_{\mathrm{d}\Gamma_N(A)} \end{aligned}$$

which shows that G is bounded with respect to the graph norm of $\mathrm{d}\Gamma_N(A)$. Then, since $D(\mathrm{d}\Gamma_N(A))$ is dense in $\mathfrak{F}_N(\mathfrak{h})$, we can choose a sequence $(\phi_n)_{n\in\mathbb{N}}$ in $D(\mathrm{d}\Gamma_N(A))$ that converges to ϕ and by boundedness of G we get for $(\psi_n)_{n\in\mathbb{N}} := (G\phi_n)_{n\in\mathbb{N}}$ which is a sequence in $G(D(\mathrm{d}\Gamma_N(A)))$ that converges to ψ, because

$$\|\psi - \psi_n\| = \|G\phi - G\phi_n\| = \|G(\phi - \phi_n)\| \leq |G\| \, \|\phi - \phi_n\| \, .$$

■

If $G \in \mathfrak{G}_N$ has closed image, $\mathfrak{F}_G(\mathfrak{h})$ is a Hilbert space and by the Lemma B.7 the restriction

$$\mathrm{d}\Gamma_G(A) := \mathrm{d}\Gamma_N(A)|_{G(D(\mathrm{d}\Gamma_N(A)))} \tag{B.26}$$

is a densely defined operator on $\mathfrak{F}_G(\mathfrak{h})$ in its own right. To simplify notation we define

$$\mathrm{d}\Gamma_{N,-}(A) := \mathrm{d}\Gamma_{S_{N,-}}(A)\,, \tag{B.27}$$
$$\mathrm{d}\Gamma_{N,+}(A) := \mathrm{d}\Gamma_{S_{N,+}}(A)\,. \tag{B.28}$$

If $\mathrm{d}\Gamma_G(A)$ is closeable, we automatically denote its closure by $\mathrm{d}\Gamma_G(A)$. If $\mathrm{d}\Gamma_{N,-}(A)$ or $\mathrm{d}\Gamma_{N,+}(A)$ are closeable, we also use the notations $\mathrm{d}\Gamma_{N,-}(A)$ and $\mathrm{d}\Gamma_{N,+}(A)$ for the closures, respectively.

Lemma B.8 (*Linearity*)

Let $G \in \mathfrak{G}_N$, $\lambda, \mu \in \mathbb{C}$ and A, B be densely defined operators, such that $\lambda A + \mu B$ is a densely defined operator. Then, for any $\phi \in D(\mathrm{d}\Gamma_G(A)) \cap D(\mathrm{d}\Gamma_G(B))$ we have

$$\mathrm{d}\Gamma_G(\lambda A + \mu B)\phi = \lambda \mathrm{d}\Gamma_G(A)\phi + \mu \mathrm{d}\Gamma_G(B)\phi\,. \tag{B.29}$$

Proof: Let ϕ be a vector of type $\phi = \bigotimes_{r=1}^N \phi_r$ with $\phi_r \in D(A)\cap D(B)$. Then, $\phi \in D(\mathrm{d}\Gamma_N(A))\cap D(\mathrm{d}\Gamma_N(B))$ as well as $\phi \in D((\lambda A + \mu B)_{N,k})$. Moreover, for any $k \in \{1, ..., N\}$ we have

$$\begin{aligned}
(\lambda A + \mu B)_{N,k}\phi &= \Big(\bigotimes_{l=1}^N (\lambda A + \mu B)^{\delta_{kl}}\Big)\Big(\bigotimes_{r=1}^N \phi_r\Big) = \bigotimes_{l=1}^N (\lambda A + \mu B)^{\delta_{kl}} \phi_l \\
&= \bigotimes_{l=1}^N (\lambda A)^{\delta_{kl}} \phi_l + \bigotimes_{l=1}^N (\mu B)^{\delta_{kl}} \phi_l = \lambda \bigotimes_{l=1}^N A^{\delta_{kl}} \phi_l + \mu \bigotimes_{l=1}^N B^{\delta_{kl}} \phi_l \\
&= \lambda \bigotimes_{l=1}^N A^{\delta_{kl}} \bigotimes_{r=1}^N \phi_r + \mu \bigotimes_{l=1}^N B^{\delta_{kl}} \bigotimes_{r=1}^N \phi_r = \lambda\, A_{N,k}\phi + \mu\, B_{N,k}\phi\,.
\end{aligned}$$

By summation over k and considering linear combinations of vectors of the type above we get the relation $\mathrm{d}\Gamma_N(\lambda A + \mu B)\phi = \lambda \mathrm{d}\Gamma_N(A)\phi + \mu \mathrm{d}\Gamma_G(B)\phi$ for any vector $\phi \in D(\mathrm{d}\Gamma_N(A)) \cap D(\mathrm{d}\Gamma_N(B))$. By restriction to vectors $D(\mathrm{d}\Gamma_G(A)) \cap D(\mathrm{d}\Gamma_G(B))$ we finally get the statement of the lemma. ■

Lemma B.9 (*Commutator*)

Let $G \in \mathfrak{G}_N$ and A, B be densely defined operators such that $[A, B]$ is a densely defined operator. Then, for any $\phi \in D(\mathrm{d}\Gamma_G(AB)) \cap D(\mathrm{d}\Gamma_G(BA))$ we have

$$[\mathrm{d}\Gamma_G(A), \mathrm{d}\Gamma_G(B)]\phi = \mathrm{d}\Gamma_G([A, B])\phi\,. \tag{B.30}$$

Proof: We consider a vector of type $\phi = \bigotimes_{r=1}^N \phi_r$ with $\phi_r \in D(AB) \cap D(BA)$. Then, it follows that $\phi \in D(\mathrm{d}\Gamma_N(AB)) \cap D(\mathrm{d}\Gamma_N(BA))$ as well as $\phi \in D(\mathrm{d}\Gamma_N([A, B]))$. Moreover, for any $k, l \in \{1, ..., N\}$ we have

$$\begin{aligned}
[A_{N,k}, B_{N,l}]\phi &= \Big(\bigotimes_{n=1}^N A^{\delta_{ij}}\Big)\Big(\bigotimes_{m=1}^N B^{\delta_{lm}}\Big)\Big(\bigotimes_{r=1}^N \phi_r\Big) - \Big(\bigotimes_{m=1}^N B^{\delta_{lm}}\Big)\Big(\bigotimes_{n=1}^N A^{\delta_{kn}}\Big)\Big(\bigotimes_{r=1}^N \phi_r\Big) \\
&= \bigotimes_{n=1}^N A^{\delta_{kn}} B^{\delta_{ln}} \phi_n - \bigotimes_{n=1}^N B^{\delta_{ln}} A^{\delta_{kn}} \phi_n = \delta_{kl} \bigotimes_{n=1}^N ([A, B])^{\delta_{kn}} \phi_n \\
&= \delta_{kl}\Big(\bigotimes_{n=1}^N ([A, B])^{\delta_{kn}}\Big)\Big(\bigotimes_{r=1}^N \phi_r\Big) = \delta_{kl}([A, B])_{N,k}\phi\,.
\end{aligned}$$

By summation over k and l, considering linear combinations of vectors of the type above and by bilinearity of the commutator $[\mathrm{d}\Gamma_N(B), \mathrm{d}\Gamma_N(A)]\phi = \mathrm{d}\Gamma_G([A, B])\phi$ for any vector $\phi \in D(\mathrm{d}\Gamma_N(AB))\cap D(\mathrm{d}\Gamma_N(BA))$. By restriction to vectors $D(\mathrm{d}\Gamma_G(AB)) \cap D(\mathrm{d}\Gamma_G(BA))$ we get the statement of the lemma. ■

Lemma B.10 (*Adjoints*)

Let A be a densely defined operator on $\mathfrak{h}$ with densely defined adjoint. Then, for any $G \in \mathfrak{G}_N$ and any $\phi \in D(\mathrm{d}\Gamma_G(A^*))$ we have $\phi \in D(\mathrm{d}\Gamma_G(A)^*)$ and

$$\mathrm{d}\Gamma_G(A^*)\phi = \mathrm{d}\Gamma_G(A)^*\phi \; . \tag{B.31}$$

Proof : We consider a vector of type $\phi = \bigotimes_{r=1}^N \phi_r$ and $\psi = \bigotimes_{s=1}^N \psi_s$ with $\phi_r \in D(A^*)$ and $\psi_s \in D(A)$ for all $r, s \in \{1, ..., N\}$. Then, it follows that $\phi \in D(\mathrm{d}\Gamma_N(A^*))$ and $\psi \in D(\mathrm{d}\Gamma_N(A))$ and for all $k \in \{1, ..., N\}$

$$\begin{aligned}
\langle A^*_{N,k}\phi, \psi\rangle &= \Big\langle \Big(\bigotimes_{l=1}^N (A^*)^{\delta_{kl}}\Big)\Big(\bigotimes_{r=1}^N \phi_r\Big), \bigotimes_{s=1}^N \psi_s \Big\rangle = \Big\langle \bigotimes_{l=1}^N (A^*)^{\delta_{kl}}\phi_l, \bigotimes_{s=1}^N \psi_s\Big\rangle \\
&= \prod_{l=1}^N \langle (A^*)^{\delta_{kl}}\phi_l, \psi_l\rangle = \prod_{l=1}^N \langle \phi_l, A^{\delta_{kl}}\psi_l\rangle = \Big\langle \bigotimes_{r=1}^N \phi_r, \bigotimes_{l=1}^N A^{\delta_{kl}}\psi_l\Big\rangle \\
&= \Big\langle \bigotimes_{r=1}^N \phi_r, \Big(\bigotimes_{l=1}^N A^{\delta_{kl}}\Big)\Big(\bigotimes_{s=1}^N \psi_s\Big)\Big\rangle = \langle \phi, A_{N,k}\psi\rangle \; .
\end{aligned}$$

By summation over k, considering linear combinations of vectors of the type above and by sesquilinearity of the scalar product we get $\langle \mathrm{d}\Gamma_N(A^*)\phi, \psi\rangle = \langle \phi, \mathrm{d}\Gamma_N(A)\psi\rangle$ for any vector $\phi \in D(\mathrm{d}\Gamma_N(A^*))$ and therefore $\psi \in D(\mathrm{d}\Gamma_N(A)^*)$. By restriction to vectors $\phi \in D(\mathrm{d}\Gamma_G(A^*))$ and $\psi \in D(\mathrm{d}\Gamma_G(A))$ we get the statement of the lemma. ■

If we assume that A is a closed operator on $\mathfrak{h}$, we have that $\mathrm{d}\Gamma_N(A)$ is closed. In addition, the restrictions of $S_{N,-}$ and $S_{N,+}$ to $D(\mathrm{d}\Gamma_N(A))$ equipped with the scalar product induced by the graph norm of $\mathrm{d}\Gamma_N(A)$ are orthogonal projections, so they have a closed image. Because closed subsets of complete spaces are complete, $\mathrm{d}\Gamma_{N,-}(A)$ and $\mathrm{d}\Gamma_{N,+}(A)$ are closed. Similarly, one can show that, if A is a self-adjoint operator on $\mathfrak{h}$, also the operators $\mathrm{d}\Gamma_{N,+}(A)$ and $\mathrm{d}\Gamma_{N,-}(A)$ are self-adjoint (RS72, Coo51).

For any bounded operator $A \in \mathscr{B}(\mathfrak{h})$ we have $\mathrm{d}\Gamma_N(A) \in \mathscr{B}(\mathfrak{F}_N(\mathfrak{h}))$, since $\|A_{N,k}\| = \|A\|$ for any $k \in \{1, ..., N\}$. We obtain $\|\mathrm{d}\Gamma_N(A)\| = \left\|\sum_{k=1}^N A_{N,k}\right\| \leq \sum_{k=1}^N \|A_{N,k}\| = N\,\|A\|$ and, in addition, for any $G \in \mathfrak{G}_N$ we have $[\mathrm{d}\Gamma_N(A), G] = 0$ as an immediate consequence of Lemma B.7.

Because $\mathrm{d}\Gamma_G(A)$ is a restriction of $\mathrm{d}\Gamma_N(A)$, we always have $\|\mathrm{d}\Gamma_G(A)\| \leq N\|A\|$. So, considering bounded operators, we get a mapping $\mathrm{d}\Gamma_G : \mathscr{B}(\mathfrak{h}) \mapsto \mathscr{B}(\mathfrak{F}_G(\mathfrak{h}))$. The properties of $\mathrm{d}\Gamma_G$ follow directly from Lemmas B.8, B.9 and B.10, respectively, by continuity of all operators involved. They are summed up in the following lemma.

Lemma B.11 (*Homomorphism*)

For any $G \in \mathfrak{G}_N$ the map $\mathrm{d}\Gamma_G : \mathscr{B}(\mathfrak{h}) \mapsto \mathscr{B}(\mathfrak{F}_G(\mathfrak{h}))$, $A \mapsto \mathrm{d}\Gamma_G(A)$ is a *- homomorphism of Lie algebras, i.e. for any $A, B \in \mathscr{B}(\mathfrak{h})$ and any $\lambda, \mu \in \mathbb{C}$

$$\mathrm{d}\Gamma_G(\lambda A + \mu B) = \lambda \mathrm{d}\Gamma_G(A) + \mu \mathrm{d}\Gamma_G(B) \; , \tag{B.32}$$

$$\mathrm{d}\Gamma_G([A, B]) = [\mathrm{d}\Gamma_G(A), \mathrm{d}\Gamma_G(B)] \; , \tag{B.33}$$

$$\mathrm{d}\Gamma_G(A^*) = \mathrm{d}\Gamma_G(A)^* \; . \tag{B.34}$$

B.2. Formalism for Arbitrary Number of Particles

B.2.1. Fock Space

According to our constructions in Section B.1 for any one-particle space $\mathfrak{h}$ we define the vacuum space as $\mathfrak{F}_0(\mathfrak{h}) := \mathbb{C}$ equipped with the usual scalar product. Moreover, we define $\mathcal{G}_0$ as the set just including the identity on $\mathbb{C}$ and $\mathfrak{G}_0$ as the algebra spanned by $\mathcal{G}_0$. Finally, for any densely defined operator A on $\mathfrak{h}$ and any $G \in \mathfrak{G}_0$ we define the operators on $\mathfrak{F}_G(\mathfrak{h}) := \mathfrak{F}_0(\mathfrak{h})$ by $\Gamma_G(A) \equiv \Gamma_0(A) := 1$ and $\mathrm{d}\Gamma_G(A) := \mathrm{d}\Gamma_0(A) := 0$. All these definitions are made in view of the notation introduced in Section B.1. Now we can define the Fock space over $\mathfrak{h}$

$$\mathfrak{F}(\mathfrak{h}) := \bigoplus_{N\in\mathbb{N}_0} \mathfrak{F}_N(\mathfrak{h}) \tag{B.35}$$

that consists of sequences $\phi = (\phi_N)_{N\in\mathbb{N}_0}$, where $\phi_N \in \mathfrak{F}_N(\mathfrak{h})$ for all $N \in \mathbb{N}_0$, such that the norm $\|\phi\|^2 := \sum_{N\in\mathbb{N}_0} \|\phi_N\|^2 < \infty$. Then, the Fock space becomes a Hilbert space for which the set $\mathcal{B} := \bigcup_{N\in\mathbb{N}_0} \mathcal{B}_N$ forms an orthonormal basis, where $\mathcal{B}_0 := \{1\}$. The algebra $\mathfrak{G} := \bigoplus_{N\in\mathbb{N}_0} \mathfrak{G}_N$ of operators on $\mathfrak{F}(\mathfrak{h})$ with finite norm has two special elements, namely

$$S_- := \bigoplus_{N\in\mathbb{N}_0} S_{N,-} \,, \tag{B.36}$$

$$S_+ := \bigoplus_{N\in\mathbb{N}_0} S_{N,+} \,, \tag{B.37}$$

which are orthogonal projections. We define subspaces for general $G = \bigoplus_{N\in\mathbb{N}_0} G_N \in \mathfrak{G}$ via

$$\mathfrak{F}_G(\mathfrak{h}) := G(\mathfrak{F}(\mathfrak{h})) = \bigoplus_{N\in\mathbb{N}_0} G_N(\mathfrak{F}_N(\mathfrak{h})) = \bigoplus_{N\in\mathbb{N}_0} \mathfrak{F}_{G_N}(\mathfrak{h}) \,. \tag{B.38}$$

The anti-symmetric and symmetric Fock spaces are given as the images of $\mathfrak{F}(\mathfrak{h})$ with respect to the projections S_- and S_+, respectively, i.e.

$$\mathfrak{F}_-(\mathfrak{h}) := S_-(\mathfrak{F}(\mathfrak{h})) = \bigoplus_{N\in\mathbb{N}_0} S_{N,-}(\mathfrak{F}_N(\mathfrak{h})) = \bigoplus_{N\in\mathbb{N}_0} \mathfrak{F}_{N,-}(\mathfrak{h}) = \mathfrak{F}_{S_-}(\mathfrak{h}) \,, \tag{B.39}$$

$$\mathfrak{F}_+(\mathfrak{h}) := S_+(\mathfrak{F}(\mathfrak{h})) = \bigoplus_{N\in\mathbb{N}_0} S_{N,+}(\mathfrak{F}_N(\mathfrak{h})) = \bigoplus_{N\in\mathbb{N}_0} \mathfrak{F}_{N,+}(\mathfrak{h}) = \mathfrak{F}_{S_+}(\mathfrak{h}) \,, \tag{B.40}$$

where $S_{0,-} = S_{0,+} = 1$. Clearly, $\mathcal{B}_- := \bigcup_{N\in N_0} \mathcal{B}_{N,-}$ is an orthonormal basis of the anti-symmetric Fock space and $\mathcal{B}_+ := \bigcup_{N\in\mathbb{N}_0} \mathcal{B}_{N,+}$ is a basis of the bosonic Fock space, where $\mathcal{B}_{0,-} = \mathcal{B}_{0,+} = \{1\}$. Next, we turn to the analogous constructions of operators to those presented in Section B.1.2.

B.2.2. Operators on Fock Space I

Second Quantisation of Unitaries

For any densely defined operator A on Hilbert space $\mathfrak{h}$ with domain $D(A)$ we construct a densely defined operator on $\mathfrak{F}(\mathfrak{h})$ by

$$\Gamma(A) := \bigoplus_{N\in\mathbb{N}_0} \Gamma_N(A) \,. \tag{B.41}$$

If $\Gamma(A)$ is closeable, we denote its closure by $\Gamma(A)$. If A is closeable, then so is $\Gamma(A)$ (RS72, Coo51). The following lemmas are immediate consequences of the direct sum structure of $\Gamma(A)$ and the analogous statements for the components $\Gamma_N(A)$.

Lemma B.12 (*Symmetry*)

Let $\mathfrak{h}$ be a densely defined operator on $\mathfrak{h}$. For any $G \in \mathfrak{G}$ we have $G(D(\Gamma(A))) \subseteq D(\Gamma(A))$. Moreover, $G(D(\Gamma(A)))$ is a dense subspace of $\mathfrak{F}_G(\mathfrak{h})$ and for any $\phi \in D(\Gamma(A))$ we have

$$G\Gamma(A)\phi = \Gamma(A)G\phi \ . \tag{B.42}$$

Due to lemma B.12 given any $G = \bigoplus_{N\in\mathbb{N}_0} G_N \in \mathfrak{G}$ we can restrict $\Gamma(A)$ and define the operator

$$\Gamma_G(A) := \bigoplus_{N\in\mathbb{N}_0} \Gamma_{G_N}(A) \ , \tag{B.43}$$

which is a densely defined operator on $\mathfrak{F}_G$ in its own right. In particular, if $G = S_-$ or $G = S_+$, we write

$$\Gamma_-(A) := \bigoplus_{N\in\mathbb{N}_0} \Gamma_{N,-}(A) = \Gamma_{S_-}(A) \ , \tag{B.44}$$

$$\Gamma_+(A) := \bigoplus_{N\in\mathbb{N}_0} \Gamma_{N,+}(A) = \Gamma_{S_+}(A) \ . \tag{B.45}$$

If $\Gamma_G(A)$ is closeable, automatically $\Gamma_G(A)$ denotes the closure. If $\Gamma_-(A)$ or $\Gamma_+(A)$ are closeable, automatically $\Gamma_-(A)$ and $\Gamma_+(A)$ denote the closures, respectively.

Lemma B.13 (*Products*)

Let A and B be densely defined operators on $\mathfrak{h}$ such that also AB is densely defined. Then, for any $G \in \mathfrak{G}$ and any $\phi \in D(\Gamma_G(AB))$ we have

$$\Gamma_G(AB)\phi = \Gamma_G(A)\Gamma_G(B)\phi \ . \tag{B.46}$$

Lemma B.14 (*Adjoints*)

Let A be a densely defined operator with densely defined adjoint. For any $G \in \mathfrak{G}$ we have $D(\Gamma_G(A^*)) \subseteq \mathrm{D}(\Gamma_G(A)^*)$ and for all $\phi \in D(\Gamma_G(A^*))$

$$\Gamma_G(A^*)\phi = \Gamma_G(A)^*\phi \ . \tag{B.47}$$

In the following we consider bounded operators on A with $\|A\| \leq 1$. Thus, for any $N \in \mathbb{N}_0$ the operator $\Gamma_N(A)$ is bounded by $\|\Gamma_N(A)\| = \|A\|^N \leq 1$ so that $\Gamma_G(A)$ exists as a bounded operator for any $G \in \mathfrak{G}$ and $\|\Gamma_G(A)\| \leq 1$. For any $A \in B_1(\mathscr{B}(\mathfrak{h}))$ and any bounded $G \in \mathfrak{G}$ we have

$$[\Gamma(A), G] = 0 \ . \tag{B.48}$$

Lemma B.15 (*Homomorphism*)

For any $G \in \mathfrak{G}$ the map $\Gamma_G : B_1(\mathscr{B}(\mathfrak{h})) \to B_1(\mathscr{B}(\mathfrak{F}_G(\mathfrak{h}))),\ A \mapsto \Gamma_G(A)$ is a *-homomorphism of semigroups, i.e. for any $A, B \in B_1(\mathscr{B}(\mathfrak{h}))$

$$\Gamma_G(AB) = \Gamma_G(A)\Gamma_G(B) \ , \tag{B.49}$$

$$\Gamma_G(A^*) = \Gamma_G(A)^* \ . \tag{B.50}$$

Moreover, the map $\Gamma_G : \mathscr{U}(\mathfrak{h}) \to \mathscr{U}(\mathfrak{F}_G(h)),\ U \mapsto \Gamma_G(U)$ is a *- homomorphism of groups.

Second Quantisation of Observables

For any densely defined operator A on Hilbert space $\mathfrak{h}$ with domain $D(A)$ we construct a densely defined operator on $\mathfrak{F}(\mathfrak{h})$ by

$$\mathrm{d}\Gamma(A) := \bigoplus_{N\in\mathbb{N}_0} \mathrm{d}\Gamma_N(A) \,. \tag{B.51}$$

If $\mathrm{d}\Gamma(A)$ is closeable, we denote its closure by $\mathrm{d}\Gamma(A)$. If A is closeable, then so is $\mathrm{d}\Gamma(A)$ (RS72, Coo51). The following lemmas are immediate consequences of the direct sum structure of $\mathrm{d}\Gamma(A)$ and the analogous statements for the components $\mathrm{d}\Gamma_N(A)$.

Lemma B.16 (*Symmetry*)

Let A be a densely defined operator. Then, for any $G \in \mathfrak{G}$ we have $G(D(\mathrm{d}\Gamma(A))) \subseteq D(\mathrm{d}\Gamma(A))$ and $G(D(\mathrm{d}\Gamma_N(A)))$ is a dense subspace of $\mathfrak{F}_G(\mathfrak{h})$. Moreover, G is a bounded operator with respect to the graph norm of $\mathrm{d}\Gamma(A)$ and for any $\phi \in D(\mathrm{d}\Gamma(A))$ we have

$$G\mathrm{d}\Gamma(A)\phi = \mathrm{d}\Gamma(A)G\phi \,. \tag{B.52}$$

So if $G \in \mathfrak{G}$ has closed image, $\mathfrak{F}_G(\mathfrak{h})$ is a Hilbert space and by the Lemma B.16 the restriction

$$\mathrm{d}\Gamma_G(A) := \mathrm{d}\Gamma(A)|_{G(D(\mathrm{d}\Gamma(A)))} \tag{B.53}$$

is a densely defined operator on $\mathfrak{F}_G(\mathfrak{h})$ in its own right. In order to simplify notation we define

$$\mathrm{d}\Gamma_-(A) := \bigoplus_{N\in\mathbb{N}_0} \mathrm{d}\Gamma_{N,-}(A) = \mathrm{d}\Gamma_{S_-}(A) \,, \tag{B.54}$$

$$\mathrm{d}\Gamma_+(A) := \bigoplus_{N\in\mathbb{N}_0} \mathrm{d}\Gamma_{N,+}(A) = \mathrm{d}\Gamma_{S_+}(A) \,. \tag{B.55}$$

If $\mathrm{d}\Gamma_G(A)$ is closeable, we automatically denote its closure by $\mathrm{d}\Gamma_G(A)$. If $\mathrm{d}\Gamma_-(A)$ or $\mathrm{d}\Gamma_+(A)$ are closeable, we also use the notations $\mathrm{d}\Gamma_-(A)$ and $\mathrm{d}\Gamma_+(A)$ for the closures, respectively.

Lemma B.17 (*Linearity*)

Let $G \in \mathfrak{G}$, $\lambda, \mu \in \mathbb{C}$ and A, B be a densely defined operator such that $\lambda A + \mu B$ is a densely defined operator. Then, for any $\phi \in D(\mathrm{d}\Gamma_G(A)) \cap D(\mathrm{d}\Gamma_G(B))$ we have

$$\mathrm{d}\Gamma_G(\lambda A + \mu B)\phi = \lambda \mathrm{d}\Gamma_G(A)\phi + \mu \mathrm{d}\Gamma_G(B)\phi \,. \tag{B.56}$$

Lemma B.18 (*Commutator*)

Let $G \in \mathfrak{G}$ and A, B be densely defined operators such that $[A, B]$ is a densely defined operator. Then, for any $\phi \in D(\mathrm{d}\Gamma_G(AB)) \cap D(\mathrm{d}\Gamma_G(BA))$ we have

$$[\mathrm{d}\Gamma_G(A), \mathrm{d}\Gamma_G(B)]\phi = \mathrm{d}\Gamma_G([A, B])\phi \,. \tag{B.57}$$

Lemma B.19 (*Adjoints*)

Let A be a densely defined operator on $\mathfrak{h}$ with densely defined adjoint. Then, for any $G \in \mathfrak{G}$ and $\phi \in D(\mathrm{d}\Gamma_G(A^*))$ we have $\phi \in D(\mathrm{d}\Gamma_G(A)^*)$ and

$$\mathrm{d}\Gamma_G(A^*)\phi = \mathrm{d}\Gamma_G(A)^*\phi \,. \tag{B.58}$$

If A is closeable, then so is $\mathrm{d}\Gamma(A)$. Since S_- and S_+ are orthogonal projections on $D(\mathrm{d}\Gamma(A))$ equipped with the scalar product induced by the graph norm with respect to $\mathrm{d}\Gamma(A)$, they have closed image, thus one obtains that $\mathrm{d}\Gamma_-(A)$ and $\mathrm{d}\Gamma_+(A)$ are closeable operators, respectively. Analogously, if A is a self-adjoint operator on $\mathfrak{h}$, one has that $\mathrm{d}\Gamma_-(A)$ and $\mathrm{d}\Gamma_+(A)$ are self-adjoint operators.
Note that there is no direct analogue of Lemma B.11 on Fock space such as Lemma B.15 is a direct consequence of Lemma B.6, because of the fact that in general, if A is any non-vanishing operator, $\mathrm{d}\Gamma(A)$ is an unbounded operator (Coo51). Nevertheless, for finite rank operators A the operator $\mathrm{d}\Gamma_-(A)$ is bounded.

B.2.3. Relation of the Constructions

We now want to relate the constructions in the following way. Roughly speaking, for arbitrary $G \in \mathfrak{G}_N$ or $G \in \mathfrak{G}$ the operations Γ_G and $\mathrm{d}\Gamma_G$ mapping operators on $\mathfrak{h}$ to those on $\mathfrak{F}_G(\mathfrak{h})$ are related to each other via differentiation, i.e. if A is the infinitesimal generator of a strongly continuous unitary group $\{U(t) : t \in \mathbb{R}\}$, then $\mathrm{d}\Gamma_G(A)$ is the infinitesimal generator of the strongly continuous unitary group $\{\Gamma_G(U(t)) : t \in \mathbb{R}\}$.
More precisely, we assume that we are given an open interval I including the origin and that $B : I \to L(\mathfrak{h})$, $t \mapsto B(t)$ is a strongly continuous mapping with $B(0) = \mathrm{id}$, such that for all vectors ϕ of a dense subspace $D(A)$ of $\mathfrak{h}$ the identity $\partial_t B(t)\phi|_{t=0} = A\phi$ holds for some operator A. Next, consider a vector $\psi = \bigotimes_{r=1}^N \psi_r$ with $\psi_r \in D(A)$ for all $r \in \{1, ..., N\}$. Then, by an application of the product rule for the differentiation of tensor products, we obtain

$$\begin{aligned}\partial_t\Gamma_N(B(t))\phi|_{t=0} &= \partial_t\Big(\bigotimes_{l=1}^N B(t)\phi_l\Big)\,|_{t=0} = \sum_{k=1}^N \bigotimes_{l=1}^N (\partial_t)^{\delta_{kl}} B(t)\phi_l|_{t=0} \\ &= \sum_{k=1}^N \bigotimes_{l=1}^N A^{\delta_{kl}}\phi_l = \sum_{k=1}^N A_{N,k}\phi = \mathrm{d}\Gamma_N(A)\phi\ .\end{aligned}$$

By linearity of all operators involved the equation above extends to all $\phi \in D(\mathrm{d}\Gamma_N(A))$ and by restriction to $\phi \in \mathrm{d}\Gamma_G(A)$ for $G \in \mathfrak{G}_N$ we get

$$\partial_t\Gamma_G(B(t))\phi|_{t=0} = \mathrm{d}\Gamma_G(A)\phi\ . \tag{B.59}$$

Taking the direct sum over N one gets the analogous statement on Fock spaces. In particular, one may think of the case, where A is the infinitesimal generator of the strongly continuous one-parameter unitary group $\{U(t) : t \in \mathbb{R}\}$. Then, Equation (B.59) states that for G having closed image $\mathrm{d}\Gamma_G(A)$ is the generator of the strongly continuous one-parameter unitary group $\{\Gamma_G(U(t)) : t \in \mathbb{R}\}$. This can also be seen the following way. Since A is the infinitesimal generator of $\{U(t) : t \in \mathbb{R}\}$, we have $U(t) = \mathrm{e}^{itA}$ for all $t \in \mathbb{R}$. Therefore, using Equation (B.12) we obtain

$$\begin{aligned}\Gamma_N(U(t)) &= \prod_{k=1}^N (U(t))_{N,k} = \prod_{k=1}^N (\exp(-\mathrm{i}tA))_{N,k} \\ &= \prod_{k=1}^N \exp(-\mathrm{i}tA_{N,k}) = \exp\Big(-\mathrm{i}t\sum_{k=1}^N A_{N,k}\Big) = \exp(-\mathrm{i}t\mathrm{d}\Gamma_N(A))\ .\end{aligned}$$

So if $G \in \mathfrak{G}_N$ or $G \in \mathfrak{G}$ has closed image, then

$$\Gamma_G(U(t)) = \exp(-\mathrm{i}t\mathrm{d}\Gamma_G(A))\ . \tag{B.60}$$

Compatibility of the two constructions Γ_G and $\mathrm{d}\Gamma_G$ also appears in the following identity. Consider A to be the a densely defined closed operator on $\mathfrak{h}$ with domain $D(A)$. Moreover, let $B \in \mathscr{B}_{\mathrm{inv}}(\mathfrak{h})$ be an operator such that $B(D(A)) \subset D(A)$. For $N \in \mathbb{N}$ we consider ϕ of the form $\phi = \bigotimes_{r=1}^{N} \phi_r \in D(\mathrm{d}\Gamma_N(A))$ and obtain

$$\begin{aligned}\Gamma_N(B)^{-1}\mathrm{d}\Gamma_N(A)\Gamma_N(B)\phi &= \Gamma_N(B^{-1})\mathrm{d}\Gamma_N(A)\Gamma_N(B)\phi \\ &= \Big(\bigotimes_{k=1}^{N} B^{-1}\Big)\Big(\sum_{l=1}^{N}\bigotimes_{m=1}^{N} A^{\delta_{lm}}\Big)\Big(\bigotimes_{n=1}^{N} B\Big)\Big(\bigotimes_{r=1}^{N}\phi_r\Big) \\ &= \sum_{l=1}^{N}\bigotimes_{k=1}^{N} B^{-1}A^{\delta_{lk}}B\phi_k = \sum_{l=1}^{N}\bigotimes_{k=1}^{N}(B^{-1}AB)^{\delta_{lk}}\phi_k \\ &= \sum_{l=1}^{N}(B^{-1}AB)_{N,l}\phi = \mathrm{d}\Gamma_N(B^{-1}AB)\phi\,.\end{aligned}$$

First by linear extension to $\phi \in D(\Gamma_G(A))$ and then by restriction to $\phi \in D(\mathrm{d}\Gamma_G(A))$ for $G \in \mathfrak{G}_N$ from the above calculation we obtain that the formula analogously holds on Fock space

$$\mathrm{d}\Gamma_G(A)\Gamma_G(B)\phi = \Gamma_G(B)\mathrm{d}\Gamma_G(B^{-1}AB)\phi\,. \tag{B.61}$$

B.2.4. Operators on Fock Space II

We introduce the so called *creation* and *annihilation* operators on Fock space. For any $\psi \in \mathfrak{h}$ the former operator is defined via linear extension of its action on vectors of $\mathfrak{F}_N(\mathfrak{h})$ that is

$$a^*(\psi)\Big(\bigotimes_{k=1}^{N}\phi_k\Big) := \sqrt{N+1}\,\Big(\bigotimes_{k=1}^{N}\phi_k\Big)\otimes\psi\,. \tag{B.62}$$

for $N \in \mathbb{N}$ and $\phi = \phi_1 \otimes \ldots \otimes \phi_N$ and $a^*(\psi)\lambda = \lambda\psi$ for any $\lambda \in \mathfrak{F}_0(\mathfrak{h})$. So, for $N \in \mathbb{N}_0$ the creation operator $a^*_-(\psi)$ maps $\mathfrak{F}_N(\mathfrak{h})$ to $\mathfrak{F}_{N+1}(\mathfrak{h})$. Automatically this forces the annihilation operator, being the adjoint of the creation operator, to act by

$$a(\psi)\Big(\bigotimes_{k=1}^{N+1}\varphi_k\Big) = \sqrt{N+1}\,\langle\psi,\varphi_{N+1}\rangle\,\Big(\bigotimes_{k=1}^{N}\varphi_k\Big) \tag{B.63}$$

on vectors $\varphi := \bigotimes_{k=1}^{N}\varphi_k \in \mathfrak{F}_{N+1}(\mathfrak{h})$ for $N \in \mathbb{N}$ by $a(\psi)\varphi = \langle\psi,\varphi\rangle$ for $\varphi \in \mathfrak{F}_1(\mathfrak{h})$ and $a(\psi)\lambda := 0$ for any $\lambda \in \mathfrak{F}_0(\mathfrak{h})$ as it can be seen from

$$\begin{aligned}\langle\varphi, a^*(\psi)(\phi)\rangle &= \sqrt{N+1}\,\Big\langle\bigotimes_{k=1}^{N+1}\varphi_k, \Big(\bigotimes_{k=1}^{N}\phi_k\Big)\otimes\psi\Big\rangle \\ &= \sqrt{N+1}\,\Big(\prod_{k=1}^{N}\langle\varphi_k,\phi_k\rangle\Big)\langle\varphi_{N+1},\psi\rangle \\ &= \Big\langle\sqrt{N+1}\,\langle\psi,\varphi_{N+1}\rangle\Big(\bigotimes_{k=1}^{N}\varphi_k\Big), \bigotimes_{k=1}^{N}\phi_k\Big\rangle = \langle a_-(\psi)\varphi,\psi\rangle\,.\end{aligned}$$

For any $G \in \mathfrak{G}$ with closed image by $S_G : \mathfrak{F}(\mathfrak{h}) \to \mathfrak{F}_G(\mathfrak{h})$ we denote the projection onto $\mathfrak{F}_G(\mathfrak{h})$. Next, we define the operators

$$a^*_G(\psi) := S_G a^*(\psi) S_G\,, \tag{B.64}$$

$$a_G(\psi) = S_G a(\psi) S_G \tag{B.65}$$

which, restricted to $\mathfrak{F}_G(\mathfrak{h})$, are operators on $\mathfrak{F}_G(\mathfrak{h})$ in their own right. Moreover, the operators in Equations (B.64) and (B.65) are densely defined on $\mathfrak{F}'_G(\mathfrak{h})$, the linear space of vectors in $\mathfrak{F}_G(\mathfrak{h})$ which are non-zero only on finitely many $\mathfrak{F}_{G_N}(\mathfrak{h})$ for $N \in \mathbb{N}_0$. Obviously, one has that the mapping $\mathfrak{h} \to \mathscr{B}(\mathfrak{F}'_G(\mathfrak{h}), \mathfrak{F}_G(\mathfrak{h}))$, $\psi \mapsto a^*_G(\psi)$ is linear and that $\mathfrak{h} \to \mathscr{B}(\mathfrak{F}'_G(\mathfrak{h}), \mathfrak{F}_G(\mathfrak{h}))$, $\psi \mapsto a_G(\psi)$ is an anti-linear mapping.

Lemma B.20

Let B be a densely defined and closed operator on $\mathfrak{h}$, $\psi \in D(B)$ and $G \in \mathfrak{G}$ have closed image. Then, for any $\phi \in (D(\Gamma_G(B)) \cap \mathfrak{F}'_G(\mathfrak{h}))$ we have

$$\Gamma_G(B) a^*_G(\psi)\phi = a^*_G(B\psi)\Gamma_G(B)\phi \,. \tag{B.66}$$

Proof: Directly from definition and linearity one obtains that for any $N \in \mathbb{N}_0$, $\psi \in D(B)$ and any $\phi = \bigotimes_{k=1}^N \phi_k \in D(\Gamma_N(B))$ the following equation holds

$$\Gamma_{N+1}(B) a^*(\psi)\phi = \Gamma_{N+1}(B)\Big(\Big(\bigotimes_{k=1}^N \phi_k\Big) \otimes \psi\Big) = \Big(\Big(\bigotimes_{k=1}^N B\phi_k\Big) \otimes B\psi\Big) = a^*(B\psi)\Gamma_N(B)\phi \,.$$

By linearity this generally holds for all $\phi \in D(\Gamma_N(B))$. Summation over $N \in \mathbb{N}_0$ yields the statement for the special case $G = \mathrm{id}$. For arbitrary $G \in \mathfrak{G}$ the statement follows considering Equation (B.52) and the definition of the creation operator in Equation (B.64). ■

Lemma B.21

Let A be a self-adjoint operator on $\mathfrak{h}$, $\psi \in D(A)$ and $G \in \mathfrak{G}$ have closed image. Then, for any $\phi \in (D(\mathrm{d}\Gamma_G(A)) \cap \mathfrak{F}'_G(\mathfrak{h}))$ we have

$$[\mathrm{d}\Gamma_G(A), a^*_G(\psi)]\phi = a^*_G(A\psi)\phi \,. \tag{B.67}$$

Proof: We consider the mapping $U : \mathbb{R} \to \mathscr{U}(\mathfrak{F}_G(\mathfrak{h}))$, $t \mapsto \mathrm{e}^{\mathrm{i}tA}$ to form a strongly continuous one parameter group. Then, by Lemma B.20 for any $t \in \mathbb{R}$ $\phi \in \mathfrak{F}'_G(\mathfrak{h})$ we have $\mathrm{e}^{\mathrm{i}t\mathrm{d}\Gamma_G(A)} = \Gamma_G(\mathrm{e}^{\mathrm{i}tA}) = \Gamma_G(U(t))$ so that

$$\mathrm{e}^{\mathrm{i}t\mathrm{d}\Gamma_G(A)} a^*_G(\psi)\phi = \Gamma_G(U(t)) a^*_G(\psi)\phi = a^*_G(U(t)\psi)\Gamma_G(U(t))\phi = a^*_G(\mathrm{e}^{\mathrm{i}tA}\psi)\mathrm{e}^{\mathrm{i}t\mathrm{d}\Gamma_G(A)}\phi \,.$$

For $\psi \in D(A)$ and $\phi \in (D(\mathrm{d}\Gamma_G(A) \cap \mathfrak{F}'_G(\mathfrak{h}))$ this equation is differentiable with respect to t at $t = 0$ and one has

$$\begin{aligned}
\mathrm{i}[\mathrm{d}\Gamma_G(A), a_G(\psi)]\phi &= \partial_t \mathrm{e}^{\mathrm{i}t\mathrm{d}\Gamma_G(A)} a^*_G(\psi)\phi|_{t=0} \\
&= \partial_t a^*_G(\mathrm{e}^{\mathrm{i}tA}\psi)\mathrm{e}^{\mathrm{i}t\mathrm{d}\Gamma_G(A)}\phi|_{t=0} \\
&= a^*_G(\mathrm{i}A\psi)\phi + \mathrm{i}a^*_G(\psi)\mathrm{d}\Gamma_G(A)\phi \,.
\end{aligned}$$

■

Canonical Anti-Commutation Relations

We focus on the special case of anti-symmetric Fock space. As an abbreviation we write

$$a^*_-(\psi) := a^*_{S_-}(\psi) = S_- a^*(\psi) S_- \,, \tag{B.68}$$

$$a_-(\psi) = a_{S_-}(\psi) = S_- a(\psi) S_- \,. \tag{B.69}$$

In this situation, it is obvious from Equation (B.8) that for any $N \in \mathbb{N}$ and $\{\mathbf{n}\} = \{n_1, ..., n_N\} \in \mathcal{P}_{N,-}(\mathcal{N})$ with $n_1 < n_2 < ... < n_N$ the creation operators create the elements of the basis $\mathcal{B}_-$ via

$$\Big(\prod_{k=1}^{N} a_-^*(\psi_{n_k})\Big)\Omega = \sqrt{N!}\, S_{N,-} \bigotimes_{k=1}^{N} \psi_{n_k} = \psi_{\{\mathbf{n}\},-} \,, \tag{B.70}$$

where $\Omega = (1, 0, 0, ...) \in \mathfrak{F}_-(\mathfrak{h})$ is the so called vacuum state. Using an orthonormal basis $(\psi)_{n\in\mathbb{N}}$ of $\mathfrak{h}$ from the above one obtains $\|a_-^*(\psi_n)\| < 1$, by testing the creation operator $a^*(\psi)$ on elements of $\mathcal{B}_-$. By linearity, we see that $a_-^*(\psi)$ is a bounded operator on $\mathfrak{F}_-(\mathfrak{h})$ for general $\psi \in \mathfrak{h}$. Automatically, also its adjoint $a_-(\psi)$ is a bounded operator.

Lemma B.22 (*CAR*)

For any $\phi, \psi \in \mathfrak{h}$ the following equations, the so called canonical anti-commutation relations (CAR), hold on anti-symmetric Fock space $\mathfrak{F}_-(\mathfrak{h})$

$$\{a_-(\phi), a_-(\psi)\} = 0 \,, \tag{B.71}$$
$$\{a_-^*(\phi), a_-^*(\psi)\} = 0 \,, \tag{B.72}$$
$$\{a_-(\phi), a_-^*(\psi)\} = \langle\phi, \psi\rangle \mathbb{1}_- \,. \tag{B.73}$$

Proof: Note that Equation (B.71) is linked to Equation (B.72) via adjunction, so we only prove Equations (B.72) and (B.73). By use of Equation (B.70) we see that for any $k, l \in \mathcal{N}$ and any $\psi_{\{\mathbf{n}\},-} \in \mathcal{B}_-$ we have

$$\begin{aligned} a_-^*(\psi_k)a_-^*(\psi_l)\psi_{\{\mathbf{n}\},-} &= -a_-^*(\psi_l)a_-^*(\psi_k)\psi_{\{\mathbf{n}\},-} \\ a_-(\psi_k)a_-^*(\psi_l)\psi_{\{\mathbf{n}\},-} &= -a_-^*(\psi_l)a_-(\psi_k)\psi_{\{\mathbf{n}\},-} + \langle\psi_k, \psi_l\rangle\, \psi_{\{\mathbf{n}\},-} \,. \end{aligned}$$

In the special cases $\phi = \psi_k$ and $\psi = \psi_l$, the Equations (B.71) - (B.73) hold. But then, by anti-linearity of $\mathfrak{h} \to \mathscr{B}(\mathfrak{F}_-(\mathfrak{h}))$, $\phi \mapsto a_-(\phi)$ and linearity of $\mathfrak{h} \to \mathscr{B}(\mathfrak{F}_-(\mathfrak{h}))$, $\psi \mapsto a_-^*(\psi)$ and on the left hand sides of Equations (B.72) and (B.73), as well as by sesquilinearity of $\mathfrak{h} \times \mathfrak{h} \to \mathbb{C}, (\phi, \psi) \mapsto \langle\phi, \psi\rangle$ on the right hand side of Equation (B.73) we see, that the Equations (B.71) - (B.73) hold, for general $\phi, \psi \in \mathfrak{h}$. ■

Lemma B.23

On fermionic Fock space creation and annihilation operators are bounded, i.e. for any $\psi \in \mathfrak{h}$

$$\|a_-(\psi)\| = \|a_-^*(\psi)\| = \|\psi\| \,. \tag{B.74}$$

Proof: From the remarks subsequent to Equation (B.70) we already know, that creation and annihilation operators are bounded. Moreover, for general $\psi \in \mathfrak{h}$ one finds

$$\begin{aligned} \|a_-^*(\psi)\|^4 &= (\|a_-^*(\psi)\|^2)^2 = \|a_-^*(\psi)a_-(\psi)\|^2 = \|(a_-^*(\psi)a_-(\psi))^2\| \\ &= \|a_-^*(\psi)a_-(\psi)a_-^*(\psi)a_-(\psi)\| = \|a_-^*(\psi)(\langle\psi, \psi\rangle - a_-^*(\psi)a_-(\psi))a_-(\psi)\| \\ &= \|\psi\|^2\, \|a_-^*(\psi)a_-(\psi)\| = \|\psi\|^2\, \|a_-^*(\psi)\|^2 \,. \end{aligned}$$

So, the equality holds true for the annihilation operator. Since $\|a_-^*(\psi)\|^2 = \|a_-^*(\psi)a_-(\psi)| = \|a_-(\psi)\|^2$, one gets that the same equality holds true for all the creation operator. ■

Next, we prove a representation formula for second quantised operators on anti-symmetric Fock space (Ber66). The action of these operators on arbitrary vectors is expressed as a quadratic polynomial in creation and annihilation operators.

Lemma B.24

Let A be a self-adjoint operator on $\mathfrak{h}$ and let $\{\psi_n : n \in \mathcal{N}\} \in D(A)$ be an orthonormal basis of $\mathfrak{h}$. Then, for any $\psi_{\{\mathbf{n}\},-} \in \mathcal{B}_-$ as defined in Equation (B.8) one has

$$\mathrm{d}\Gamma_-(A)\psi_{\{\mathbf{n}\},-} = \sum_{n\in\mathcal{N}} a_-^*(A\psi_n)a_-(\psi_n)\psi_{\{\mathbf{n}\},-} \ . \tag{B.75}$$

Proof: For any $N \in \mathbb{N}$ and $\{\mathbf{n}\} = \{n_1, ..., n_N\}$ with $n_1 < n_2 < ... < n_N$ we apply $\mathrm{d}\Gamma_-(A)$ to the element $\psi_{\{\mathbf{n}\},-}$. The statement is the result of the following calculation

$$\begin{aligned}
\mathrm{d}\Gamma_-(A)\psi_{\{\mathbf{n}\},-} &= \sqrt{N!}\,\mathrm{d}\Gamma_-(A)S_{N,-}\bigotimes_{k=1}^{N}\psi_{n_k} = \sqrt{N!}\,S_{N,-}\mathrm{d}\Gamma(A)\bigotimes_{k=1}^{N}\psi_{n_k} \\
&= \sqrt{N!}\,S_{N,-}\sum_{l=1}^{N}A_{N,l}\bigotimes_{k=1}^{N}\psi_{n_k} = \sum_{l=1}^{N}\sqrt{N!}\,S_{N,-}\bigotimes_{k=1}^{N}A^{\delta_{k,l}}\psi_{n_k} \\
&= \sum_{l=1}^{N}\Big(\prod_{k=1}^{l-1}a_-^*(\psi_{n_k})\Big)a_-^*(A\psi_{n_l})\,\{a_-(\psi_{n_l}), a_-^*(\psi_{n_l})\}\Big(\prod_{m=l+1}^{N}a_-^*(\psi_{n_m})\Big)\Omega \\
&= \sum_{l=1}^{N}a_-^*(A\psi_{n_l})a_-(\psi_{n_l})\Big(\prod_{m=1}^{N}a_-^*(\psi_{n_m})\Big)\Omega = \sum_{l=1}^{N}a_-^*(A\psi_{n_k})a_-(\psi_{n_k})\psi_{\{\mathbf{n}\},-} \\
&= \sum_{n\in\mathcal{N}}a_-^*(A\psi_n)a_-(\psi_n)\psi_{\{\mathbf{n}\},-} \ .
\end{aligned}$$

■

In particular, the so called *particle number operator* is of certain interest. For arbitrary $\psi \in \mathfrak{h}$ it is defined by

$$N_-(\psi) := a_-^*(\psi)a_-(\psi) \ . \tag{B.76}$$

The name particle number operator origins from the fact, that if $\psi \in \mathfrak{h}$ is a one-particle state, i.e. $||\psi|| = 1$, the operator $N_-(\psi)$ implements the measurement of the number of particles in the one-particle state ψ. In this case one has $N_-(\psi) = \mathrm{d}\Gamma_-(P_\psi)$, where P_ψ is the orthogonal projection onto the space spanned by ψ. If $(\psi_n)_{n\in\mathbb{N}}$ is an orthonormal basis, one has

$$N_- := \mathrm{d}\Gamma_-(\mathbb{1}) \ , \tag{B.77}$$

where the sum converges in weak operator topology. The operator N_- implements a measurement of the total particle number.

List of Symbols

Number Systems

$\mathbb{C}$	complex numbers
$\mathbb{N}$	natural numbers
$\mathbb{N}_0$	non-negative integer numbers
$\mathbb{R}$	real numbers
$\mathbb{Z}$	integer numbers

Operator Algebraic Objects

$\mathrm{Aut}(\mathfrak{A})$	automorphisms on operator algebra $\mathfrak{A}$
$\mathrm{Der}(\mathfrak{S})$	derivations on subalgebra $\mathfrak{S}$ of operator algebra $\mathfrak{A}$
$\mathrm{Sta}(\mathfrak{A})$	states on C^*-algebra $\mathfrak{A}$

Spaces of Operators

$\mathscr{B}(X)$	bounded linear operators on normed space X
$\mathscr{B}_{\mathrm{inv}}(X)$	invertable bounded linear operators on normed spaces X and Y
$\mathscr{L}(X, Y)$	linear operators between normed space X and Y
$\mathscr{U}(\mathfrak{H})$	unitary operator on Hilbert space $\mathfrak{H}$

Spaces of Functions

$\mathcal{BM}(X, Y)$	bounded measurable mappings between measure spaces X and Y
$C(X, Y)$	continuous mappings between Hausdoff spaces X and Y
$C(X)$	complex-valued and continuous mappings on Hausdorff space X
$C_0(X)$	mappings in $C(X)$ that vanish at infinity
$C_c^\infty(\mathbb{R}^d)$	compactly supported smooth functions on $\mathbb{R}^d$
$\mathcal{E}(\mathbb{R}, \mathbb{R}^d)$	space of electric fields
$\mathcal{M}(X, Y)$	measurable mappings between measure spaces X and Y

Second Quantisation

$\mathfrak{F}(\mathfrak{h})$	Fock space over Hilbert space $\mathfrak{h}$
$\mathfrak{F}_-(\mathfrak{h})$	anti-symmetric Fock space over Hilbert space $\mathfrak{h}$
$\mathfrak{F}_+(\mathfrak{h})$	symmetric Fock space over Hilbert space $\mathfrak{h}$
$\mathfrak{F}_G(\mathfrak{h})$	Fock space with respect to $G \in \mathfrak{G}$ or $G \in \mathfrak{G}_N$
$\mathfrak{F}_N(\mathfrak{h})$	N-particle space over Hilbert space $\mathfrak{h}$
$\mathfrak{F}_{N,-}(\mathfrak{h})$	anti-symmetric N-particle space over Hilbert space $\mathfrak{h}$
$\mathfrak{F}_{N,+}(\mathfrak{h})$	symmetric N-particle space over Hilbert space $\mathfrak{h}$
$\mathcal{G}$	permutation group on $\mathfrak{F}(\mathfrak{h})$
$\mathfrak{G}$	group algebra of $\mathcal{G}$
$\mathcal{G}_N$	permutation group on $\mathfrak{F}_N(\mathfrak{h})$
$\mathfrak{G}_N$	group algebra of $\mathcal{G}_N$

Model

$\mathfrak{B}$	algebra of bounded linear operators on $\mathfrak{h}$
$\mathfrak{B}_c$	elements of $\mathfrak{B}$ with finite support
$\mathfrak{B}_-$	Fermi algebra on $\mathfrak{h}$
$\mathfrak{B}_{c,-}$	elements of $\mathfrak{B}_-$ with finite support
$\mathfrak{h}$	space $\ell^2(\mathbb{Z}^d)$ of square sumable sequences on $\mathbb{Z}^d$
$\mathfrak{h}_c$	elements of $\mathfrak{h}$ with finite support
$\mathcal{K}^\infty$	space of covariant operators
$\mathcal{K}_c^\infty$	elements of $\mathcal{K}^\infty$ with invariant subspace $\mathfrak{h}_c$
$\mathcal{K}^2$	space of covariant operators

Standard Notation

$B_1(X)$	closed unit ball on normed space X
$\mathcal{B}(X)$	Borel σ-algebra of topological space X
$D(A)$	domain of an operator A on Banach space X
$\hat{f}$	Fourier transform of a function f
$\Gamma_N(U)$	N-particle operator corresponding to unitary U
$\mathrm{d}\Gamma_N(A)$	N-particle operator corresponding to observable A
$\Gamma(U)$	second quantisation of unitary U
$\mathrm{d}\Gamma(A)$	second quantisation of observable A
$\Gamma_G(U)$	second quantisation of unitary U with respect to $G \in \mathfrak{G}$
$\mathrm{d}\Gamma_G(A)$	second quantisation of observable A with respect to $G \in \mathfrak{G}$
$\Gamma_{N,-}(A)$	fermionic N-particle operator corresponding to unitary$U$
$\mathrm{d}\Gamma_{N,-}(A)$	fermionic N-particle operator sorresponding to observable A
$\Gamma_{N,+}(U)$	bosonic N-particle operator corresponding to unitary U
$\mathrm{d}\Gamma_{N,+}(A)$	bosonic N-particle operator sorresponding to observable A
$\Gamma_-(U)$	second quantisation of unitary U on fermionic Fock space
$\mathrm{d}\Gamma_-(A)$	second quantisation of observable A on fermionic Fock space
$\Gamma_+(U)$	second quantisation of unitaray U on bosonic Fock space
$\mathrm{d}\Gamma_+(A)$	second quantisation of observable A on bosonic Fock space
$M_d(\mathbb{C})$	algebra of $d \times d$-matrices with complex entries.

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