Irreversible Dynamics in Quantum Mechanics by the Introduction of a Time Scale

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Chapter 1

Introduction

More than half a century has passed since Erwin Schrödinger introduced for the first time his by now celebrated and extensively studied wave equation. An equation whose interpretation was from the very beginning problematic. During all these years quantum mechanics has proven to be strikingly successful and has provided the explanation for marvelous experiments. The relativistic extension of this theory, quantum field theory, has also led to amazing achievements, both with regard to experimental precision and to the understanding of nuclear and subnuclear structures. Still, one cannot feel actually satisfied, due to the fact that there are still great conceptual difficulties in the understanding of the foundations of quantum mechanics. And also quantum field theory is burdened with very serious interpretative difficulties, only partially circumvented by the useful recipe of renormalization. Many formal and interpretative schemes have been proposed, but neither seems to be prevailing or liable to be definitely proved or disproved by realizable experiments. It is not even clear what notions and objects should be taken as fundamental; a lack of rigor and clarity is felt to undermine the whole theory, and in particular the problem of measurement [1]. Quantum mechanics is said to be the theory of microsystems, but taking well-known experimental evidences into account one is lead to realize that, contrary to what is often tacitly believed, no direct objectivity can be attributed to microsystems, such as for example particles. This should be clear if one considers the manifestations of wave-particle duality; the existence of quantum correlations which, as stressed at the very beginning of quantum mechanics by Schrödinger himself [2], through the phenomenon of entanglement (*Verschränkung*) make the attribution of properties to part of a system problematic; the famous E.P.R. paradox [3]; recent experiments in which the particle picture seems to lead to inconsistencies, e.g., the heavily debated superluminal photonic tunneling experiments [4]. The dissatisfaction with this situation and the necessity to reconsider the notion of particle has been recently stressed also by Haag, who has proposed to take as fundamental the notion of *event* [5]. A possible alternative approach was elaborated by Ludwig: according to his axiomatic foundations of quantum mechanics the basic elements of reality are not microsystems, but rather the macroscopic setup of any real experiment, which he divided in preparation and registration apparatuses. His approach gives a solid basis to the point of view, initially expressed by Bohr, according to which the internal coherence of quantum mechanics and closeness to experimental reality demand that microsystems should be anchored to the objective reality of macroscopic systems. About the connection between the quantum and the classical description let us only mention a recent review on the subject [6], paying particular attention to the problem of decoherence, together with a recently proposed approach, in which quantum and classical observables are jointly considered and a notion of *event* is also introduced [7].

Sharing Ludwig's viewpoint one should start with a phenomenological, objective, and in this sense classical, description of macrosystems, macroscopic exactly in the sense that they are liable to be objectively described. In particular Ludwig envisaged this objective description in terms of trajectories for suitable observables or parameters connected to the system. Such a description is however still lacking, even though much progress has been made thanks to the theory of continuous measurement, mathematically based on the theory of stochastic processes, which has led to the introduction of the notion of trajectory in quantum mechanics. Indeed the very definition of a finite isolated macroscopic system is slippery, because of the existence of quantum correlations. The way in which isolation from the environment is obtained belongs, in our opinion, to the very definition of the system. If one does not take some approximations into account, the concept of isolated system can only be an asymptotic one. Considering a finite preparation time means that some memory loss is operatively necessary, the price of some coarse graining of the dynamical description must be paid: to do this we associate in a systematic way to the preparation procedure a suitable time scale. The relevant role of the preparation procedure means a breaking of basic space-time symmetry by suitable boundary conditions which introduce the peculiarities of the system, hiding the more universal behavior of local or short range interactions. The field theoretical approach, that is anyway mandatory in the relativistic case, is best suited to express the interplay of local universality and peculiar boundary conditions. The time scale has to be long enough in order to break up the correlations with the environment and make the idealized boundary conditions physically meaningful. On this time scale one considers the subdynamics of suitable slow variables. According to the level of description, the fundamental fields may be associated to molecules as fundamental constituents or, in a more refined description, to nuclei and electrons. The physically relevant observables, slowly varying on the given time scale, typically densities of conserved charges, should be connected to the objective properties to be ascribed to the system. The time scale associated to the preparation procedure, necessary in order to actually define and isolate the system, accounts for irreversibility, reflected in the structure of the equations for the relevant variables and connected to the directedness between preparation and registration. In a completely sharp description of the dynamics of a subsystem the physics of the whole universe would enter, correlations could not be neglected. The proposal is to tune the formalism of quantum mechanics to this situation, emphasizing already in the formalism that only coarse grained descriptions make sense: obviously the striving to lower the time scale and to push cutoffs farther still remains, but should not be based only on formal procedures like thermodynamic limit and renormalization.

My PhD studies, that have been strongly influenced by the works of Ludwig on the foundations of quantum mechanics, have been devoted to make the first steps in the concrete realization of this research program. The main effort has been toward the development of a general formalism, inside non relativistic quantum field theory, for the description of the reduced dynamics of slowly varying degrees of freedom. Such a description should be meaningful on a time scale determined by the choice of relevant observables.

The formalism has already been developed in detail in the case of a microsystem interacting with a macroscopic system, which can be seen as the simplest perturbation of matter at equilibrium, a first step in the direction of the description of non equilibrium systems. One obtains for the statistical operator describing the microsystem a dynamical semigroup in which the operators determining the structure of the generator are linked to the T-matrix describing the interaction between the particle and the macroscopic system. The generator has the Lindblad form, accounting for complete positivity, a property which seems to be particularly relevant in the one-particle quantum mechanical framework, and that we have tried to extend to the case of macroscopic systems. The mixture term in the Lindblad generator accounts for irreversibility and is typical of a quantum description. The result has been considered in the framework of modern one particle experiments and has been applied to two very different cases, neutron matter interaction near the optical regime and Brownian motion, thus showing the wide range of validity of the obtained expression. In the case of neutron matter interaction particular attention has been devoted to incoherent effects in the dynamics, keeping in mind the recent beautiful neutron interferometry experiments made by the group of Rauch in Wien [8]. Also possible experimental consequences of our analysis of the contribution to incoherent scattering have been suggested. Considering Brownian motion, a typical example of irreversible interaction, we have recovered some results already obtained in the literature in the attempt to give a quantum description of the phenomenon.

This formal approach has been pursued further in order to apply it to macroscopic systems. In this case the reduced dynamics pertains to some degrees of freedom (e.g., distribution function in a kinetic description; densities of mass, energy and momentum in a hydrodynamic description) that are slowly varying on the chosen time scale, much longer than the typical time of microphysical interactions. The obtained equations are formally very similar to those derived for the case of the microsystem, so that a kind of unified description may be envisaged. It appears that, considering slow variables, the time evolution satisfies a generalization of the complete positivity property. A first application of these calculations in the homogeneous case leads to a Boltzmann equation with complete quantum statistical corrections (Uehling – Uhlenbeck equation). The formalism can however be applied also to the non-homogeneous case, as we intend to do in the next future. The structure of the generator, with a commutator term linked to the self-adjoint part of the T-matrix, makes it a promising candidate for the description of both a kinetic regime and a coherent, typically quantum, regime, analogously to what has been done in the case of the particle interacting with matter. Such an interplay between these two regimes seems to be particularly important for example in the extremely interesting case of Bose Einstein condensation, a field in which new and extraordinary experimental results have been reached in the last few years [9]. In fact analogous equations have been recently obtained with a very different treatment, aiming at an explanation of Bose Einstein condensation in a gas of trapped alkali atoms [10], in which the dynamics should be governed by a competition between the coherent quantum dynamics of atoms in the condensate and the incoherent kinetic dynamics of the other atoms.

The conceptual and formal scheme that we have proposed for the description of reduced degrees of freedom inside a field theoretical formalism, based on a selection of relevant observables, typically densities of conserved charges slowly varying on a given time scale, can be applied to very different physical situations and levels of description. In this thesis we have considered the case of a particle interacting with matter and of a medium of molecules interacting via a two body short range potential. The next natural step, apart from further improvements and applications to particular situations, would consist in considering more refined degrees of freedom, for example charged nuclei and electrons interacting through the electromagnetic field, thus building a hierarchy of theories at a deeper and deeper level.

The thesis is organized as follows. In Chap. 2 we have tried to write a brief but self-consistent survey of Ludwig's axiomatic approach to the notion of microsystem appearing in the directed interaction of objectively described macroscopic systems. This is simply intended to give the reader who is not acquainted with Ludwig's works a compact reference, which is, at least to our knowledge, still not available. In Chap. 3 the abovementioned formalism is developed in the case of a microsystem interacting with matter, while Chap. 4 is devoted to the application in the fields of neutron optics and quantum Brownian motion. Chap. 5 is devoted to the extension of the same formalism to the much more complex problem of macroscopic systems. References to written contributions in which the results presented in this thesis have already been reported are listed at the end of the bibliography [70, 71, 72, 73, 74]. Appendix A is devoted to a more profound analysis of the axiom of quantization introduced in Chap. 2, while Appendix B simply gives a list of the introduced axioms, together with their names in Ludwig's books.

Chapter 2

Microsystems as Interaction Carriers

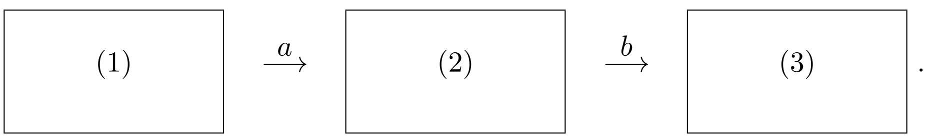
2.1 Introduction

In this chapter we briefly introduce Ludwig's axiomatic approach to the notion of microsystem and connected to this the natural appearance of such notion in considering the directed interaction of macroscopic systems, which are supposed to be described objectively. Our presentation will certainly be lacking and incomplete, both because of the huge amount of material to be concentrated in a few pages and because of mathematical and physical subtleties inherent in the very subject. We therefore apologize to the reader from the very beginning, referring him to the original papers and books by Ludwig [11, 12, 13, 14, 15]. This exposition is simply intended to give a compact review of the subject, which, at least to our knowledge, is at present not available. The reader interested in Ludwig's work is still bound to work his way through many (often huge and difficult) volumes before he gains at least an overview of the main points of this axiomatic approach and of the achievements of Ludwig's studies. This brief résumé is therefore meant to make the highlights of this approach available to a larger audience, stressing the points which will be of relevance to the sequel and that have proven to be worth mentioning after so many years and so much experimental and theoretical work about the foundations of quantum mechanics. Our hope is that this brief exposition may arise in the reader at least the curiosity to dwell a little longer on the original work by Ludwig. In the sequel we will suppose that the reader is already familiar with the notion of ensemble and effect, together with the basics of the connected rich mathematical structures [16, 17, 18].

According to Ludwig the main difficulties in the interpretation of quantum mechanics arise because one takes as fundamental concepts the notions of *state* and *observable*, notions that have to be defined by quantum mechanics itself. While in Newtonian mechanics one can safely speak of position and momentum of a given planet or of any material system, and in order to measure position and momentum one does not have to take Newtonian mechanics into account, this is not so in quantum mechanics. Both the notion of state and observable of a system are to be indicated by quantum mechanics itself. The very notion of particle, as stressed in Chap. 1, cannot be taken as fundamental, due to wave-particle duality and E.P.R. correlations, linked respectively to interference and entanglement (*Verschränkung*). As a matter of fact, every experiment with single microsystems is in any case an experiment using macrosystems, explaining what has happened between macrosystems in terms of microsystems, often envisaged as particles. Microsystems like single electrons, single atoms or single molecules appear only indirectly in real experiments. Ludwig intended to give what he called an Axiomatic Basis to quantum mechanics, where by axiomatic basis of a physical theory he meant a construction of the considered theory based on elements of reality which can be described without the theory itself, only in terms of what he called Pretheories (for example classical mechanics is a pretheory for classical electrodynamics and both are pretheories for quantum mechanics).

2.2 The Notion of Microsystem

In his axiomatic approach to the foundations of quantum mechanics Ludwig proposed to take as fundamental domain of the theory the statistical experiments with single microsystems and the frequencies of the related phenomena. Instead of the particles themselves one considers the macroscopic setup of any real experiment, which can be divided in a preparation procedure and a registration procedure, both to be described in terms of pretheories. A simple example of preparation apparatus could be an accelerator plus target, while a typical registration apparatus could be a bubble chamber. Once this experimental setup is suitably described, one considers the rate according to which microsystems prepared with the given preparation apparatus trigger the assigned registration apparatus: these are the frequencies to be compared with the quantum mechanical laws. One may argue whether every experimental arrangement for an experiment with a single microsystem consists of a preparation apparatus and a registration apparatus. This is indeed the case even though such a subdivision is in no way unique in the case of a complicated experiment. Let us consider the following scheme:



In (1) the microsystem a is produced, which then produces b interacting with the macroscopic system (2). The microsystem b is then registered by (3). We may now consider (1) as the preparation apparatus for the microsystem a, which is then registered by (2) plus (3), but we may also consider (1) plus (2) as the preparation apparatus for the microsystem b, which is then registered by (3).

In this spirit we want to introduce the notion of microsystem as of something which has been prepared by a preparation apparatus and registered by a registration apparatus. To do this we need a statistical theory, in terms of which the general structures of preparation and registration, which can be applied both to microsystem and macrosystem, can be described.

2.2.1 Statistics

Let M be the set having as elements the representatives of the physical features whose statistics we want to describe (in the present case it will become the set of microsystems). The statistics is related to selection procedures, by which special features may be selected. A selection procedure is to be described by a subset $a \subset M$, corresponding to the subset of features (microsystems) that satisfy the given selection procedure. We define as SELECTION PROCEDURE the following mathematical structure: a set M and a subset $\mathcal{S} \subset \mathcal{P}(M)$ such that (**S** standing for statistics)

S 1.1 $a, b \in \mathcal{S}, a \subset b \Rightarrow b \backslash a \in \mathcal{S}$

S 1.2 $a, b \in \mathcal{S} \Rightarrow a \cap b \in \mathcal{S}$.

We call selection procedure both $\mathcal{S}$ and an element a of $\mathcal{S}$. **S 1.2** says that the selection procedure consisting in selecting both according to a and b exists. If $a \subset b$ we say that a is *finer* than b. **S 1.1** says that if we use two selection procedures a and b, where a is finer than b, the rest of the objects $x \in b$, which do not satisfy the finer criterion a, still constitute a selection procedure. Note that in this construction it is not necessarily $M \in \mathcal{S}$. In fact $a \in \mathcal{S}$, $M \in \mathcal{S}$ would lead to $M \backslash a \in \mathcal{S}$ contrary to physical meaningfulness. Let us consider in fact a modern electron accelerator: for the selected set of electrons a we may make important assertions about the experiments for which the electrons are used, but what assertions can we make about the electrons which are not prepared by the accelerator? Thus it is meaningful not to require that M be a selection procedure. Let us note that $\mathcal{S}(a) \equiv \{b \in \mathcal{S} | b \subset a\}$ is a Boolean ring, while $\mathcal{S}$ need not even be a lattice, because $a, b \in \mathcal{S}$ does not automatically imply $a \cup b \in \mathcal{S}$. In particular two selection procedures $a, b \in \mathcal{S}$ are called COEXISTENT relative to c if both $a \subset c$ and $b \subset c$.

It often happens in applications that two selection procedures a and b, where b is finer than a, are not statistically independent. Consider for example an experiment in which of the N systems prepared according to the selection procedure a, N_1 also satisfy the selection criterion of b: we say that N_1/N is the relative frequency of b relative to a. If this frequency shows to be reproducible and it is confirmed by experiments with great number of systems, we say that b is statistically dependent from a. Let $\mathcal{S} \subset \mathcal{P}(M)$ be a selection procedure, for which **S 1** holds, and let $\mathcal{T} \equiv \{(a,b)|a,b \in \mathcal{S}, b \subset a, a \neq \emptyset\}$: we say that $\mathcal{S}$ is a Statistical Selection Procedure whenever a real function $\lambda(a,b)$ with $0 \leq \lambda(a,b) \leq 1$ is defined on $\mathcal{T}$ such that

S 2.1 $a_1, a_2 \in \mathcal{S}, a_1 \cap a_2 = \emptyset, a_1 \cup a_2 \in \mathcal{S} \Rightarrow \lambda(a_1 \cup a_2, a_1) + \lambda(a_1 \cup a_2, a_2) = 1$

S 2.2 $a_1, a_2, a_3 \in \mathcal{S}, a_1 \supset a_2 \supset a_3, a_2 \neq \emptyset \Rightarrow \lambda(a_1, a_3) = \lambda(a_1, a_2)\lambda(a_2, a_3)$

S 2.3 $a_1, a_2 \in \mathcal{S}, a_1 \supset a_2, a_2 \neq \emptyset \Rightarrow \lambda(a_1, a_2) \neq 0$.

$\lambda(a,b)$ is usually called the *conditional probability* of b relative to a and represents the frequency with which systems selected by a also satisfy b. If $a_1 \cup a_2$ is a selection procedure, both a_1 and a_2 are finer than $a_1 \cup a_2$; if $a_1 \cap a_2 = \emptyset$ they exclude each other. If N systems are selected according to $a_1 \cup a_2$, of which N_1 also satisfy a_1 and N_2 satisfy a_2, because of $a_1 \cap a_2 = \emptyset$ we have $N_1 + N_2 = N$: this explains **S 2.1**. If for three selection procedures we have $a_1 \supset a_2 \supset a_3$ and N_1 systems are selected according to a_1, between these N_2 according to a_2, between these again N_3 according to a_3, we simply have $N_3/N_1 = (N_2/N_1)(N_3/N_2)$, that is to say **S 2.2**. If $a_1 \supset a_2 \neq \emptyset$, of the N systems chosen according to a_1 certainly finitely many will also satisfy a_2, which is **S 3.3**. From these axioms follows $\lambda(a_1, 0) = 0$ and $\lambda(a_1, a_1) = 1$; moreover, if $a_2 \cap a_3 = \emptyset$, $a_2, a_3 \subset a_1$, we have $\lambda(a_1, a_2 \cup a_3) = \lambda(a_1, a_2) + \lambda(a_1, a_3)$.

Before going back to the notion of microsystem, let us introduce the notion of *additive measure on a boolean ring*, which will be useful later on, in deriving the concept of observable. A real function $\mu(q)$ on a Boolean ring Q such that $0 \leq \mu(q) \leq 1$, $\mu(e) = 1$ (where e is the unit element) and $\mu(q_1 \vee q_2) = \mu(q_1) + \mu(q_2)$ for $q_1 \wedge q_2 = 0$ is called an additive measure on Q. As an example $\mu(b) = \lambda(a,b)$ is an additive measure on the Boolean ring $\mathcal{S}(a)$ and for $a \supset a_1 \supset a_2$ we have $\lambda(a_1, a_2) = \mu(a_2)/\mu(a_1)$. On the Boolean ring $\mathcal{S}(a)$ one can therefore recover all the conditional probabilities $\lambda(a,b)$ from the probability function $\mu(b)$.

We now introduce a mathematical expression for the notion of experimental mixture. Considering a selection procedure $\mathcal{S}$, a partition of $a \in \mathcal{S}$ of the form $a = \cup_{i=1}^{n} b_i$, with $b_i \in \mathcal{S}$ and mutually disjoint is called a Decomposition of a in the b_i, and a is called a Mixture of the b_i. Since the set $\mathcal{S}(a)$ is a Boolean ring a decomposition of a is simply a disjoint partition of the unit element a of $\mathcal{S}(a)$. With the above defined additive measure $\mu(b)$ over $\mathcal{S}(a)$ we have $\sum_{i=1}^{n} \mu(b_i) = 1$, $\mu(b_i) = \lambda(a, b_i)$ being the weights of b_i in a. If we experimentally choose N systems according to a, and of these N_i are further selected according to b_i, the relations $N_i/N \approx \mu(b_i)$ must be verified in physical approximation. This should however not induce the reader to confuse the notion of selection procedure with that of ensemble, which will be introduced later on.

2.2.2 Physical Systems

Exploiting the above defined notions of selection procedure and of statistical selection procedure we want to introduce on M (which is expected to become the set of microsystems) suitable mathematical structures, so as to interpret its elements as physical systems, in that they can be prepared and registered. Let a structure $\mathcal{Q} \subset \mathcal{P}(M)$ be given on M, which we call PREPARATION PROCEDURE, such that (**A** standing for axiom)

A 1 $\mathcal{Q}$ is a statistical selection procedure.

The elements of $\mathcal{Q}$ are representatives of well-defined technical processes, to be described by pretheories and not by quantum mechanics itself, thanks to which microsystems can be produced in large numbers. The mathematical relation $x \in a$ $(a \in \mathcal{Q})$ means: x has been obtained according to the preparation procedure a. There are very many examples of preparation procedures, e.g., an ion-accelerator together with the apparatus which generates the ion-beam. We denote by $\lambda_{\mathcal{Q}}(a, b)$ the probability function defined over $\mathcal{Q}$. We now consider a specific physical example, in order to make this construction clearer. We take an experimental apparatus which generates couples (1,2) of spin 1/2 particles with total spin 0 and emits them in opposite directions. As preparation procedure for the system 1 we consider the apparatus consisting of the preparation apparatus for the couple (1,2) and an apparatus detecting the z component of the spin of system 2. This apparatus gives us three different preparation procedures for the system 1. Preparation procedure a_1^3: all prepared systems 1 independent of the detection on system 2; preparation procedure a_1^{3+}: all systems 1, by which a positive z component has been detected for system 2; preparation procedure a_1^{3-}: all systems 1, by which a negative z component has been detected for system 2. We obviously have $a_1^{3+} \subset a_1^3$, $a_1^{3-} \subset a_1^3$, $a_1^{3+} \cap a_1^{3-} = \emptyset$ and $a_1^3 = a_1^{3-} \cup a_1^{3+}$ represents a decomposition of a_1^3. In this particular case the weights are given by $\mu(a_1^{3\pm}) = \lambda(a_1^3, a_1^{3\pm}) = 1/2$.

We now want to introduce the notion of registration. Let there be on M two further structures, the set of REGISTRATION PROCEDURES $\mathcal{R} \subset \mathcal{P}(M)$ and the set of REGISTRATION METHODS $\mathcal{R}_0 \subset \mathcal{P}(M)$, satisfying

A 2 $\mathcal{R}$ is a selection procedure

A 3 $\mathcal{R}_0$ is a statistical selection procedure

A 4.1 $\mathcal{R}_0 \subset \mathcal{R}$

A 4.2 To each $b \in \mathcal{R}$ there exists a $b_0 \in \mathcal{R}_0$ for which $b \subset b_0$.

These two structures correspond to the two steps of a typical registration process: the construction and utilization of the registration apparatus and the selection according to the changes which have occurred or not occurred in the registration apparatus. Let us consider for example a proportional counter: $b_0 \in \mathcal{R}_0$ is the set of all microsystems which have been applied to the counter; the elements of $\mathcal{R}_0$ characterize therefore the construction of the registration apparatus and its application to microsystems. For a particular microsystem $x \in b_0$ the counter may or may not respond: let b_+ (with $b_+ \subset b_0$) be the selection procedure of all $x \in b_0$ for which the counter has responded and b_- the set of all $x \in b_0$ for which the counter has not responded. b_+ and b_- are elements of $\mathcal{R}$. **A 3** accounts for the fact that there could be correlations between the different apparatuses.

It is extremely important that we do not require $\mathcal{R}$ to be a statistical selection procedure. To understand this point let us come back to the previous example. The counter characterized by b_0 may respond or not, so that b_0 is decomposed in the two sets b_+ and b_-, such that $b_0 = b_+ \cup b_-$ and $b_+ \cap b_- = \emptyset$. There is however in nature no reproducible frequency $\lambda_{\mathcal{R}}(b_0, b_+)$; in fact if in a real experiment N microsystems $x_1, x_2, \ldots, x_N$ are applied to the counter, i.e., $x_1 \in b_0, x_2 \in b_0, \ldots, x_N \in b_0$, and for N_+ of these the counter has responded, the frequency N_+/N depends in an essential way on the previous history of the microsystems, it cannot be reproduced on the basis of the registration procedure alone. The experimental frequencies depend on the preparation procedure, as expressed by the next axiom

A 5 For all $a \in \mathcal{Q}$, $a \neq \emptyset$ and for all $b_0 \in \mathcal{R}_0$, $b_0 \neq \emptyset$ we have $a \cap b_0 \neq \emptyset$; to each $b \in \mathcal{R}$, $b \neq \emptyset$ there is at least an $a \in \mathcal{Q}$ such that $a \cap b \neq \emptyset$.

$a \cap b_0$ with $a \in \mathcal{Q}$ and $b_0 \in \mathcal{R}_0$ is the set of microsystems which have been prepared according to the procedure a and that have been applied to the registration method b_0. $a \cap b_0 \neq \emptyset$ means therefore that it is physically possible to combine every preparation procedure a with every registration method b_0. This is certainly not realistic because of causality relations and the problem of the time-ordering between preparation and registration procedure. For the sake of simplicity however we shall keep the simpler axiom **A 5**, a minor mathematical idealization which, as we shall see, will not have severe consequences on the following. The second part of **A 5** simply says that, if microsystems exist, which applied to b_0 trigger it according to b, they can also be prepared.

Let us call $\mathcal{S}$ the smallest set of selection procedures containing all $a \cap b$ with $a \in \mathcal{Q}$ and $b \in \mathcal{R}$ (remember that $a \cap b$ is the set of all microsystems that have been prepared according to a and registered according to b). We have $\mathcal{S} \subset \mathcal{P}(M)$, but in the general case neither $\mathcal{Q} \subset \mathcal{S}$ nor $\mathcal{R} \subset \mathcal{S}$ will be true. We now come to a most important statement, according to which preparation *and* registration procedures together give reproducible frequencies

A 6 $\mathcal{S}$ is a statistical selection procedure.

Of course there will be some relations between the statistics in $\mathcal{S}$ and those in $\mathcal{Q}$ and $\mathcal{R}_0$. We now want to express the fact that preparation procedures and registration methods are independent of each other; denoting with $\lambda_{\mathcal{S}}(c, c')$ the probability function in $\mathcal{S}$ we have

A 7.1 If $a, a' \in \mathcal{Q}$, $a' \subset a$ and $b_0 \in \mathcal{R}_0$ then $\lambda_{\mathcal{S}}(a \cap b_0, a' \cap b_0) = \lambda_{\mathcal{Q}}(a, a')$

A 7.2 If $a \in \mathcal{Q}$ and $b_0, b_0' \in \mathcal{R}_0$, $b_0' \subset b_0$, then $\lambda_{\mathcal{S}}(a \cap b_0, a \cap b_0') = \lambda_{\mathcal{R}_0}(b_0, b_0')$.

$\lambda_{\mathcal{Q}}(a, a')$ is the frequency with which microsystems prepared according to a satisfy the finer selection a'. If to the microsystems prepared according to a the registration method b_0 is applied, this should be independent from the fact that they also satisfy a'. Thus **A 7.1** expresses the directedness of the interaction of the preparation on the registration apparatus, and similarly for **A 7.2**.

We are now ready to exactly define the notion of Physical System: a set M with three structures $\mathcal{Q} \subset \mathcal{P}(M)$, $\mathcal{R} \subset \mathcal{P}(M)$, $\mathcal{R}_0 \subset \mathcal{P}(M)$, satisfying **A 1** to **A 7** is a set of physical systems. As stressed at the beginning of this section the structures we have used to introduce the notion of physical system are not restricted to the case of microsystems, they can describe macroscopic systems as well. Thanks to the axioms **A 1** to **A 7**, implying the independence of the preparation procedure with respect to the registration procedure, the facts that we have called physical systems have some reality beyond that of the direct interpretation in terms of preparation and registration procedures. Intuitively this means that in the preparation "something" is produced which can be afterwards detected by the registration apparatus. Nevertheless the physical systems that we have introduced are still closely related to the associated production and detection methods; it does not seem that they can be described in terms of the objective properties that we are accustomed to ascribe to physical systems. Speaking of self-existing objects which do not suffer or exert any influence on the rest of the world would be physically meaningless and, from a logical point of view, self-contradictory. Nevertheless in physics one seeks to describe portions of the world as if they were isolated, in the sense that on a given description level their interactions with the rest of the world may be neglected. To the extent that this is possible one may attribute objective properties to the considered system. The introduced scheme is so far very general, being applicable both to macrosystems and microsystems: the selection procedures in $\mathcal{S}$ describe a conventional "classical statistics", not exhibiting the "typical" quantum mechanical structure. The transition to quantum statistics will be made only later with axiom **QM** (or more precisely with **L 5** in Appendix A), thus coming to the notion of microsystem. We are able to describe the structure of a physical system only to the extent that it can be prepared and registered. In mathematical terms this amounts to introducing the following axioms

A 8.1 $M = \bigcup_{a\in\mathcal{Q}} a$

A 8.2 $M = \bigcup_{b\in\mathcal{R}} b$,

stating that every physical system interacts with the outside world at least once (**A 8.1**) and again (**A 8.2**).

2.2.3 Ensembles and Effects

From **S 2** and **A 7** one can prove that the probability function $\lambda_{\mathcal{S}}(c, c')$ is uniquely determined by $\lambda_{\mathcal{Q}}$ and by the special values

$$\lambda_{\mathcal{S}}(a \cap b_0, a \cap b), \tag{2.2.1}$$

with $a \in \mathcal{Q}$, $b \in \mathcal{R}$, $b_0 \in \mathcal{R}_0$ and $b \subset b_0$. $\lambda_{\mathcal{S}}(a \cap b_0, a \cap b)$ gives the frequencies with which microsystems prepared by a and applied to the apparatus characterized by b_0 trigger it according to b. The values (2.2.1) are just the values the experimental physicist obtains to compare with the theory: N systems are prepared according to the preparation procedure a and applied to the registration method specified by b_0, then one counts the number N_+ of microsystems which trigger the registration apparatus in a definite way, specified by b. Within physical approximations the number N_+/N should agree with (2.2.1): the whole statistics of experiments with microsystems is contained in (2.2.1).

To proceed further let us introduce the set $\mathcal{F}$ of Effect Processes: $\mathcal{F} \equiv \{(b_0, b) | b_0 \in \mathcal{R}_0, b_0 \neq \emptyset, b \in \mathcal{R}, b \subset b_0\}$. A couple (b_0, b) in $\mathcal{F}$ exactly describes the experimental situation corresponding to the generation of an effect. We may now write in a simpler way the function (2.2.1): denoting by $g = (b_0, b)$ a couple in $\mathcal{F}$ we define $\lambda_{\mathcal{S}}(a \cap b_0, a \cap b) = \mu(a, g)$, where thanks to **A 5** the function $\mu(a, g)$ is defined on the whole $\mathcal{Q}' \times \mathcal{F}$ (the prime denoting the set without the element $\emptyset$). According to $\mu(a_1, g) = \mu(a_2, g)$ for all $g \in \mathcal{F}$ an equivalence relation $a_1 \sim a_2$ is defined on $\mathcal{Q}$, which allows to partition it into equivalence classes. We call $\mathcal{K}$ the set of all equivalence classes in $\mathcal{Q}$: an element of $\mathcal{K}$ is called Ensemble (or *state*) and $\mathcal{K}$ is the set of ensembles. This is one of the main definitions, which has been made possible by the idealized axiom **A 5**. In fact one can partition $\mathcal{Q}$ into equivalence classes even when **A 5** is replaced by more physical axioms, keeping the problem of combination of preparation and registration procedures into account: for this reason we kept **A 5**, thus making the exposition much more compact. Let us stress the fact that an ensemble $w \in \mathcal{K}$ is not a subset of M, that is to say, an ensemble w is not a set of prepared microsystems: it is a class of sets a of prepared microsystems. The difference between ensembles and preparation procedures is very important, as we shall see focusing on the E.P.R. paradox. Analogously to what has been done in $\mathcal{Q}$, one can introduce an equivalence relation in $\mathcal{F}$: $g_1 \sim g_2$ whenever $\mu(a, g_1) = \mu(a, g_2)$ for all $a \in \mathcal{Q}'$. We denote by $\mathcal{L}$ the set of all equivalence classes in $\mathcal{F}$: an element $f \in \mathcal{L}$ is called EFFECT and $\mathcal{L}$ is the set of all effects. Once again one should not confuse effects and effect processes. Through $\tilde{\mu}(w, f) = \mu(a, g)$ for $w \in \mathcal{K}$, $f \in \mathcal{L}$ and $a \in w$, $g \in f$ a function $\tilde{\mu}(w, f)$ is defined on $\mathcal{K} \times \mathcal{L}$ (in the following we will simply write μ instead of $\tilde{\mu}$). For the real function $\mu(w, f)$ on $\mathcal{K} \times \mathcal{L}$ we have:

1. $0 \leq \mu(w, f) \leq 1$,
2. $\mu(w_1, f) = \mu(w_2, f)\ \forall f \in \mathcal{L} \Rightarrow w_1 = w_2$,
3. $\mu(w, f_1) = \mu(w, f_2)\ \forall w \in \mathcal{K} \Rightarrow f_1 = f_2$,
4. $\exists!\ f_0 \in \mathcal{L}$ (also denoted by $\mathbf{0}$) such that $\mu(w, f_0) = 0\ \forall w \in \mathcal{W}$,
5. $\exists!\ f_1 \in \mathcal{L}$ (also denoted by $\mathbf{1}$) such that $\mu(w, f_1) = 1\ \forall w \in \mathcal{W}$.

We denote by ϕ the map which to each element $a \in \mathcal{Q}'$ associates the corresponding equivalence class $w \in \mathcal{K}$; analogously we define a map ψ from $\mathcal{F}$ to $\mathcal{L}$, often writing $\psi(g)$ instead of $\psi(b_0, b)$ whenever $g = (b_0, b)$. In particular, considering a decomposition of a ($a = \cup_{i=1}^{n} a_i$, with $a_i \in \mathcal{Q}'$ and mutually disjoint), we have for all $g \in \mathcal{F}$:

$$\mu(a, g) = \sum_{i=1}^{n} \lambda_{\mathcal{Q}}(a, a_i)\mu(a_i, g) \qquad \sum_{i=1}^{n} \lambda_{\mathcal{Q}}(a, a_i) = 1,$$

which may be rewritten as

$$\mu(\phi(a), f) = \sum_{i=1}^{n} \lambda_{\mathcal{Q}}(\phi(a), \phi(a_i))\mu(\phi(a_i), f) \quad \forall f \in \mathcal{L}. \tag{2.2.2}$$

The introduced partitions into equivalence classes of the sets $\mathcal{Q}'$ and $\mathcal{F}$ are most important. These partitions do not simply amount to make the theory of the considered physical systems independent from inessential features in the construction of the apparatuses $a \in \mathcal{Q}'$ and $b_0 \in \mathcal{R}_0$. They have a much deeper significance with regard to the physical theory. For example the partition of $\mathcal{Q}'$ depends in an essentially way on which and how many effect processes are physically realizable. Restricting the set $\mathcal{F}$ to a subset $\widetilde{\mathcal{F}}$ could imply a coarser partition of $\mathcal{Q}'$. Axioms about the extension of the sets $\mathcal{Q}'$ and $\mathcal{F}$ amount to specify the theory one is dealing with, thus indirectly identifying the described physical systems and the possible realizable experiments.

2.2.4 Ensembles and Effects in Quantum Mechanics

So far we have introduced the quantities that connect theory and experiment, that is to say the elements of $\mathcal{Q}$, $\mathcal{R}$, $\mathcal{R}_0$ and the functions $\lambda_{\mathcal{Q}}$, $\lambda_{\mathcal{R}_0}$, $\lambda_{\mathcal{S}}$. Note that contrary to the usual formulations of quantum mechanics, neither the statistical operators (or in particular the pure states) nor the self-adjoint operators (describing the so-called observables) will be used for direct comparison with experiment: the relationship between mathematical description and experiment exclusively rests upon the preparation and the registration procedures and the probability function $\lambda_{\mathcal{S}}$. We now add an axiom connecting this general theoretical scheme to the usual Hilbert space quantum mechanics (**QM** standing for quantum mechanics).

QM There is a bijective map β of $\mathcal{K}$ onto the set K of positive self-adjoint operators W on a Hilbert space $\mathcal{H}$ with $\mathrm{Tr}(W) = 1$ and a bijective map γ of $\mathcal{L}$ onto the set L of all self-adjoint operators with $\mathbf{0} \leq F \leq \mathbf{1}$, so that $\mu(w, f) = \mathrm{Tr}(WF)$ holds where $W = \beta w$, $F = \gamma f$.

Because of **QM** one simply identifies $\mathcal{K}$ with K, $\mathcal{L}$ with L and $\mu(w, f)$ with $\mathrm{Tr}(WF)$, so that we can write $\phi(a) = W \in K$, $\psi(g) = F \in L$. The convex set K is the base of the base-norm space T of trace-class operators on $\mathcal{H}$, while L is the order unit interval of the order unit space B of bounded operators on $\mathcal{H}$. The Banach space B is the dual of the Banach space T, the canonical bilinear form being given by $\langle W, A\rangle = \mathrm{Tr}(W^\dagger A)$ with $W \in T$ and $A \in B$. The axiom **QM** cannot be physically understood or explained in a simple way, and at this level it can only be guessed on the basis of the correspondence principle. This axiom can be also deduced as a theorem from physically more motivated axioms, as shown in Appendix A. In this alternative deduction of the Hilbert space structure the notion of Face of the convex set K plays a major role. The "finiteness" of quantum mechanics, typically expressed by the existence of quantized states and not reflected by the infinite dimensionality of the spaces one is dealing with, is there connected to the notion of finite face as typical feature of quantum mechanics as opposed to classical mechanics.

Thanks to the identification of $\mathcal{K}$ with K, $\mathcal{L}$ with L and the embedding of K in the set T of trace-class operators on the Hilbert space $\mathcal{H}$ we may rewrite (2.2.2) in the form

$$\phi(a) = \sum_{i=1}^{n} \lambda_{\mathcal{Q}}(\phi(a), \phi(a_i))\phi(a_i), \tag{2.2.3}$$

that is to say a decomposition of $\phi(a) \in K$. Introducing the set $\check{K} \equiv \{A \in T | A \geq 0, \mathrm{Tr}A \leq 1\}$ we shall say that a set ($\nu = 1, 2, \ldots, r$) of decompositions of a $W \in K$ of the form $W = \sum_{i=1}^n W_i^{(\nu)}$ with $W_i^{(\nu)} \in \check{K}$ is a set of Coexistent Decompositions provided there exists a Boolean ring Σ and an additive measure $W(\sigma)$ over Σ with $W(\sigma) \in \check{K}$ such that all $W_i^{(\nu)}$ build a subset of all $W(\sigma)$ and for the unit element e of Σ the relation $W(e) = W$ holds.

After the introduction of **QM** we call M the set of MICROSYSTEMS. On the basis of the above formulation of the foundations of quantum mechanics it is clear that the Hilbert space does not directly describe a physical structure. It is a mathematical tool which permits us to cleverly handle the structure of the convex set K. Since the positive affine functionals on K are identical to the elements of the positive cone of B (of which L is the basis), it is the structure of K alone which determines the physical structure of microsystems. The structure of K also contains the so-called "wave character" of microsystems: the Schrödinger equation and the vectors in a Hilbert space are mathematical tools to better "handle" this "wave character".

2.2.5 Coexistent Effects and the Notion of Observable

Up to now we have described measurements in terms of yes-no responses by suitable registration apparatuses, which were supposed to describe all possible registration procedures. This approach seems to be somehow in contrast with the usual attitude of taking as fundamental the notion of measurement scale associated to each observable. The importance attributed to the notion of observable with a measurement scale is however due to the relevance that the correspondence principle assumed in the early developments of quantum mechanics, rather than to well-founded physical reasons. Starting from Ludwig's attempt to a better formulation of the foundations of quantum mechanics we will see how the notion of observable (a generalized one) comes out as a result of the existence of different registration procedures *coexistent* with respect to the same registration method b_0. The statement that b' and b'' are coexistent relative to a given b_0 amounts to say that it is possible to JOINTLY MEASURE, for every single microsystem x which has been registered according to b_0, whether b' *and* b'' have given the answer yes (i.e., $x \in b' \cap b''$), whether b' *or* b'' have given the answer yes (i.e., $x \in b' \cup b''$), and similarly for the other possible combinations. Given a fixed $b_0 \in \mathcal{R}_0$ we call a set of *coexistent effect processes* the set of all couples $(b_0, b) \in \mathcal{F}$ with $b \subset b_0$; the set of all $b \subset b_0$ will be denoted by $\mathcal{R}(b_0)$. The registration procedures $b \in \mathcal{R}(b_0)$ are said to be *coexistent* with respect to the registration method b_0. The set $\mathcal{R}(b_0)$ is a Boolean ring, the so called *Boolean switching algebra*. Such coexistent effect processes are very common in physics. Take for example as b_0 an array of counters, which may or may not be triggered by a microsystem passing by: $\mathcal{R}(b_0)$ is then the set of all possible logical combinations of yes or no responses for each single counter, accounting for all possible joint measurements. We define as additive measure over a Boolean ring Σ a map χ from Σ to a linear ordered vector space such that $\mathbf{0} \leq \chi(\sigma) \leq \mathbf{1}$ and $\chi(\sigma_1 \cup \sigma_2) = \chi(\sigma_1) + \chi(\sigma_2)$ for $\sigma_1 \cap \sigma_2 = \emptyset$. As a consequence the map $\psi(b_0, b)$, interpreted for fixed b_0 as a map of $\mathcal{R}(b_0)$ in L is a positive measure over the Boolean ring $\mathcal{R}(b_0)$:

we have in fact, for $b \subset b_0$, $b = b' \cup b''$, $b' \cap b'' = \emptyset$

$$\psi(b_0, b) = \psi(b_0, b') + \psi(b_0, b''). \tag{2.2.4}$$

This last equation leads us to the definitions of sets of coexistent effects and commensurable decision effects. We say that a set $A \subset L$ is called a set of COEXISTENT EFFECTS if there exists a Boolean ring Σ with additive measure $F : \Sigma \to L$ for which $A \subset F\Sigma$. In the very particular case in which the apparatus characterized by b_0 is so constructed that the $\psi(b_0, b)$ are decision effects we may introduce a more restrictive definition: a set $A \subset G$ (where G is the lattice of decision effects) is called a set of COMMENSURABLE DECISION EFFECTS if there exists a Boolean ring Σ with additive measure $F : \Sigma \to G$ for which $A \subset F\Sigma$. According to (2.2.4) all b's that may be jointly registered by a common registration method b_0 always lead to coexistent effects or even to commensurable decision effects. One expects that the converse is also true, in correspondence to each set of coexistent effects (or commensurable decision effects) it should be physically possible to build up an apparatus where these effects jointly appear. To this end we introduce the following

A 9 To each set A of coexistent effects there corresponds an $\mathcal{R}(b_0)$ so that A is a subset of all $\psi(b_0, b)$ with $b \in \mathcal{R}(b_0)$.

Before going over to define what is meant by an observable in Ludwig's approach and the relations to the usual definition, let us stress the fact that the introduced concept of joint measurements must not be confused with the so called *simultaneous measurements* which play such a relevant role in the standard formulation. The different yes-no responses in the apparatus b_0 need not arise at the same time, on the contrary in many experiments it is important to consider the time interval between different responses: consider for example the different droplets forming at different space-time points in a bubble chamber.

We call OBSERVABLE a Boolean ring Σ with an additive vector measure $F(\sigma)$ with $F(\sigma) \in L$ (for example the abovementioned $\psi : \mathcal{R}(b_0) \to L$), indicating it briefly by $A \equiv A(\Sigma, F(\sigma))$. In particular we call DECISION OBSERVABLE a Boolean ring Σ with an additive vector measure $E(\sigma)$ with $E(\sigma) \in G$. Note that we have not identified observables and self-adjoint operators. If the Boolean ring Σ is defined in terms of subsets of a parameter space the parameters are called the scale values of the observable $(\Sigma, F(\sigma))$, or of the decision observable $(\Sigma, E(\sigma))$. As a matter of fact every Boolean ring may be represented through subsets of a parameter space so that scales do not unduly restrict the notion of observable.

The more familiar description of decision observables in terms of self-adjoint operators is obtained as follows. Consider a one-dimensional scale for a decision observable. Let λ be the parameter of this scale; instead of the whole additive vector measure we can only specify the measures for the intervals $-\infty < \ldots \leq \lambda$, which we call $E(\lambda)$. The $E(\lambda)$ build a spectral family to which corresponds the following uniquely defined self-adjoint operator

$$A = \int_{-\infty}^{+\infty} \lambda \, dE(\lambda), \tag{2.2.5}$$

and conversely each self-adjoint operator A uniquely determines the whole spectral family $E(\lambda)$ and therefore the additive measure on the Boolean ring generated by the intervals $-\infty < \ldots \leq \lambda$. The physical meaning of (2.2.5) lies in the fact that all possible expectation values with respect to the scale λ of any function $f(\lambda)$, for a fixed statistical operator W may be obtained in terms of the operator A

$$\mathrm{Exp}(f(\lambda)) = \int f(\lambda) \, d\mu(W, E(\lambda)) = \mu(W, f(A)).$$

This is not true in the case of a general observable, because then one has to use instead of spectral measures the more general notion of Positive Operator Valued Measure (p.o.v. measure), for which $F(\lambda) \in L$ (but non necessarily $F(\lambda) \in G$), so that one still has

$$\mathrm{Exp}(f(\lambda)) = \int f(\lambda) \, d\mu(W, E(\lambda)),$$

but $\mathrm{Exp}(f(\lambda)) = \mu(W, f(A))$ no more holds with an operator given by

$$A = \int_{-\infty}^{+\infty} \lambda \, dF(\lambda).$$

We still have $\mathrm{Exp}(\lambda) = \mu(W, A)$, but generally $\mathrm{Exp}(\lambda^2) \neq \mu(W, A^2)$.

2.3 Microsystems as Interaction Carriers

If one considers real experimental setups, one realizes that every experiment with microsystems is in reality a complicated arrangement of macrosystems, together with the detection of definite macroscopic processes taking place in the laboratory. So all experiments take place in a macroscopic background and may be interpreted only indirectly in terms of microsystems. Keeping this simple fact into account we now schematically show how Ludwig obtained the concept of microsystem as introduced in Sect. 2.2 starting from the directed interaction of two macroscopic systems.

2.3.1 Preparation and Registration of Two Combined Macrosystems

We introduce two sets M_1, M_2 corresponding to macrosystems of type 1 and 2. We suppose that both sets may be interpreted as sets of physical systems, i.e., the structures of preparation procedure, registration method and registration procedure are defined on them (denoted by the usual symbols with a superscript (1) or (2)). We denote two different experiments with the same system through two different elements of M_1 (M_2), corresponding to the fact that the experiment has to be prepared every time anew. As a consequence the combined systems form only a subset of $M_1 \times M_2$: if $x_1 \in M_1$ is combined with $x_2 \in M_2$, it cannot be combined with any other $x_2' \in M_2$. Further restrictions are due to the impossibility of putting two macrosystems in the very same place. Calling M_c the set of combined systems we have: $M_c \subset M_1 \times M_2$; moreover $(x_1, x_2) \in M_c, (x_1', x_2) \in M_c$ implies $x_1 = x_1'$ and similarly $(x_1, x_2) \in M_c, (x_1, x_2') \in M_c$ implies $x_2 = x_2'$.

Let us consider two preparation procedures, $a^{(1)} \in \mathcal{Q}^{(1)}$ and $a^{(2)} \in \mathcal{Q}^{(2)}$, for systems 1 and 2 respectively: we say that these preparation procedures may be COMBINED provided for any $\bar{a}^{(1)} \in \mathcal{Q}^{(1)}, \bar{a}^{(2)} \in \mathcal{Q}^{(2)}$ such that $\emptyset \neq \bar{a}^{(1)} \subset a^{(1)}, \emptyset \neq \bar{a}^{(2)} \subset a^{(2)}$ the relation $\bar{a}^{(1)} \times \bar{a}^{(2)} \cap M_c \neq \emptyset$ holds. The structure of selection procedures over M_c generated by $\Gamma = \{a^{(1)} \times a^{(2)} \cap M_c | a^{(1)}, a^{(2)}$ may be combined$\}$ will be denoted by $\mathcal{Q}_c$. According to experience we ask that to any $a^{(1)} \in \mathcal{Q}^{(1)\prime}$ corresponds at least one $a^{(2)} \in \mathcal{Q}^{(2)\prime}$ that can be combined with $a^{(1)}$ and similarly in the reverse direction. Setting (for $a^{(1)} \times a^{(2)} \cap M_c \neq \emptyset$)

$$\lambda_{\mathcal{Q}_c}(a_1^{(1)} \times a_1^{(2)} \cap M_c, a_2^{(1)} \times a_2^{(2)} \cap M_c) = \lambda_{\mathcal{Q}_1}(a_1^{(1)}, a_2^{(1)}) \lambda_{\mathcal{Q}_2}(a_1^{(2)}, a_2^{(2)})$$

a probability function $\lambda_{\mathcal{Q}_c}$ is uniquely defined on M_c in terms of the probability functions $\lambda_{\mathcal{Q}_1}$ on M_1 and $\lambda_{\mathcal{Q}_2}$ on M_2. $\mathcal{Q}_c$ is therefore the preparation procedure for the combined systems.

To obtain registration procedures and registration methods for the combined systems we start from the structures $\mathcal{R}^{(1)}, \mathcal{R}_0^{(1)}$ and $\mathcal{R}^{(2)}, \mathcal{R}_0^{(2)}$ on the sets M_1 and M_2 respectively. We suppose that if $a^{(1)} \in \mathcal{Q}^{(1)\prime}, a^{(2)} \in \mathcal{Q}^{(2)\prime}, b_0^{(1)} \in \mathcal{R}_0^{(1)\prime}, b_0^{(2)} \in \mathcal{R}_0^{(2)\prime}$, where $a^{(1)}$ and $a^{(2)}$ may be combined, the relation $(a^{(1)} \cap b_0^{(1)}) \times (a^{(2)} \cap b_0^{(2)}) \cap M_c \neq \emptyset$ holds, that is to say, the registrations on the two subsystems 1 and 2 do not disturb each other. The system of registration procedures generated by $b^{(1)} \times b^{(2)} \cap M_c$ with $b^{(1)} \in \mathcal{R}^{(1)}$, $b^{(2)} \in \mathcal{R}^{(2)}$ will be indicated by $\mathcal{R}_c$, while the system of registration methods generated by $b_0^{(1)} \times b_0^{(2)} \cap M_c$ with $b_0^{(1)} \in \mathcal{R}_0^{(1)}$, $b_0^{(2)} \in \mathcal{R}_0^{(2)}$ will be indicated by $\mathcal{R}_{0c}$. The probability function $\lambda_{\mathcal{R}_{0c}}$ on $\mathcal{R}_{0c}$ is determined by asking

$$\lambda_{\mathcal{R}_{0c}}(b_{01}^{(1)} \times b_{01}^{(2)} \cap M_c, b_{02}^{(1)} \times b_{02}^{(2)} \cap M_c) = \lambda_{\mathcal{R}_{01}}(b_{01}^{(1)}, b_{02}^{(1)}) \lambda_{\mathcal{R}_{02}}(b_{01}^{(2)}, b_{02}^{(2)}),$$

with an obvious notation. One can show that $\mathcal{R}_{0c}, \mathcal{R}_c$ satisfy axioms **A 2** to **A 4**, while we still postulate **A 5** for $\mathcal{Q}_c, \mathcal{R}_{0c}, \mathcal{R}_c$, which indirectly represents a postulate on M_c.

We denote by $\mathcal{S}_c$ the system of selection procedures generated by all $a \cap b$ with $a \in \mathcal{Q}_c, b \in \mathcal{R}_c$. According to **A 6** we ask $\mathcal{S}_c$ to be a statistical selection procedure with probability function $\lambda_{\mathcal{S}_c}$ satisfying **A 7**. Contrary to the probability functions for the other statistical selection procedures we do not ask $\lambda_{\mathcal{S}_c}$ to satisfy (with $\lambda_{\mathcal{S}_1}, \lambda_{\mathcal{S}_2}$ the probability functions for the uncoupled systems 1 and 2 respectively)

$$\lambda_{\mathcal{S}_c}(a^{(1)} \times a^{(2)} \cap M_c \cap b_0^{(1)} \times b_0^{(2)}, a^{(1)} \times a^{(2)} \cap M_c \cap b^{(1)} \times b^{(2)}) =$$

$$\lambda_{\mathcal{S}_1}(a^{(1)} \cap b_0^{(1)}, a^{(1)} \cap b^{(1)})\lambda_{\mathcal{S}_2}(a^{(2)} \cap b_0^{(2)}, a^{(2)} \cap b^{(2)}),$$

because this equation would correspond to the too simple case according to which the two systems are not in interaction.

2.3.2 Directed Interaction

We consider the slightly more complicated situation of a Directed Interaction between the two systems: that is to say we consider couples (x_1, x_2) such that x_1 acts on x_2, but the converse is not true. This is expressed in mathematical terms by the following equation for $\lambda_{\mathcal{S}_c}$

$$\lambda_{\mathcal{S}_c}(a^{(1)} \times a^{(2)} \cap M_c \cap b_0^{(1)} \times b_0^{(2)}, a^{(1)} \times a^{(2)} \cap M_c \cap b^{(1)} \times b_0^{(2)}) = \lambda_{\mathcal{S}_1}(a^{(1)} \cap b_0^{(1)}, a^{(1)} \cap b^{(1)}). \quad (2.3.1)$$

Equation (2.3.1) expresses the fact that the effect process $(b_0^{(1)}, b^{(1)})$ when applied to 1 gives frequencies that are independent from the selection $a^{(2)} \cap b_0^{(2)}$ of the combined system 2. The registration on system 1 depends neither on which system 2 is put nearby nor on the method used to register 2. When (2.3.1) holds we have

$$\lambda_{\mathcal{S}_c}(a^{(1)} \times a^{(2)} \cap M_c \cap b_0^{(1)} \times b_0^{(2)}, a^{(1)} \times a^{(2)} \cap M_c \cap b^{(1)} \times b^{(2)}) =$$

$$\lambda_{\mathcal{S}_c}(a^{(1)} \times a^{(2)} \cap M_c \cap b_0^{(1)} \times b_0^{(2)}, a^{(1)} \times a^{(2)} \cap M_c \cap b^{(1)} \times b_0^{(2)})$$

$$\times \lambda_{\mathcal{S}_c}(a^{(1)} \times a^{(2)} \cap M_c \cap b^{(1)} \times b_0^{(2)}, a^{(1)} \times a^{(2)} \cap M_c \cap b^{(1)} \times b^{(2)}) =$$

$$\lambda_{\mathcal{S}_1}(a^{(1)} \cap b_0^{(1)}, a^{(1)} \cap b^{(1)})\lambda_{\mathcal{S}_c}(a^{(1)} \times a^{(2)} \cap M_c \cap b^{(1)} \times b_0^{(2)}, a^{(1)} \times a^{(2)} \cap M_c \cap b^{(1)} \times b^{(2)}).$$

The second factor of the last term indicates a conditional probability and may be rewritten

$$\lambda_{\mathcal{S}_c}(a^{(1)} \times a^{(2)} \cap M_c \cap b^{(1)} \times b_0^{(2)}, a^{(1)} \times a^{(2)} \cap M_c \cap b^{(1)} \times b^{(2)}) \equiv \tilde{\lambda}_{\mathcal{S}_c}(a^{(1)} \cap b^{(1)}; a^{(2)} \cap b_0^{(2)}, a^{(2)} \cap b^{(2)}) \quad (2.3.2)$$

giving the probability for a registration on system 2 under the condition that system 1 has been selected according to $a^{(1)} \cap b^{(1)}$. It seems physically reasonable to assume that the influence of 1 on 2 depends not only on the way 1 has been prepared, but also on the result of a registration on it.

2.3.3 Interaction Carrier

Exploiting the structures defined on M_1 and M_2 we have introduced on M_c the structures $\mathcal{Q}_c$, $\mathcal{R}_{0c}$, $\mathcal{R}_c$ which allow us to interpret the elements of M_c as combined physical systems. We now want to see how the same mathematical structure can be read in a different way, thus leading to the notion of interaction carrier.

To avoid confusion we introduce a set M and a bijective map j of M_c onto M. All structures on M have to be introduced through the map j. Supposing directed interactions the probability function over $\mathcal{S}_c$ is fixed by the values in (2.3.2). Setting $\tilde{a} = [(a^{(1)} \cap b^{(1)}) \times M_2] \cap M_c$, $\tilde{b}_0 = [M_1 \times (a^{(2)} \cap b_0^{(2)})] \cap M_c$, $\tilde{b} = [M_1 \times (a^{(2)} \cap b^{(2)})] \cap M_c$ we have the more compact notation

$$\lambda_{\mathcal{S}_c}(a^{(1)} \times a^{(2)} \cap M_c \cap b^{(1)} \times b_0^{(2)}, a^{(1)} \times a^{(2)} \cap M_c \cap b^{(1)} \times b^{(2)}) = \lambda_{\mathcal{S}_c}(\tilde{a} \cap \tilde{b}_0, \tilde{a} \cap \tilde{b}).$$

We can now introduce the following structures on M:

$$\mathcal{Q} = \{a | a = j(\tilde{a}), \tilde{a} = (c \times M_2) \cap M_c \text{ with } c \in \mathcal{S}^{(1)}\}, \tag{2.3.3}$$

where $\mathcal{S}^{(1)}$ is the selection procedure generated by all $a^{(1)} \cap b^{(1)}$ with $a^{(1)} \in \mathcal{Q}^{(1)}, b^{(1)} \in \mathcal{R}^{(1)}$;

$$\mathcal{R}_0 = \{b_0 | b_0 = j(\tilde{b}_0), \tilde{b}_0 = (M_1 \times c) \cap M_c \text{ with } c \in \mathcal{D}^{(2)}\}, \tag{2.3.4}$$

where $\mathcal{D}^{(2)}$ is the selection procedure generated by all $a^{(2)} \cap b_0^{(2)}$ with $a^{(2)} \in \mathcal{Q}^{(2)}, b_0^{(2)} \in \mathcal{R}_0^{(2)}$;

$$\mathcal{R} = \{b | b = j(\tilde{b}), \tilde{b} = (M_1 \times c) \cap M_c \text{ with } c \in \mathcal{S}^{(2)}\}, \tag{2.3.5}$$

with $\mathcal{S}^{(2)}$ defined analogously to $\mathcal{S}^{(1)}$. Since $\mathcal{S}^{(1)}, \mathcal{D}^{(2)}, \mathcal{S}^{(2)}$ are selection procedures, $\mathcal{Q}, \mathcal{R}_0, \mathcal{R}$ are also selection procedures. Equation (2.3.3) establishes a bijective relation h between $\mathcal{S}^{(1)}$ and $\mathcal{Q}$, thanks to which we can introduce a probability function $\lambda_{\mathcal{Q}}$ setting $\lambda_{\mathcal{Q}}(a_1, a_2) = \lambda_{\mathcal{S}^{(1)}}(c_1, c_2)$. Correspondingly (2.3.4) establishes a bijective relation between $\mathcal{D}^{(2)}$ and $\mathcal{R}_0$ so that for $c_1, c_2 \in \mathcal{D}^{(2)}$ we may define a probability function over $\mathcal{R}_0$ through the relation $\lambda_{\mathcal{R}_0}(b_{01}, b_{02}) = \lambda_{\mathcal{S}^{(2)}}(c_1, c_2)$. According to property **A 7** for $\lambda_{\mathcal{S}^{(2)}}$ we have for $a_2^{(2)} \subset a_1^{(2)}$ and $b_{02}^{(2)} \subset b_{01}^{(2)}$

$$\lambda_{\mathcal{S}^{(2)}}(a_1^{(2)} \cap b_{01}^{(2)}, a_2^{(2)} \cap b_{02}^{(2)}) = \lambda_{\mathcal{Q}^{(2)}}(a_1^{(2)}, a_2^{(2)}) \lambda_{\mathcal{R}_0^{(2)}}(b_{01}^{(2)}, b_{02}^{(2)}),$$

so that $\lambda_{\mathcal{R}_0}$ is determined solely by $\lambda_{\mathcal{Q}^{(2)}}$ and $\lambda_{\mathcal{R}_0^{(2)}}$.

Exploiting the structures defined on the set M_1 and M_2 one can therefore show that for $\mathcal{Q}$, $\lambda_{\mathcal{Q}}$, $\mathcal{R}_0$, $\lambda_{\mathcal{R}_0}$, $\mathcal{R}$ the relations **A 1** to **A 4** hold. Due to the fact that not all $a^{(1)}$ and $a^{(2)}$ may be combined, **A 5** will not hold in the general case. This is not disappointing, since we had already stressed the fact that this axiom expresses an idealization. To circumvent this difficulty we say that $a \in \mathcal{Q}$ and $b_0 \in \mathcal{R}_0$ may be *combined* when $\tilde{a} \in \mathcal{Q}, \tilde{b}_0 \in \mathcal{R}_0$ and $\emptyset \neq \tilde{a} \subset a, \emptyset \neq \tilde{b}_0 \subset b_0$ implies $\tilde{a} \cap \tilde{b}_0 \neq \emptyset$, setting $C \equiv \{(a, b_0)|a, b_0$ may be combined$\}$. We shall call $\mathcal{S}$ the selection procedure generated by the set $\{a \cap b|a \in \mathcal{Q}, b \in \mathcal{R}$ and there is a $b_0 \in \mathcal{R}_0$ such that $b \subset b_0$ and $(a, b_0) \in C\}$. The relations (2.3.3) and (2.3.5) then imply that $c = j(\tilde{c})$ with $\tilde{c} \in \mathcal{S}_c$ represents a bijective map between $\mathcal{S}$ and $\mathcal{S}_c$, so that the probability function $\lambda_{\mathcal{S}_c}$ may be transported as λ on $\mathcal{S}$. In such a way also **A 6** and **A 7** are satisfied thanks to the directedness of the interaction. As seen in the previous section the statistics is completely determined by $\lambda_{\mathcal{Q}}$ and the function

$$\mu(a, (b_0, b)) = \lambda_{\mathcal{S}}(a \cap b_0, a \cap b). \qquad (2.3.6)$$

We introduce further the set $\mathcal{C} = \{(a, g)|a \in \mathcal{Q}, g = (b_0, b) \in \mathcal{F}$ and $(a, b_0) \in C\}$, over which the function $\mu(a, g)$ is defined.

We have therefore shown that $\mathcal{Q}, \mathcal{R}_0, \mathcal{R}$ together with the probability functions $\lambda_{\mathcal{Q}}, \lambda_{\mathcal{R}_0}$ and $\lambda_{\mathcal{S}}$ define on M a structure of preparation and registration satisfying the axioms given in Sect. 2.2 (apart from **A 5**). However the physical meaning of the elements of $\mathcal{Q}, \mathcal{R}_0, \mathcal{R}$, as well as of the probability functions $\lambda_{\mathcal{Q}}, \lambda_{\mathcal{R}_0}, \lambda_{\mathcal{S}}$, is already given by the macroscopic situation of the combined systems with directed interaction. With respect to Sect. 2.2 we have done a further step in that the set M with the structures $\mathcal{Q}, \mathcal{R}_0, \mathcal{R}$ has been derived more precisely from the pretheories in terms of which the two macroscopic systems are supposed to be described. Given this construction one can understand why the elements of M can be interpreted as INTERACTION CARRIERS. Of course on this basis one is not led to state the independent existence of these interaction carriers: what one is really confronted with are in fact the two interacting macroscopic systems. This may seem disappointing, but it is a natural consequence of the structure of any real experiment, in which one is actually dealing with different arrangements of macroscopic systems.

Although **A 5** is no more valid, one can show that under definite not too restrictive conditions on C the relation

$$a_1 \sim a_2 \quad \text{whenever} \quad \mu(a_1, g) = \mu(a_2, g) \quad \text{for all } g \text{ such that} \quad (a_1, g), (a_2, g) \in \mathcal{C}$$

is in fact an equivalence relation. We introduce as before $\mathcal{K}$ as the set of equivalence classes; through

$$\tilde{\mu}(w, g) = \mu(a, g) \quad \text{with} \quad a \in w$$

we may define a function on all couples w, g such that there is at least an element $a \in w$ satisfying $(a, g) \in \mathcal{C}$. If it is physically meaningful to ask that for each couple $(w, g) \in \mathcal{K} \times \mathcal{F}$ there is an $a \in w$ such that $(a, g) \in \mathcal{C}$ the function $\tilde{\mu}$ is defined on the whole $\mathcal{K} \times \mathcal{F}$ and

$$\tilde{\mu}(w, g_1) = \tilde{\mu}(w, g_2) \quad \text{for all} \quad w \in \mathcal{K}$$

gives an equivalence relation on $\mathcal{F}$. As usual we denote with $\mathcal{L}$ the set of these equivalence classes. Slightly generalizing the definition introduced at the end of Sect. 2.2.2 we say that the elements of a set M with the structures $\mathcal{Q}, \mathcal{R}_0, \mathcal{R}$ represent PHYSICAL SYSTEMS provided the set $\mathcal{K}$ of ensembles and $\mathcal{L}$ of effects may be introduced as shown above. We can also say that the action of system 1 on system 2 is carried by physical systems.

2.3.4 Microsystems as Interaction Carriers

We shall now see in more detail how the notion of microsystem, as something which has been prepared and registered, comes out of this description of the directed interaction between macroscopic systems.

The structure of M_c allows the introduction of a map $\pi : M_1 \to M_c$ defined by $x_1 \to (x_1, x_2)$. Through the map j defined in the previous paragraph we can construct the composed map $j\pi : M_1 \stackrel{\pi}{\to} M_c \stackrel{j}{\to} M$. $x = j\pi(x_1)$ is then the microsystem x prepared from the preparation system x_1. Exploiting the bijective map $h : \mathcal{S}^{(1)} \to \mathcal{Q}$ defined thanks to (2.3.3) for $c \in \mathcal{S}^{(1)}$ we have $h(c) = j\pi(c)$, where $j\pi(c) = \bigcup_{x \in c} j\pi(x)$. Using the identification of $\mathcal{K}$ with K and the map ϕ we have the composed map $\phi h : \mathcal{S}^{(1)\prime} \stackrel{h}{\to} \mathcal{Q}' \stackrel{\phi}{\to} K$. $W = \phi h(c)$ is then called the *ensemble* of microsystems prepared by the preparation systems in c. We recall that it is sufficient to know the map ϕh for the special values $c = a^{(1)} \cap b^{(1)}$ with $a^{(1)} \in \mathcal{Q}^{(1)}, b^{(1)} \in \mathcal{R}^{(1)}$. This poses the so called *preparation problem*, that is to develop a theory which makes it possible to calculate $W = \phi h(a^{(1)} \cap b^{(1)})$ starting from a macroscopic description of the systems in M_1.

Analogously we can introduce a map $\rho : M_2 \to M_c$ defined by $x_2 \to (x_1, x_2)$. Through the map j we come to $j\rho : M_2 \stackrel{\rho}{\to} M_c \stackrel{j}{\to} M$. $x = j\rho(x_2)$ then means that the microsystem x was registered by the registration system x_2. Through (2.3.5) a map $k : \mathcal{S}^{(2)} \to \mathcal{R}$ is defined, which restricted to $\mathcal{D}^{(2)}$ describes a bijective map of $\mathcal{D}^{(2)}$ onto $\mathcal{R}_0$. For $c \in \mathcal{S}^{(2)}$ we then have $k(c) = j\rho(c)$. We now introduce the subset of $\mathcal{D}^{(2)} \times \mathcal{S}^{(2)}$ given by $\mathcal{N}^{(2)} = \{(c_0, c) | c_0 \in \mathcal{D}^{(2)}, c \in \mathcal{S}^{(2)} \text{ and } c \subset c_0\}$. Through the definition $k(c_0, c) = (k(c_0), k(c))$ is defined a map $k : \mathcal{N}^{(2)} \to \mathcal{F}$, which may be composed with the map ψ thus giving $\psi k : \mathcal{N}^{(2)} \stackrel{k}{\to} \mathcal{F} \stackrel{\psi}{\to} L$, where we have identified $\mathcal{L}$ with L. $F = \psi k(c_0, c)$ is the *effect* defined by the registration system c_0 together with the registration c. Once again it is sufficient to know the map ψk for the special values $c_0 = a^{(2)} \cap b_0^{(2)}$ with $a^{(2)} \in \mathcal{Q}^{(2)}, b_0^{(2)} \in \mathcal{R}^{(2)}$ and $c = a^{(2)} \cap b^{(2)}$ with $b^{(2)} \in \mathcal{R}^{(2)}, b^{(2)} \subset b_0^{(2)}$. This poses the so called *registration problem*, also called *measurement problem*: to develop a theory which makes it possible, starting from a macroscopic description of the systems in M_2, to calculate $F = \psi k(a^{(2)} \cap b_0^{(2)}, a^{(2)} \cap b^{(2)})$.

Once we have obtained the expression for the ensemble $W = \phi h(c)$ with $c \in \mathcal{S}^{(1)}$ and for the effect $F = \psi k(c_0, c)$ with $(c_0, c) \in \mathcal{N}^{(2)}$ we can neglect the precise structure of preparation and registration apparatus and simply speak in terms of microsystems, that is simply deal with the more familiar *quantum mechanics of microsystems.* However we are now interested in the connection between the probabilities $\mathrm{Tr}(WF)$ and the macroscopic processes taking place between the interacting systems. Exploiting axiom **QM**, for $a \in \mathcal{Q}', g \in \mathcal{F}$, with the function μ as defined in (2.3.6) we have $\mu(a, g) = \mathrm{Tr}(\phi(a)\, \psi(g))$. According to the previously introduced relations, for $c_1 \in \mathcal{S}^{(1)}, (c_0, c_2) \in \mathcal{N}^{(2)}$ we may write $\phi(a) = \phi h(c_1)$, $\psi(g) = \psi k(c_0, c_2)$ and therefore, using (2.3.6) and (2.3.2) with $c_1 = a^{(1)} \cap b^{(1)}, c_0 = a^{(2)} \cap b_0^{(2)}, c_2 = a^{(2)} \cap b^{(2)}$:

$$\lambda_{\mathcal{S}_c}(a^{(1)} \times a^{(2)} \cap M_c \cap b^{(1)} \times b_0^{(2)}, a^{(1)} \times a^{(2)} \cap M_c \cap b^{(1)} \times b^{(2)}) =$$

$$\mathrm{Tr}\left(\phi h(a^{(1)} \cap b^{(1)})\, \psi k(a^{(2)} \cap b_0^{(2)}, a^{(2)} \cap b^{(2)})\right). \tag{2.3.7}$$

This equation may be denoted as the *interpretation formula for quantum mechanics*: to the left we have a probability for macroscopic processes, to the right a quantum-mechanical probability for the appearance of the effect $F = \psi k(a^{(2)} \cap b_0^{(2)}, a^{(2)} \cap b^{(2)})$ in the ensemble $W = \phi h(a^{(1)} \cap b^{(1)})$. The l.h.s. of (2.3.7) knows nothing about microsystems, while the r.h.s. is just a statement about microsystems.

2.4 Einstein-Podolsky-Rosen Paradox

After this brief presentation of how quantum mechanics can be based, according to Ludwig's approach, on the objective description of macroscopic devices, we intend to show how sharing this point of view the E.P.R. paradox becomes no more paradoxical. In keeping with the literature we take the usual case of two particles with spin 1/2, restricting our description to the spin variables.

We consider a preparation procedure generating correlated couples (1,2) of particles with spin 1/2 in such a way that their total spin is 0. Moreover we suppose, in accordance with experimental feasibility, that the two particles are emitted in opposite directions, so that they can be measured without further interaction between the two. The prepared ensemble is given by

$$P_\phi \quad \text{with} \quad \phi = \frac{1}{\sqrt{2}}\left[u_+(1)u_-(2) - u_-(1)u_+(2)\right], \tag{2.4.1}$$

where $u_\pm$ are eigenvectors for the z component of the spin operator. When the particles are far apart, we measure on particle 2 the spin in the z direction, that is to say the decision effect $P_{u_+(2)}$. According to this effect we can select the ensemble

$$W_1 = \frac{1}{2}P_{u_+(1)} + \frac{1}{2}P_{u_-(1)} \tag{2.4.2}$$

for 1 in that we put in the same group all systems 1 for which the effect $P_{u+(2)}$ has given a positive result, that is to say the corresponding system 2 had spin $+1/2$ along the z direction. Instead of measuring the spin of particle 2 in the z direction, we can measure its spin along the x direction as well. Denoting by $v_\pm$ the eigenvectors of the x component of the spin operator the state given by (2.4.1) can also be expressed as

$$\phi = \frac{1}{\sqrt{2}} \left[v_+(1)v_-(2) - v_-(1)v_+(2) \right].$$

Selecting now particle 2 according to $P_{v+(2)}$ we obtain for the same ensemble W_1 as in (2.4.2) the decomposition

$$W_1 = \frac{1}{2} P_{v+(1)} + \frac{1}{2} P_{v-(1)}, \tag{2.4.3}$$

where the subcollection $\frac{1}{2}P_{v-(1)}$ corresponds to the registration of effect $P_{v+(2)}$ for particle 2. The two decompositions (2.4.2) and (2.4.3) are however not coexistent, they cannot be performed together.

The fact that an ensemble W_1 of systems 1 can be decomposed in different ways without any interaction with these systems, only exploiting the correlations with another system and the effects measured on this other system, is a certainly intriguing quantum-mechanical feature, typical of scattering experiments. It is however by itself non-contradictory: the paradox emerges with the following "plausible reasoning".

An ensemble as described for example by W_1 in (2.4.2) is given by a big number of particles, let us say N. The set M^1 of the N particles corresponding to W_1 can be obviously partitioned in two subsets in different ways, for example $M^1 = M^1_{3+} \cup M^1_{3-}$ with $M^1_{3+} \cap M^1_{3-} = \emptyset$, where M^1_{3+} is the set of particles 1 for which the corresponding particle 2 has given a positive z component of the spin, and correspondingly M^1_{3-} those for which the correlated particle 2 has given a negative result. The set M^1_{3+} represents an ensemble $P_{u-(1)}$ and the set M^1_{3-} an ensemble $P_{u+(1)}$. Let us stress again that this decomposition is possible without any interaction with particle 1, simply making measurements on 2. The same set M^1 however can be partitioned also in the form $M^1 = M^1_{1+} \cup M^1_{1-}$ with $M^1_{1+} \cap M^1_{1-} = \emptyset$, where M^1_{1+} is the set of particles 1 for which the corresponding particle 2 has given a positive x component of the spin, and similarly for M^1_{1-}. M^1_{1+} corresponds to the ensemble $P_{v-(1)}$ and M^1_{1-} to $P_{v+(1)}$. One might think that both partitions of the same set should be (at least in thought) possible, in fact one can decide "after" the couples have been generated whether to measure on particle 2 the z or the x component of the spin, and this is possible without any interaction with system 1. Taking both partitions one obtains as a consequence the further partition

$$M^1 = (M^1_{3+} \cap M^1_{1+}) \cup (M^1_{3+} \cap M^1_{1-}) \cup (M^1_{3-} \cap M^1_{1+}) \cup (M^1_{3-} \cap M^1_{1-})$$

where not all four sets may be empty: let for example $(M^1_{3+} \cap M^1_{1+}) \neq \emptyset$. Then $(M^1_{3+} \cap M^1_{1+})$ is a set of systems 1 in which both the z and the x component of the spin are sharply defined. However the existence of such a set is even in principle impossible in quantum mechanics, thus leading to a contradiction.

The mistake lies in the failure to clearly distinguish between a collection of microsystems obtained by means of a preparation procedure and an ensemble, where the latter is represented by a statistical operator, and in the use of everyday language to describe experiments with microsystems. In quantum mechanics one has no fundamental mathematical quantity linked to microsystems, only ensemble appears.

Let us now reexamine the experiment in terms of preparation and registration procedure and exploiting the notion of ensemble as equivalence class. Given the preparation apparatus a for the couple and introducing another apparatus measuring the z component of the spin of particle 2 we obtain three different preparation procedures for system 1: a^3_1 all systems 1 independent of the result of the measurement on 2; a^{3+}_1 all systems 1 by which 2 has given a positive value for the spin along z; a^{3-}_1 the corresponding set in case of a negative value. We have $a^3_1 = a^{3+}_1 \cup a^{3-}_1$ and $a^{3+}_1 \cap a^{3-}_1 = \emptyset$. Moreover $\lambda_{\mathcal{Q}}(a^3_1, a^{3+}_1) = \lambda_{\mathcal{Q}}(a^3_1, a^{3-}_1) = 1/2$. $a^3_1 = a^{3+}_1 \cup a^{3-}_1$ therefore represents a decomposition of the preparation procedure a^3_1 with equal weights: to this preparation procedure is associated an ensemble $\phi(a^3_1)$ given in the spin space by W_1 as in (2.4.2). To the decomposition $a^3_1 = a^{3+}_1 \cup a^{3-}_1$ of the preparation procedure a^3_1 corresponds according to (2.2.3) a decomposition of the ensemble

$$\phi(a^3_1) = \tfrac{1}{2}\phi(a^{3+}_1) + \tfrac{1}{2}\phi(a^{3-}_1), \tag{2.4.4}$$

giving (2.4.2) in spin space. One can however build different preparation procedures, adding to the apparatus a an apparatus measuring the component of the spin of particle 2 along the x direction, thus obtaining other three preparation procedures: a^1_1 all systems 1 independent of the result of the measurement on 2; a^{1+}_1 all systems 1 by which 2 has given a positive value for the spin along x; a^{1-}_1 the corresponding set in case of a negative value. Again $a^1_1 = a^{1+}_1 \cup a^{1-}_1$ represents a decomposition of a^1_1 with equal weights. It is now fundamental to note that $\phi(a^1_1) = \phi(a^3_1)$. In spite of this $a^1_1 = a^{1+}_1 \cup a^{1-}_1$ gives a different decomposition of $\phi(a^1_1) = \phi(a^3_1)$:

$$\phi(a^1_1) = \tfrac{1}{2}\phi(a^{1+}_1) + \tfrac{1}{2}\phi(a^{1-}_1), \tag{2.4.5}$$

corresponding in spin space to the decomposition (2.4.3). We have now two different decompositions of the set of microsystems:

$$a^3_1 = a^{3+}_1 \cup a^{3-}_1 \quad \text{and} \quad a^1_1 = a^{1+}_1 \cup a^{1-}_1, \tag{2.4.6}$$

similarly to the previously obtained partitions:

$$M^1 = M_1^{3+} \cup M_1^{3-} \quad \text{and} \quad M^1 = M_1^{1+} \cup M_1^{1-}. \tag{2.4.7}$$

Between (2.4.6) and (2.4.7) there is however an important difference: in (2.4.7) we have partitioned the same set, while in (2.4.6) we are considering two different preparation procedures. Note that we are not allowed to deduce from $\phi(a_1^1) = \phi(a_1^3)$ the relation $a_1^1 = a_1^3$. It is fundamental to take into account the fact that different preparation procedures may correspond to the same ensemble, the last being an equivalence class. Keeping track of this let us try to follow the "plausible reasoning" which previously led us to a contradiction starting from (2.4.6). From (2.4.6) follows

$$a_1^3 \cap a_1^1 = (a_1^{3+} \cap a_1^{1+}) \cup (a_1^{3+} \cap a_1^{1-}) \cup (a_1^{3-} \cap a_1^{1+}) \cup (a_1^{3-} \cap a_1^{1-}), \tag{2.4.8}$$

apparently the same as before. Being $a_1^{3+} \cap a_1^{1+} \in \mathcal{Q}$, if also $a_1^{3+} \cap a_1^{1+} \neq \emptyset$ we could define an ensemble according to $\phi(a_1^{3+} \cap a_1^{1+})$. Exploiting the identities $a_1^{3+} = (a_1^{3+} \cap a_1^{1+}) \cup \tilde{a}_1^{3+}$, with $\tilde{a}_1^{3+} = a_1^{3+} \backslash (a_1^{3+} \cap a_1^{1+})$, and $a_1^{1+} = (a_1^{3+} \cap a_1^{1+}) \cup \tilde{a}_1^{1+}$, with $\tilde{a}_1^{1+} = a_1^{1+} \backslash (a_1^{3+} \cap a_1^{1+})$, the following decompositions should exist

$$\phi(a_1^{3+}) = \lambda \phi(a_1^{3+} \cap a_1^{1+}) + (1-\lambda)\phi(\tilde{a}_1^{3+}) \qquad \phi(a_1^{1+}) = \mu \phi(a_1^{3+} \cap a_1^{1+}) + (1-\mu)\phi(\tilde{a}_1^{1+}),$$

leading in spin space to the decompositions

$$P_{u_-(1)} = \lambda W' + (1-\lambda) W'' \qquad P_{v_-(1)} = \mu W' + (1-\mu) W''.$$

But $P_{u_-(1)}$ and $P_{v_-(1)}$ are extreme points of K, they cannot be further decomposed, so that we must have either $\lambda = 0$ and therefore $a_1^{3+} \cap a_1^{1+} = \emptyset$ or $\phi(a_1^{3+} \cap a_1^{1+}) = P_{u_-(1)}$. But if $a_1^{3+} \cap a_1^{1+} \neq \emptyset$ we would also have $\phi(a_1^{3+} \cap a_1^{1+}) = P_{v_-(1)}$ which is impossible because $P_{u_-(1)} \neq P_{v_-(1)}$. We have therefore $a_1^{3+} \cap a_1^{1+} = \emptyset$. The same follows for all other intersections, so that from (2.4.8) we have

$$a_1^3 \cap a_1^1 = \emptyset. \tag{2.4.9}$$

Instead of a contradiction we have now obtained (2.4.9) saying that the two preparation procedures a_1^3 and a_1^1 together do not lead to any preparation procedure apart from the empty one: there is no microsystem which can be selected both according to a_1^3 and to a_1^1. We have therefore seen that through the map ϕ, leading from the subsets a of microsystems corresponding to the preparation procedures to the equivalence classes, that is to say the ensembles, something of the structure of a is lost.

A set of preparation procedures coexistent with respect to $a \in \mathcal{Q}'$ can always be seen as subset of the Boolean ring $\mathcal{Q}(a) \equiv \{\tilde{a} | \tilde{a} \in \mathcal{Q}, \tilde{a} \subset a \in \mathcal{Q}'\}$. Let us therefore consider the ensembles $\phi(\tilde{a})$

with $\tilde{a} \in \mathcal{Q}(a)$. If $\tilde{a} = \tilde{a}_1 \cup \tilde{a}_2$ is a decomposition of such an $\tilde{a}$ (i.e., $\tilde{a}_1 \cap \tilde{a}_2 = \emptyset$) according to (2.2.3) we have, setting $\lambda = \lambda_{\mathcal{Q}}(\tilde{a}, \tilde{a}_1)$

$$\phi(\tilde{a}) = \lambda\phi(\tilde{a}_1) + (1-\lambda)\phi(\tilde{a}_2). \tag{2.4.10}$$

Defining the following map of $\mathcal{Q}(a)$ in $\check{K}$

$$\check{\phi}(\tilde{a}) = \lambda_{\mathcal{Q}}(a, \tilde{a})\phi(\tilde{a}),$$

so that (2.4.10) becomes

$$\check{\phi}(\tilde{a}) = \check{\phi}(\tilde{a}_1) + \check{\phi}(\tilde{a}_2),$$

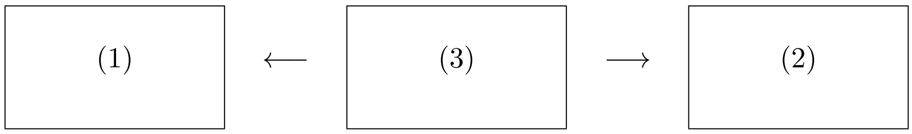
we see that $\check{\phi}$ is an additive measure on the Boolean ring $\mathcal{Q}(a)$ with $\check{\phi}(a) = \phi(a)$. Considering two different decompositions of the same $a \in \mathcal{Q}'$, $a = a_1 \cup a_2$ and $a = \tilde{a}_1 \cup \tilde{a}_2$, we have the following well defined decomposition of a (equal to (2.4.8) for the case $a_1^3 = a_1^1$)

$$a = (a_1 \cap \tilde{a}_1) \cup (a_1 \cap \tilde{a}_2) \cup (a_2 \cap \tilde{a}_1) \cup (a_2 \cap \tilde{a}_2).$$

Furthermore we have the decompositions $a_1 = (a_1 \cap \tilde{a}_1) \cup (a_1 \cap \tilde{a}_2)$, $a_2 = (a_2 \cap \tilde{a}_1) \cup (a_2 \cap \tilde{a}_2)$ and similar ones. All such decompositions go over to decompositions of the corresponding ensembles $\phi(a)$, $\phi(a_1)$, $\phi(a_2)$ and so on. What was impossible for a_1^3, a_1^1 is now possible for a single fixed a. Many decompositions of the ensemble $\phi(a)$ associated to a may be performed together. However not all decompositions of the ensemble $\phi(a)$ may be obtained from a decomposition $a = \bigcup_{i=1}^n a_i$ in terms of disjoint members of the Boolean ring $\mathcal{Q}(a)$. Together with a there are other preparation procedures $c \in \mathcal{Q}'$ such that $\phi(a) = \phi(c)$ but which could possibly lead to different decompositions of the ensemble. This clarifies the physical meaning of the definition of coexistent decomposition of an ensemble given at the end of Sect. 2.2.4.

For the ensembles $W \in K$ there are also non-coexistent decompositions and such decompositions can only be obtained with two different preparation procedures. In particular, with reference to the example with the two spin 1/2 particles, we may introduce the notion of COMPLEMENTARY DECOMPOSITION. We say that two decompositions $W = \sum_{i=1}^n W_i, W_i \in \check{K}$ and $W = \sum_{i=1}^n \tilde{W}_i, \tilde{W}_i \in \check{K}$ are complementary if, given $a, \tilde{a} \in \mathcal{Q}'$ with $\phi(a) = \phi(\tilde{a}) = W$ and a decomposition $a = \bigcup_{i=1}^n a_i$ of a and $\tilde{a} = \bigcup_{k=1}^m a_k$ of $\tilde{a}$, with $\check{\phi}(a_i) = W_i, \check{\phi}(a_k) = \tilde{W}_k$, the relation $a \cap \tilde{a} = \emptyset$ necessarily follows. The two decompositions (2.4.4) and (2.4.5) of $\phi(a_1^1) = \phi(a_1^3)$ are therefore complementary. Every preparation of two complementary decompositions of an ensemble W necessarily requires the introduction of two mutually exclusive preparation procedures.

The actual paradox in E.P.R. situations comes out if one still believes that microsystems can be envisaged as "particles" (kind of "tiny spheres") flying through space and carrying objective properties, that is being already distinguishable with respect to a definite property. This picture may hold in classical physics, where objective properties can be ascribed to physical systems. In that framework the possibility to determine some property of a system simply by making an observation on another physical system, exploiting some correlation given by a conservation law, worries nobody. The problem in quantum mechanics arises because of the existence of non-coexistent decompositions, and is particularly striking if one considers complementary decompositions of an ensemble obtained by the measurement of a non dispersive decision effect as in the example of the two correlated spin 1/2 particles. This difficulty disappears if one considers microsystems as arising from a structure of preparation and registration: then one can no more burden the microsystems with intrinsic properties pertaining to them without reference to a registration. What one actually observes in such experiments is the occurrence of two correlated macroscopic processes. The typical setup is given by the following scheme,



where system (3) directly interacts with (1) and (2). One may then consider (3) plus (1) as a preparation procedure with respect to the registration procedure (2) (or, according to the experimental conditions, (3) plus (2) as a preparation procedure for (1)). The registration on (2) depends on the possible decompositions of the given preparation procedure and only coexistent decompositions may be performed. Complementary decompositions require the introduction of a different preparation, that is of a different apparatus (1). Nevertheless the same ensemble may correspond to these two different preparation procedures, as seen above. Note that in such a description of the E.P.R. experiment one need not even mention particles or microsystems: one simply considers a suitable scheme of directed interactions between macroscopic systems and the resulting correlations between the realization of different registrations in separate space-time regions.

2.5 Summary

In this chapter we have briefly outlined Ludwig's axiomatic approach to quantum mechanics along the following line. In Sect. 2.2 we have tried to introduce the notion of microsystem as something which has been prepared by a preparation apparatus and registered by a registration apparatus. In particular Sect. 2.2.1 has been devoted to the construction of a suitable statistical theory, which has allowed the introduction of the notion of selection procedure and statistical selection procedure, in terms of which preparation and registration procedures can be built. In Sect. 2.2.2 we have defined a physical system as a set M with three structures $\mathcal{Q} \subset \mathcal{P}(M)$ (preparation procedures), $\mathcal{R} \subset \mathcal{P}(M)$ (registration procedures), $\mathcal{R}_0 \subset \mathcal{P}(M)$ (registration methods) satisfying axioms **A1** to **A7**. In Sect. 2.2.3 we have constructed ensembles and effects as equivalence classes of preparation and registration procedures respectively. In Sect. 2.2.4 we have introduced axiom **QM** determining the connection between these sets of equivalence classes and the Hilbert space formulation of quantum mechanics, reserving the name microsystem to the sets M having the three structures $\mathcal{Q}, \mathcal{R}, \mathcal{R}_0$ and satisfying axioms **A1** to **A7** together with **QM**. The set K of ensembles is then the convex set of positive trace-class operators with trace one, while the set L of effects is given by the set of positive bounded operators smaller than the unit operator. The usual definition of observable is recovered in Sect. 2.2.5, together with the more general notion of coexistent effects. In Sect. 2.3 we have sketched how the given structure of microsystem can be recovered from the description of the directed interaction of two macroscopic systems. In Sect. 2.3.1 we have shown how to describe the preparation anf registration procedures pertaining to two combined macrosystems, restricting ourselves in Sect. 2.3.2 to the case of a directed interaction. In Sect. 2.3.3 we have seen how the obtained structure might be reinterpreted in terms of a set M with the structures $\mathcal{Q}, \mathcal{R}, \mathcal{R}_0$, thus leading to the notion of interaction carrier, considering the particular case of microsystems (that is physical systems satisfying also axiom **QM**) as interaction carriers in Sect. 2.3.4. The link between the macroscopic and the microphysical interpretation of the observed experimental frequencies is given by equation (2.3.7). Finally in Sect. 2.4 we have considered the E.P.R. paradox inside this approach to the foundations of quantum mechanics. The paradoxical aspects of E.P.R. experiments are simply avoided provided one does not confuse preparation procedures and ensembles (that is to say equivalence classes of preparation procedures), so that the possible decompositions of preparation procedures pertaining to a given apparatus are not erroneously identified with the decompositions of the corresponding ensembles.

In Appendix A we have given a set of axioms alternative to axiom **QM**, allowing a much deeper understanding of the physical origin of this axiom connecting the equivalence classes of preparations and registrations to the Hilbert space structure of quantum mechanics.

Chapter 3

A Microsystem Interacting with Matter

3.1 Introduction

In the previous chapter we have tried to briefly outline the main results of Ludwig's axiomatic approach to quantum mechanics and in particular: the mathematical structure of the space of *states* (to be identified with the set of statistical operators) and *observables* (to be identified with the set of effect valued measures) that naturally comes out of this axiomatic foundation; the role of the notion of microsystem and macrosystem together with their mutual interplay in the foundations and the very structure of quantum mechanics. These two notions appear to be very deeply intertwined. On the one hand, as suggested by Bohr and substantiated by the extensive studies of Ludwig, the internal coherence of quantum mechanics and closeness to experimental reality demand that microsystems should be anchored to the objective reality of macroscopic systems (see in particular Sect. 2.4 about the E.P.R. paradox), on the other hand the success of many-particle quantum mechanics in many fields of physics shows that some basic features in the description of the behavior of macroscopic systems can be obtained from the usual quantum mechanical description of its microphysical constituents, simply exploiting the notion of tensor product of Hilbert spaces. However complex it may be, the relation between microsystems and macrosystems is of utmost importance and deserves further investigation.

In this spirit, taking advantage of the modern formulation of quantum mechanics that has naturally grown out of the studies of Ludwig and of many other authors (see for example [16, 17, 18] and references quoted therein), and also trying to keep in mind the lesson of Ludwig on quantum mechanics, we have tackled the problem of the description of the interaction of a microsystem with a system having many degrees of freedom, typically matter at equilibrium. The purpose of this study is twofold. On the one hand, exploiting a simple mechanism in order to obtain the dynamics of the microsystem from the dynamics of the full macroscopic system, we see that a typical preparation procedure is indeed to be represented by a statistical operator and not by a pure state. The accompanying dynamics is much more general and also irreversibility in the interaction can be accounted for, expressing the directedness of the interaction between the preparation procedure and a final registration. This study has been developed in the framework of modern single particle experiments, whose impressive richness and precision require a detailed quantum mechanical description. In particular we have considered interferometric experiments, typically neutron interferometry, which should be most relevant in this connection. Such experiments are particularly sensitive to the problem of decoherence, which plays a major role in many interpretations of quantum mechanics (for a recent review see [6]) and is very important also in connection with the feasibility of quantum computing [19]. The more general expression for the dynamics we obtain allows in fact the description of incoherent effects in the interaction, a point we will deal with particularly in Sect. 4.2.2. On the other hand the emphasis in the calculation is toward the individuation of a general scheme for the description of subdynamics in nonrelativistic quantum field theory. The key point is the choice of a time scale and of suitably slowly varying variables on this time scale. In a sense one has to adjust the temporal evolution to the chosen variables, which are the ones liable to experimental observation. The necessity to introduce such a time scale, especially in the case of macroscopic systems, is linked to the very definition of an isolated system, a point we will explain in more detail in Chap. 5. It appears to us that this attitude might be useful in order to obtain a quantum mechanical description of macroscopic systems. In fact it does not seem that the huge set of preparation anf registration procedures, and therefore indirectly of states and observables, that arise if one tries to extrapolate quantum mechanics to a many-particle system by the tensor product method, are physically realizable. On the contrary the actual set of states and observables should be tuned to the possible registrations and preparations, which actually define the system.

The reader should not expect our work to be a direct application or straightforward concrete realization of the notion of microsystem as obtained by Ludwig. Neither have we solved the Titanic problem of obtaining a definite state or effect starting simply from some phenomenological macroscopic description of a preparation or registration apparatus. We have simply done an attempt, with an eye both to modern experiments and to typical quantum field theoretical structures, to a better understanding of some concrete problem of quantum mechanics which might shed some light on the questions of the notion of particle and of the description of macroscopic systems.

3.2 Experiments with Microsystems

Consider a source, emitting practically only one particle each time, feeding an interferometer; one of the most impressing features of quantum mechanics is the fact that the record in a detector of the output of the interferometer, during a suitable time interval, shows an interference pattern. If the experimental setup allows detectable events to be produced during the time the particle takes to pass through the interferometer, thus showing which way the particle went, a two component pattern is found, respectively affected and not affected by interference. Seemingly the interfering part can be strongly attenuated, if the probability of detecting events is enhanced, still retaining its visibility. Let us mention some of the experiments of relevance to the question carried out in different fields in the last years [20, 21, 22, 23]. It was sometimes claimed, and also appears in textbooks, that the very possibility of such a detection forces the interference pattern to disappear; such a somewhat strange expectation is rooted in an exaggerated faith in the so-called state reduction postulate of quantum mechanics. This postulate is a strongly idealized description of what happens to a quantum system due to the interaction with a device measuring a given observable of the system; using this postulate a shorthand explanation of measurement is usually given, based on the idea that a quantum system must be represented by a *state vector* $\psi(t)$. A much more comfortable situation is met if, instead of a state vector, a statistical operator $\varrho(t)$ is taken as the basic mathematical representation of a quantum system [24], as also suggested by the axiomatic foundation of quantum mechanics surveyed in Chap. 2. This attitude is sometimes considered suitable for applications, e.g., quantum optics, but not fine enough for more fundamental problems; it is often implicitly assumed that a statistical operator applies only to the description of a statistical mixture of a large number of microsystems, while in modern experiments often only one or very few relevant microsystems are present altogether in the experimental device. In this single-particle experiments it is often argued [25, 26] that the system is to be described by a state vector. In our opinion, instead, one-particle quantum mechanics, no matter if one uses $\psi(t)$ or $\varrho(t)$, refers in principle to a statistical experiment in which repeatedly a single particle is produced, prepared and observed under fixed macroscopic conditions; this does not oppose the fact that a beam of particles whose interactions are negligible and whose correlations are irrelevant may be treated in many experimental situations as effectively equivalent to the former preparation. It is just the modalities of the statistical experiment, which remain unchanged during the different runs of the experiment, that are represented by the statistical operator (or by the state vector, when this higher idealization works); this is indeed the striking difference with classical mechanics, where to each run of the statistical experiment corresponds a trajectory in phase space. In this context a completely different point of view seems to underlie the so-called many-Hilbert-space quantum mechanics, that was recently proposed [27]. In this framework a wave function is associated to each single-run of a statistical experiment and for example in a Young's interference experiment random phase shifts between the two branch waves may arise in the repeated experimental runs, due to interaction with matter along one of the two branches, leading to attenuation of the interference pattern [25].

As it is well known state vectors $\psi \in \mathcal{H}$, via the one dimensional projections P_ψ on $\mathcal{H}$, correspond to the subset of extreme points of the convex set $\mathcal{K}$ of statistical operators in $\mathcal{H}$: they cannot be interpreted as mixtures of other possible preparations and any $\varrho \in \mathcal{K}$ can be represented as $\varrho = \sum_j p_j P_{\psi_j}$. For this reason state vectors $\psi \in \mathcal{H}$ are also called *pure states*. Let us recall a relevant mathematical result, whose demonstration can be found in [12, 17]: any invertible affine mapping $\mathcal{M}$ on $\mathcal{K}$ onto $\mathcal{K}$ has the form

$$\mathcal{M}\varrho = M\varrho M^\dagger,$$

M being a unitary (or antiunitary) operator on $\mathcal{H}$; then, if time evolution is represented by such a mapping [28], the basic role of pure states for the dynamics becomes obvious and consequently also the relevance of the Schrödinger equation, of the Hamilton operator and finally the correspondence with classical mechanics and classical field theory. Summing up in formulae:

$$\varrho_t = \mathcal{M}_{tt_0}\varrho_{t_0} = U(t,t_0)\varrho_{t_0}U^\dagger(t,t_0) = \sum_j p_j P_{\psi_j(t)}$$

$$\psi_t = U(t,t_0)\psi_{t_0}, \qquad i\hbar\frac{d\psi_t}{dt} = H_t\psi_t.$$

In fact the main part of the physics of microsystems can be developed almost neglecting the concept of statistical operator; a noteworthy exception, however, is given by the definition of the quantum collision cross-section (a point rarely stressed in quantum mechanics textbooks). The use of an improper eigenvector $u_{\mathbf{p}_0}(\mathbf{x})$ of $\mathcal{H}$ to represent an incoming particle of momentum $\mathbf{p}_0$ in a scattering experiment is a very useful and in many cases perfectly justified shorthand replacement of a statistical operator ϱ, built as a mixture of wave packets

$$\psi_{\mathbf{b}}(\mathbf{x}) = \int d^3p \; c(\mathbf{p})\, e^{-\frac{i}{\hbar}\mathbf{p}_\perp\cdot\mathbf{b}}\, u_{\mathbf{p}}(\mathbf{x}),$$

$\mathbf{p}_\perp$ denoting the orthogonal component of $\mathbf{p}$ with respect to $\mathbf{p}_0$, with $c(\mathbf{p})$ suitably peaked around $\mathbf{p}_0$, the mixture being performed over the impact parameter $\mathbf{b}$; in this way one can represent the fact that in the statistical experiment the prepared incoming particle has a large delocalization, large with respect to the range of the interaction with the scattering center. Just in this way the concept of cross section emerges from the formalism and apart from the dependence on $\mathbf{p}_0$

substantial independence from the shape of the wave packet is achieved [13, 29]. In conclusion any time the plane wave picture of the preparation of a particle proves to be working one is dealing in fact with a statistical operator and not with a pure state.

A reversible dynamics however is to be expected only for an isolated system. If interaction with an environment is not negligible during the time evolution the question to be raised is whether this evolution can be simply described by a mapping $\mathcal{M}_{tt_0}$ on $\mathcal{K}$; i.e., whether ϱ_t is uniquely determined by ϱ_{t_0} and not by the whole history $\{\varrho_{t'}; t' \leq t_0\}$ before t_0, recorded via interaction by this environment. In this general situation the system becomes the whole complex of particle plus environment and no disentanglement of the particle's degrees of freedom is possible. On the contrary a neat and extremely relevant simplification occurs if such a mapping $\mathcal{M}_{tt_0}$ exists: then the one-particle Hilbert space $\mathcal{H}$ and not the Fock-space of the whole system is the relevant mathematical framework. Let us assume that this simplification occurs, typically due to the fact that the aforementioned history is forgotten during the time elapsed before ϱ_t varies appreciably, as in the case of Markovian dynamics; nevertheless one can no longer expect $\mathcal{M}_{tt_0}$ to be invertible: then the statistical operator ϱ_t acquires a primary role. In differential form the evolution equation for ϱ_t is:

$$\frac{d\varrho_t}{dt} = \mathcal{L}_t \varrho_t, \qquad \mathcal{L}_t = \lim_{\tau \to 0} \frac{\mathcal{M}(t+\tau, t) - \mathcal{I}}{\tau},$$

$$\mathcal{M}_{tt_0} = \mathrm{T}\left(\exp \int_{t_0}^{t} dt'\, \mathcal{L}(t')\right). \tag{3.2.1}$$

In Sect. 3.2.1 we explicitly construct the generator $\mathcal{L}_t$ of the temporal evolution for the microsystem showing in a general way how it can be obtained starting from the Hamiltonian describing the local interaction between microsystem and macrosystem. An essential step is the introduction of a time scale on which the system is to be described, linked to the irreversibility of the interaction. To develop the calculations we rely upon a reformulation of the theory of scattering based on superoperators, that is mappings defined on the algebra generated by creation and annihilation operators acting in the Fock-space. Quantum statistics is readily accounted for and the mapping $\mathcal{T}(z)$ [see (3.2.16)], strictly connected to the transition operator of the quantum theory of scattering, plays a central role from the very beginning. The use of the Heisenberg picture, consistent with the concentration of one's attention on the microsystem's observables, allows to keep the whole complex structure of the macrosystem into account. The generator obtained is of the Lindblad type, though allowing for unbounded operators. The general structure of such generators, ensuring that $\mathcal{M}_{tt_0}$ maps $\mathcal{K}$ into $\mathcal{K}$, is the following [30, 31]:

$$\mathcal{L}_t \varrho = -\frac{i}{\hbar}\left(H_t \varrho - \varrho H_t\right) - \frac{1}{\hbar}\left(A_t \varrho + \varrho A_t\right) + \frac{1}{\hbar}\sum_j L_{tj} \varrho L_{tj}^{\dagger} \tag{3.2.2}$$

$$H_t = H_t^\dagger, \quad A_t \geq 0, \quad L_{tj} \quad \text{being operators in } \mathcal{H} \quad .$$

The relation:

$$A_t = \frac{1}{2}\sum_j L_{tj}^\dagger L_{tj}, \tag{3.2.3}$$

must be satisfied in order that $\mathrm{Tr}\varrho_t$ be conserved. If the particle can be absorbed (3.2.3) is replaced by

$$A_t \geq \frac{1}{2}\sum_j L_{tj}^\dagger L_{tj}. \tag{3.2.4}$$

If the last term in (3.2.2) is neglected, for a pure state $\varrho_t = |\psi_t\rangle\langle\psi_t|$ (3.2.1) yields the Schrödinger equation:

$$i\hbar\frac{d\psi_t}{dt} = (H_t - iA_t)\,\psi_t; \tag{3.2.5}$$

this is the basis for the wavelike description of propagation of a particle inside matter. Setting $H_t - iA_t = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}, t)$ one can define

$$n(\mathbf{x}, \nu, t) = \sqrt{1 - \frac{V(\mathbf{x}, t)}{h\nu}} \tag{3.2.6}$$

as refractive index of the medium, where $h\nu$ is to be identified with the energy of the incoming particle: such a description is usually adopted in interferometric experiments to explain how a block of matter, whose properties are accounted for by the phenomenological macroscopic potential $V(\mathbf{x}, t)$, placed in one of the two branches can induce a phase shift in the corresponding branch-wave, or, in the case of an imaginary potential, cause absorption [8]. Only in the very special case of $A_t = 0$, i.e., for a real "macroscopic" potential $V(\mathbf{x}, t)$, by (3.2.3) or (3.2.4) one has $L_{tj} = 0$ and (3.2.5) is exactly equivalent to (3.2.2). In presence of absorption $A_t \neq 0$ implies by (3.2.3) $L_{tj} \neq 0$ for some j; but also in absence of absorption one cannot expect that $L_{tj} = 0$. Notice that, if one is not aware of the basic role of (3.2.2) and of the importance of the last term at its r.h.s., by (3.2.5) one could be confirmed in the erroneous belief that non-reality of the potential V is exclusively linked to absorption processes. To grasp the significance of the term $\frac{1}{\hbar}\sum_j L_{tj}\varrho L_{tj}^\dagger$ for the dynamics of ϱ let us write the evolution of ϱ due to it in a small time interval τ in the form:

$$\Delta\varrho = \frac{\tau}{\hbar}\mathrm{Tr}\,(2A_t\varrho)\sum_j \tilde{L}_{tj}\varrho\tilde{L}_{tj}^\dagger, \qquad \tilde{L}_{tj} = \frac{L_{tj}}{\sqrt{\mathrm{Tr}\,(2A_t\varrho)}}; \tag{3.2.7}$$

The statistical operator $\sum_j \tilde{L}_{tj}\varrho\tilde{L}_{tj}^\dagger$ is a mixture of subcollections $\tilde{L}_{tj}\varrho\tilde{L}_{tj}^\dagger$ related to outcome channels labeled by the index j; it bears some resemblance with the statistical operator $\sum_j P_j\varrho P_j$ which represents, by the previously mentioned reduction postulate, the system after the measurement of an observable $A = \sum_j a_j P_j$; $(1/\hbar)\mathrm{Tr}\,(2A_t\varrho)$ expresses the strength of the coupling to the incoherent regime. More generally a mapping whose infinitesimal generator is of the form (3.2.2) admits measuring decompositions that have been characterized in the context of *continuous measurement theory*, initiated by Davies for the counting processes [32, 33] and developed later in full generality [34, 35, 36, 37, 38] (for a recent review see [24, 39]). These decompositions are related to the operators L_{tj}, responsible for the irreversible dynamics, and clarify what is meant by the measuring character of a mapping describing the temporal evolution of a system. We will see in Sect. 3.2.5 that (3.2.2) couples very simply the typical wave dynamics, which is responsible for interference phenomena, with a *non-coherent* regime. Obviously in many instances the main interest is to put the wavelike behavior in major evidence; this amounts to make L_{tj} negligible, so that (3.2.5) is indeed suitable to describe the dynamics. On the contrary more recent investigations, e.g., neutron interferometry in presence of stray absorption in one path of the interferometer [20, 21], aim at investigating the competition between wavelike coherent behavior and which-way detection: then (3.2.1) and (3.2.2) must be considered. In Sect. 3.2.5 the physical interpretation of the dynamics thus obtained for the microsystem is discussed, showing the interplay between a "purely optical" regime [such as in (3.2.5) and (3.2.6)] and an "events producing" one, strictly connected to the presence of the incoherent contribution in the r.h.s. of (3.2.2).

3.2.1 Construction of the Generator

We assume for simplicity that the whole system is confined, e.g., in a box; eventually we can get rid of this confinement letting the size of the box go to infinity. The microsystem is described in a Hilbert space $\mathcal{H}^{(1)}$; energy eigenvalues are E_f, energy eigenstates u_f, spanning the space $\mathcal{H}^{(1)}$. In the following we shall make use of the formalism of non-relativistic quantum field theory, which will prove to play an essential role in order to obtain a general procedure leading from the second quantized Hamiltonian H of the whole system, acting in the global Fock-space $\mathcal{H}_F$, to the generator of the semigroup $\mathcal{L}$ acting in $\mathcal{T}(\mathcal{H}^{(1)})$ (the set of trace-class operators in $\mathcal{H}^{(1)}$).

We shall set:

$$H = H_0 + H_{\rm m} + V$$

$$H_0 = \sum_f E_f a_f^\dagger a_f \qquad\qquad \left[a_f, a_g^\dagger\right]_\mp = \delta_{fg}$$

where a_f is the annihilation operator for the microsystem, either a Fermi or a Bose particle, in the state u_f; $H_{\rm m}$ is the Hamilton operator for the sole macrosystem ($[H_{\rm m}, a_f] = 0$), also containing the potential determining the internal structure of the macrosystem; V represents the interaction between the two systems. We shall assume in this paper that no absorption process of the microsystem occurs: then $N = \sum_h a_h^\dagger a_h$ is a constant, $[N, H] = [N, V] = 0$. The present treatment is non-relativistic due to the role played by particle number conservation.

Having in mind to describe situations in which only one particle is observed in each experimental run, or equivalently a collection of noninteracting particles in each run, we assume for the statistical operator the following expression:

$$\rho = \sum_{gf} a_g^\dagger \varrho_{\mathrm{m}} a_f \varrho_{gf}, \tag{3.2.8}$$

where ϱ_{m} is a statistical operator in the subspace $\mathcal{H}_F^0$ of $\mathcal{H}_F$ in which $N = 0$, representing the macrosystem and therefore:

$$a_f \varrho_{\mathrm{m}} = 0 \quad \varrho_{\mathrm{m}} a_f^\dagger = 0 \quad \forall f, \tag{3.2.9}$$

while ρ is a statistical operator in the subspace $\mathcal{H}_F^1$ of $\mathcal{H}_F$ in which $N = 1$. As far as the microsystem is concerned, the dynamics of the macrosystem is not appreciably perturbed by the presence of the microsystem itself, so we can assume that

$$\frac{d\varrho_{\mathrm{m}}(t)}{dt} = -\frac{i}{\hbar}[H_{\mathrm{m}}, \varrho_{\mathrm{m}}(t)].$$

The coefficients ϱ_{gf} build a positive, trace one matrix, which can be considered as the representative of a statistical operator $\hat{\varrho}$ in the Hilbert space $\mathcal{H}^{(1)}$ spanned by the states u_f, $\varrho_{gf} = \langle u_g|\hat{\varrho}|u_f\rangle$ (operators in the one particle Hilbert space $\mathcal{H}^{(1)}$ will be denoted by a sans serif letter with a hat). Equation (3.2.9) indicates that the system has charge $Q = \sum_f a_f^\dagger a_f$ with value zero, i.e., it does not contain the microsystem, while equation (3.2.8) represents the fact that the system has been perturbed by the additional particle

$$Q\varrho_{\mathrm{m}} = 0, \qquad Q\rho = \rho$$

and it therefore presents a new dynamical behavior contained in the coefficients ϱ_{gf} that can be picked out studying the time evolution of observables of the form

$$A = \sum_{hk} a_h^\dagger A_{hk} a_k = \sum_{hk} a_h^\dagger \langle h|\hat{\mathsf{A}}|k\rangle a_k, \tag{3.2.10}$$

where A_{hk} is the matrix element of the corresponding operator acting in $\mathcal{H}^{(1)}$. Since we are interested in the subdynamics of the microsystem we will make use of the following reduction formula from $\mathcal{H}_F$ to $\mathcal{H}^{(1)}$ for the expectation value of an observable A of the form (3.2.10) in the state (3.2.8):

$$\mathrm{Tr}_{\mathcal{H}_F}(A\rho) = \sum_{hk} A_{hk}\varrho_{kh} = \mathrm{Tr}_{\mathcal{H}^{(1)}}\left(\hat{\mathsf{A}}\hat{\varrho}\right) \tag{3.2.11}$$

Considering in particular the operator $A = a_f^\dagger a_g$ we have:

$$\mathrm{Tr}_{\mathcal{H}_F}(A\rho) = \varrho_{gf}.$$

To individuate the generator of the semigroup we will consider the evolution of the statistical operator on a time scale τ much longer than the correlation time for the macrosystem, thus approximating $d\varrho_{gf}(t)/dt$ by:

$$\frac{\Delta\varrho_{gf}(t)}{\tau} = \frac{1}{\tau}\left[\varrho_{gf}(t+\tau) - \varrho_{gf}(t)\right] = \frac{1}{\tau}\left[\mathrm{Tr}_{\mathcal{H}_F}\left(a^\dagger_f a_g e^{-\frac{i}{\hbar}H\tau}\varrho(t)e^{\frac{i}{\hbar}H\tau}\right) - \varrho_{gf}(t)\right]. \tag{3.2.12}$$

Exploiting the cyclicity of the trace we will work in Heisenberg picture, shifting the action of the temporal evolution operator on the simple expression $a^\dagger_f a_g$, thus considerably simplifying the calculation without introducing restrictive assumptions on the structure of ϱ_{m} or of the interaction. One has to study the expression $e^{\frac{i}{\hbar}Ht}a^\dagger_h a_k e^{-\frac{i}{\hbar}Ht}$, exploiting the fact that the expectation values $\langle A\rangle_t$ are "slowly varying" if the matrix A_{hk} is "quasi-diagonal" (if $A_{hk} = \delta_{hk}$, A is a conserved charge). To proceed further we introduce the following superoperators (the prime denoting the adjoint mapping in Heisenberg picture)

$$\mathcal{H}' = \frac{i}{\hbar}[H,\cdot], \quad \mathcal{H}'_0 = \frac{i}{\hbar}[H_0 + H_{\mathrm{m}},\cdot], \quad \mathcal{V}' = \frac{i}{\hbar}[V,\cdot], \tag{3.2.13}$$

acting on the algebra generated by creation and annihilation operators. Note that the operators $(a^\dagger_{h_1})^{n_1}(a^\dagger_{h_2})^{n_2}\ldots(a^\dagger{}_{h_r})^{n_r}(a_{k_1})^{m_1}(a_{k_2})^{m_2}\ldots(a_{k_s})^{m_s}$ are "eigenstates" of the superoperator $\mathcal{H}'_0$ with eigenvalues $\frac{i}{\hbar}\left(\sum_{i=1}^r n_i E_{h_i} - \sum_{i=1}^s m_i E_{k_i}\right)$, in particular:

$$\mathcal{H}'_0 a_h = -\frac{i}{\hbar}E_h a_h \qquad \mathcal{H}'_0 a^\dagger_h = +\frac{i}{\hbar}E_h a^\dagger_h.$$

To calculate (3.2.12), setting $\mathcal{U}'(t) = e^{\mathcal{H}'t}$ we evaluate $\mathcal{U}'(t)\left(a^\dagger_h a_k\right)$ with the help of the following integral representation:

$$\begin{aligned}\mathcal{U}'(t)\left(a^\dagger_h a_k\right) &= \left(\mathcal{U}'(t)a^\dagger_h\right)\left(\mathcal{U}'(t)a_k\right)\\ &= \int_{-i\infty+\eta}^{+i\infty+\eta}\frac{dz_1}{2\pi i}\,e^{z_1 t}\left[\left(z_1 - \mathcal{H}'\right)^{-1}a^\dagger_h\right]\int_{-i\infty+\eta}^{+i\infty+\eta}\frac{dz_2}{2\pi i}\,e^{z_2 t}\left[\left(z_2 - \mathcal{H}'\right)^{-1}a_k\right].\end{aligned}$$

Let us stress at this point the relevance of the formalism of second quantization. The operator quantities of interest can be expressed in terms of products of creation and annihilation operators. The study of their time evolution may thus be reconducted to evaluation of field operators of the form $e^{\mathcal{H}'t}a^\dagger_h$ connecting in the Fock-space subspaces with n and $n+1$ particles (and similarly for $e^{\mathcal{H}'t}a_k$ connecting subspaces with n and $n-1$ particles). Thus, even recovering at the end the usual one particle quantum mechanics, the Fock-space structure plays a central role and accounts for the similarities between this simple case and the description of macroscopic systems (see Chap. 5). For the mappings defined in (3.2.13) identities hold that are reminiscent of the usual ones in scattering theory:

$$\left(z - \mathcal{H}'\right)^{-1} = \left(z - \mathcal{H}'_0\right)^{-1}\left[1 + \mathcal{V}'\left(z - \mathcal{H}'\right)^{-1}\right] = \left[1 + \left(z - \mathcal{H}'\right)^{-1}\mathcal{V}'\right]\left(z - \mathcal{H}'_0\right)^{-1}. \tag{3.2.14}$$

In particular we can introduce the superoperator $\mathcal{T}(z)$

$$\mathcal{T}(z) \equiv \mathcal{V}' + \mathcal{V}'(z-\mathcal{H}')^{-1}\mathcal{V}', \tag{3.2.15}$$

satisfying

$$(z-\mathcal{H}')^{-1} = (z-\mathcal{H}'_0)^{-1} + (z-\mathcal{H}'_0)^{-1}\mathcal{T}(z)(z-\mathcal{H}'_0)^{-1}$$

and

$$\mathcal{T}(z) = \mathcal{V}' + \mathcal{V}'(z-\mathcal{H}'_0)^{-1}\mathcal{T}(z), \tag{3.2.16}$$

corresponding to the Lippman-Schwinger equation for the T-matrix. Taking into account the fact that $[H,N]=0$ one can see that the restriction to $\mathcal{H}^1_F$ of the operator $\mathcal{T}(z)[a_k]$ has the simple general form:

$$i\hbar\mathcal{T}(z)[a_k]_{|\mathcal{H}^1_F} = \sum_f T^k_f\,(i\hbar z)\,a_f, \tag{3.2.17}$$

and similarly, taking the adjoint

$$-\,i\hbar\mathcal{T}(z^*)[a^\dagger_h]_{|\mathcal{H}^0_F} = \sum_f \left[T^h_f\,(i\hbar z)\right]^\dagger a^\dagger_f \equiv \sum_f T^{h\dagger}_f\,(i\hbar z)a^\dagger_f.$$

where $T^k_f\,(z)$ is an operator in the subspace $\mathcal{H}^0_F$. This restriction is the only part of interest to us, since we are considering a single microsystem. One can also express $T^k_f\,(z)$ in terms of $\mathcal{T}(z)$ as:

$$\begin{aligned} i\hbar\mathcal{T}(z)[a_k]a^\dagger_{h|\mathcal{H}^0_F} &= T^k_h(i\hbar z) \\ -i\hbar a_h\mathcal{T}(z)[a^\dagger_k]_{|\mathcal{H}^0_F} &= T^{k\dagger}_h(i\hbar z^*). \end{aligned} \tag{3.2.18}$$

Denoting by $|\lambda\rangle \equiv |0\rangle\otimes|\lambda\rangle$ the basis of eigenstates of $H_{\rm m}$ spanning $\mathcal{H}^0_F$, $H_{\rm m}|\lambda\rangle = E_\lambda|\lambda\rangle$, and exploiting (3.2.17) we obtain the following explicit representation of $\mathcal{U}'(t)a_{k|\mathcal{H}^1_F}$ as a mapping of $\mathcal{H}^1_F$ into $\mathcal{H}^0_F$:

$$\begin{aligned} \mathcal{U}'(t)a_{k|\mathcal{H}^1_F} &= \int_{-i\infty+\eta}^{+i\infty+\eta}\frac{dz}{2\pi i}\,e^{zt}\left[\frac{1}{z-\mathcal{H}'_0} + \frac{1}{z-\mathcal{H}'_0}\mathcal{T}(z)\frac{1}{z-\mathcal{H}'_0}\right]a_{k|\mathcal{H}^1_F} \\ &= \int_{-i\infty+\eta}^{+i\infty+\eta}\frac{dz}{2\pi i}\,e^{zt}\frac{1}{z+\frac{i}{\hbar}E_k}\left[a_k + \frac{1}{z-\mathcal{H}'_0}\frac{1}{i\hbar}\sum_f T^k_f(i\hbar z)a_f\right] \\ &= e^{-\frac{i}{\hbar}E_k t}a_k + \frac{1}{i\hbar}\sum_{\substack{\lambda\lambda' \\ f}}\int_{-i\infty+\eta}^{+i\infty+\eta}\frac{dz}{2\pi i}\,e^{zt}\frac{|\lambda'\rangle\langle\lambda'|T^k_f(i\hbar z)|\lambda\rangle\langle\lambda|}{\left(z+\frac{i}{\hbar}E_k\right)\left(z+\frac{i}{\hbar}(E_f+E_\lambda-E_{\lambda'})\right)}a_f. \end{aligned}$$

Since these expression will be considered for values of the complex variable z of the form $iy + \eta$, we can replace $E_k \to E_k + i\varepsilon$, $E_f \to E_f + 2i\varepsilon$, $\eta > \varepsilon > 0$, without introducing singularities and obtaining an expression that depends smoothly on the parameter ε:

$$e^{-\frac{i}{\hbar}E_k t} a_k + \frac{1}{i\hbar} \sum_{\substack{\lambda\lambda' \\ f}} \int_{-i\infty+\eta}^{+i\infty+\eta} \frac{dz}{2\pi i} e^{zt} \frac{|\lambda'\rangle\langle\lambda'|T_f^k(i\hbar z)|\lambda\rangle\langle\lambda|}{\left(z + \frac{i}{\hbar}E_k - \frac{\varepsilon}{\hbar}\right)\left(z + \frac{i}{\hbar}(E_f + E_\lambda - E_{\lambda'}) - 2\frac{\varepsilon}{\hbar}\right)} a_f.$$

The operator $\mathcal{T}(z)$ has poles on the imaginary axis for $z = (i/\hbar)(e_\alpha - e_\beta)$, e_α being the eigenvalues of H. In the calculation we shall assume that the function $\mathcal{T}(z)$ for $\mathrm{Re}\, z \approx \varepsilon$ with $\varepsilon \gg \delta$ (δ typical spacing between the poles) is smooth enough, so that the only relevant contribution stems from the singularities of $(z - \mathcal{H}_0')^{-1}$; this smoothness property is linked to the fact that the set of poles of $(z - \mathcal{H}')^{-1}$ goes over to a continuum if the confinement is removed yielding an analytic function with a cut along the imaginary axis, that can be continued across the cut without singularities if no absorption of the microsystem occurs. More precisely $\mathcal{T}(iy + \varepsilon)$ is considered practically constant for variations $\Delta y \approx \hbar/\tau_0$, where τ_0 has to be interpreted as a collision time. We thus come to

$$\begin{aligned} \mathcal{U}'(t) a_{k|\mathcal{H}_F^1} \approx\ & e^{-\frac{i}{\hbar}E_k t} a_k \\ & + \sum_{\substack{\lambda\lambda' \\ f}} |\lambda'\rangle \left[\frac{e^{-\frac{i}{\hbar}E_k t + \frac{\varepsilon}{\hbar}t} - e^{-\frac{i}{\hbar}(E_f + E_\lambda - E_{\lambda'})t + 2\frac{\varepsilon}{\hbar}t}}{E_k + E_{\lambda'} - E_f - E_\lambda - i\varepsilon} \langle\lambda'|T_f^k(E_k + i\varepsilon)|\lambda\rangle \right. \\ & \left. + e^{-\frac{i}{\hbar}(E_f - E_\lambda - E_{\lambda'})t + 2\frac{\varepsilon}{\hbar}t} \frac{\langle\lambda'|T_f^k(E_f + E_\lambda - E_{\lambda'} + 2i\varepsilon) - T_f^k(E_k + i\varepsilon)|\lambda\rangle}{[E_f + E_\lambda - E_{\lambda'} + 2i\varepsilon] - [E_k + i\varepsilon]} \right] \langle\lambda| a_f. \end{aligned}$$

The last term of this expression is a sum, with different phase factors, of increments of the $T_f^k(z)$ operator with respect to its energy dependence and may be considered negligible on a time scale t much longer than the correlation time for the macrosystem: we are thus working on a time scale long enough to ignore fluctuations from the non-perturbed state for the macrosystem. We are left with

$$\begin{aligned} \mathcal{U}'(t) a_{k|\mathcal{H}_F^1} \approx\ & e^{-\frac{i}{\hbar}E_k t} a_k \\ & + \sum_{\substack{\lambda\lambda' \\ f}} \frac{e^{-\frac{i}{\hbar}E_k t + \frac{\varepsilon}{\hbar}t} - e^{-\frac{i}{\hbar}(E_f + E_\lambda - E_{\lambda'})t + 2\frac{\varepsilon}{\hbar}t}}{E_k + E_{\lambda'} - E_f - E_\lambda - i\varepsilon} |\lambda'\rangle\langle\lambda'|T_f^k(E_k + i\varepsilon)|\lambda\rangle\langle\lambda| a_f, \end{aligned}$$

and similarly for the adjoint map

$$\begin{aligned} \mathcal{U}'(t) a^\dagger_{h|\mathcal{H}_F^0} \approx\ & e^{+\frac{i}{\hbar}E_h t} a_h^\dagger \\ & + \sum_{\substack{\alpha\alpha' \\ g}} a_g^\dagger |\alpha\rangle\langle\alpha|T_g^{h\dagger}(E_h + i\varepsilon)|\alpha'\rangle\langle\alpha'| \frac{e^{\frac{i}{\hbar}E_h t + \frac{\varepsilon}{\hbar}t} - e^{\frac{i}{\hbar}(E_g + E_\alpha - E_{\alpha'})t + 2\frac{\varepsilon}{\hbar}t}}{E_h + E_{\alpha'} - E_g - E_\alpha + i\varepsilon}. \end{aligned}$$

Multiplying the two expressions we have

$$\begin{aligned}
\mathcal{U}'(t)\,(a_h^\dagger a_k)_{|\mathcal{H}_F^1} &= e^{\frac{i}{\hbar}(E_h-E_k)t} a_h^\dagger a_k \\
&+ \sum_{\substack{\lambda\lambda' \\ f}} \frac{e^{\frac{i}{\hbar}(E_h-E_k)t+\frac{\varepsilon}{\hbar}t} - e^{\frac{i}{\hbar}(E_h+E_{\lambda'}-E_f-E_\lambda)t+2\frac{\varepsilon}{\hbar}t}}{E_k+E_{\lambda'}-E_f-E_\lambda-i\varepsilon} a_h^\dagger |\lambda'\rangle\langle\lambda'|T_f^k(E_k+i\varepsilon)|\lambda\rangle\langle\lambda|a_f \\
&+ \sum_{\substack{\alpha\alpha' \\ g}} \frac{e^{\frac{i}{\hbar}(E_h-E_k)t+\frac{\varepsilon}{\hbar}t} - e^{\frac{i}{\hbar}(E_g+E_\alpha-E_{\alpha'}-E_k)t+2\frac{\varepsilon}{\hbar}t}}{E_h+E_{\alpha'}-E_g-E_\alpha+i\varepsilon} a_g^\dagger |\alpha\rangle\langle\alpha|T_g^{h\dagger}(E_h+i\varepsilon)|\alpha'\rangle\langle\alpha'|a_k \\
&+ \sum_{\substack{\lambda\alpha\alpha' \\ gf}} a_g^\dagger|\alpha\rangle \frac{\langle\alpha|T_g^{h\dagger}(E_h+i\varepsilon)|\alpha'\rangle}{E_g+E_\alpha-E_h-E_{\alpha'}-i\varepsilon} \frac{\langle\alpha'|T_f^k(E_k+i\varepsilon)|\lambda\rangle}{E_f+E_\lambda-E_k-E_{\alpha'}+i\varepsilon}\langle\lambda|a_f \\
&\quad\times\Big[e^{\frac{i}{\hbar}(E_h-E_k)t+2\frac{\varepsilon}{\hbar}t} - e^{\frac{i}{\hbar}(E_h+E_{\alpha'}-E_f-E_\lambda)t+3\frac{\varepsilon}{\hbar}t} \\
&\quad\quad -e^{\frac{i}{\hbar}(E_g+E_\alpha-E_k-E_{\alpha'})t+3\frac{\varepsilon}{\hbar}t} + e^{\frac{i}{\hbar}(E_g+E_\alpha-E_f-E_\lambda)t+4\frac{\varepsilon}{\hbar}t}\Big]. \qquad (3.2.19)
\end{aligned}$$

On a time scale t, $\tau_0 \ll t \ll \tau_1$, where τ_1 represents the typical variation time inside the reduced description, i.e., considering suitable slow variables, so that

$$\frac{|E_h-E_k|}{\hbar} \ll \frac{1}{\tau_0}, \qquad \frac{|E_h+E_{\lambda'}-E_f-E_\lambda|}{\hbar} \ll \frac{1}{\tau_0}, \qquad (3.2.20)$$

we keep only the linear contribution in t for the first three terms of (3.2.19), while the last expression requires a more complex handling. In the limit of no confinement the set of eigenvalues $\{E_g\}$ and $\{E_\lambda\}$ becomes a continuum, expressions of the form $\langle\alpha'|T_f^k(z)|\lambda\rangle$ become analytic functions for Re $z > 0$, having a cut on the imaginary axis and the existence of the limit $\delta \to 0$ (δ being the typical spacing between the poles) can be reasonably assumed. The analytic continuation across the cut can be considered and one can assume that the singularities of this continuation are located in the left half-plane far enough from the imaginary axis to give contributions that rapidly decay on a time scale t much larger than the correlation time for the macrosystem. In this way a further simplification of the last term of (3.2.19) becomes clear: if the sum over $E_{\alpha'}$ is eventually replaced by an integral and the integration path shifted inside the complex $E_{\alpha'}$ plane, the contribution of the term $\exp[(i/\hbar)(E_h+E_{\alpha'}-E_f-E_\lambda)t+3(\varepsilon/\hbar)t]$ can be calculated by shifting the integration path for $E_{\alpha'}$ in the upper half-plane; then only the contribution of the singularity $1/(E_k+E_{\alpha'}-E_f-E_\lambda-i\varepsilon)$ lying in the upper half-plane must be considered, so that replacing $E_{\alpha'}$ by $E_{\alpha'} = (E_\lambda+E_f-E_k+i\varepsilon)$ the term becomes $\exp[(i/\hbar)(E_h-E_k)t+2(\varepsilon/\hbar)t]$, and similarly for the other terms. The last contribution of (3.2.19) keeping (3.2.20) into account becomes

$$\approx 2\frac{\varepsilon}{\hbar}t \sum_{\substack{\lambda\alpha\alpha' \\ gf}} a_g^\dagger |\alpha\rangle \frac{\langle\alpha|T_g^{h\dagger}(E_h+i\varepsilon)|\alpha'\rangle}{E_g+E_\alpha-E_h-E_{\alpha'}-i\varepsilon} \frac{\langle\alpha'|T_f^k(E_k+i\varepsilon)|\lambda\rangle}{E_f+E_\lambda-E_k-E_{\alpha'}+i\varepsilon} \langle\lambda|a_f.$$

We have finally, denoting by $\mathcal{L}'$ the generator of the time evolution in Heisenberg picture

$$\begin{aligned} \mathcal{U}'(t)\left(a_h^\dagger a_k\right)_{|\mathcal{H}_F^1} &= a_h^\dagger a_k + t\mathcal{L}'\left(a_h^\dagger a_k\right) \\ &= a_h^\dagger a_k + \frac{i}{\hbar}t(E_h-E_k)a_h^\dagger a_k \\ &\quad - \frac{i}{\hbar}t\sum_f a_h^\dagger T_f^k(E_k+i\varepsilon)a_f + \frac{i}{\hbar}t\sum_g a_g^\dagger T_g^{h\dagger}(E_h+i\varepsilon)a_k \\ &\quad + 2\frac{\varepsilon}{\hbar}t \sum_{\substack{\lambda\alpha\alpha' \\ gf}} a_g^\dagger |\alpha\rangle \frac{\langle\alpha|T_g^{h\dagger}(E_h+i\varepsilon)|\alpha'\rangle}{E_g+E_\alpha-E_h-E_{\alpha'}-i\varepsilon} \frac{\langle\alpha'|T_f^k(E_k+i\varepsilon)|\lambda\rangle}{E_f+E_\lambda-E_k-E_{\alpha'}+i\varepsilon} \langle\lambda|a_f. \end{aligned} \tag{3.2.21}$$

Let us define the operators

$$\begin{aligned} T^{[1]} &= \sum_{gr} a_r^\dagger T_g^r(E_r+i\varepsilon)a_g \\ T^{[1]\dagger} &= \sum_{gr} a_r^\dagger T_r^{g\dagger}(E_g+i\varepsilon)a_g \\ R_{k\lambda}^{[1]} &= \sum_f R_{k\lambda f}a_f = \sum_f \left[\sqrt{2\varepsilon}\langle\lambda|T_f^k(E_k+i\varepsilon)\frac{1}{E_f+H_{\mathrm{m}}-E_k-E_\lambda+i\varepsilon}\right]a_f \\ R_{h\lambda}^{[1]\dagger} &= \sum_g a_g^\dagger R_{h\lambda g}^\dagger = \sum_g a_g^\dagger \left[\sqrt{2\varepsilon}\frac{1}{E_g+H_{\mathrm{m}}-E_h-E_\lambda-i\varepsilon}T_g^{h\dagger}(E_h+i\varepsilon)|\lambda\rangle\right], \end{aligned} \tag{3.2.22}$$

so that we can write

$$\mathcal{L}'\left(a_h^\dagger a_k\right) = \frac{i}{\hbar}\left[H_0, a_h^\dagger a_k\right] + \frac{i}{\hbar}\left[T^{[1]\dagger}, a_h^\dagger\right]a_k + \frac{i}{\hbar}a_h^\dagger\left[T^{[1]}, a_k\right] + \frac{1}{\hbar}\sum_\lambda R_{h\lambda}^{[1]\dagger}R_{k\lambda}^{[1]}.$$

Introducing the following one-particle operators

$$\begin{aligned} V^{[1]} &= \textstyle\sum_{gr} a_r^\dagger V_{rg}a_g &= \tfrac{1}{2}\left[T^{[1]}+T^{[1]\dagger}\right] &= \textstyle\sum_{gr} a_r^\dagger \tfrac{1}{2}\left[T_g^r(E_r+i\varepsilon)+T_r^{g\dagger}(E_g+i\varepsilon)\right]a_g \\ \Gamma^{[1]} &= \textstyle\sum_{gr} a_r^\dagger \Gamma_{rg}a_g &= \tfrac{i}{2}\left[T^{[1]}-T^{[1]\dagger}\right] &= \textstyle\sum_{gr} a_r^\dagger \tfrac{i}{2}\left[T_g^r(E_r+i\varepsilon)-T_r^{g\dagger}(E_g+i\varepsilon)\right]a_g \end{aligned} \tag{3.2.23}$$

so that

$$T^{[1]} = V^{[1]} - i\Gamma^{[1]}, \qquad V^{[1]} = V^{[1]\dagger}, \qquad \Gamma^{[1]} = \Gamma^{[1]\dagger}$$

the generator of the time evolution may be written

$$\mathcal{L}'\left(a_h^\dagger a_k\right) = \frac{i}{\hbar}\left[H_0 + V^{[1]}, a_h^\dagger a_k\right] - \frac{1}{\hbar}\left\{\left[\Gamma^{[1]}, a_h^\dagger\right] a_k - a_h^\dagger\left[\Gamma^{[1]}, a_k\right]\right\} + \frac{1}{\hbar}\sum_\lambda R_{h\lambda}^{[1]\dagger} R_{k\lambda}^{[1]}. \qquad (3.2.24)$$

Let us observe that V_{rg} and Γ_{rg} are not c-number coefficients, but operators acting in the Fock-space for the macrosystem; they are connected respectively to the self-adjoint and anti-self-adjoint part of what can be considered as an operator valued T-matrix. The last contribution displays the "bilinear structure" of the third term in the r.h.s. of (3.2.2), connected to irreversibility and complete positivity and not reproducible in the Hilbert space formalism, even resorting to an interaction potential which is not self-adjoint.

3.2.2 Particle Number Conservation and Complete Positivity

We now want to check that (3.2.24) accounts for particle number conservation, that is to say $\mathcal{L}'(N) = 0$ and therefore $\mathcal{U}'(t)(N) = N$ within the approximations so far introduced. Due to

$$\sum_h \left[\Gamma^{[1]}, a_h^\dagger\right] a_h = \Gamma^{[1]}, \qquad \sum_h a_h^\dagger\left[\Gamma^{[1]}, a_h\right] = -\Gamma^{[1]}$$

we have

$$\mathcal{L}'(N) = -\frac{2}{\hbar}\Gamma^{[1]} + \frac{1}{\hbar}\sum_{h\lambda} R_{h\lambda}^{[1]\dagger} R_{h\lambda}^{[1]},$$

which is equal to zero provided

$$\Gamma^{[1]} \approx \frac{1}{2}\sum_{h\lambda} R_{h\lambda}^{[1]\dagger} R_{h\lambda}^{[1]},$$

that is to say

$$\Gamma_{sr} = \frac{1}{2}\sum_{h\lambda} R_{h\lambda s}^\dagger R_{h\lambda r} \qquad (3.2.25)$$

or

$$i\left[T_r^s(E_s + i\varepsilon) - T_s^{r\dagger}(E_r + i\varepsilon)\right] = 2\varepsilon \sum_{\substack{\alpha\lambda\\ \eta h}} |\alpha\rangle \frac{\langle\alpha|T_s^{h\dagger}(E_h + i\varepsilon)|\eta\rangle}{E_s + E_\alpha - E_h - E_\eta - i\varepsilon}\frac{\langle\eta|T_r^h(E_h + i\varepsilon)|\lambda\rangle}{E_r + E_\lambda - E_h - E_\eta + i\varepsilon}\langle\lambda|.$$

The r.h.s. may we written

$$2\varepsilon \sum_{\substack{\alpha\lambda\\ \eta h}} |\alpha\rangle \frac{\langle\alpha|a_s\mathcal{T}\left(\frac{i}{\hbar}E_h + \frac{\varepsilon}{\hbar}\right)\left[a_h^\dagger\right]|\eta\rangle}{\left[\frac{i}{\hbar}\left(E_h + E_\eta - E_s - E_\alpha\right) - \frac{\varepsilon}{\hbar}\right]}\frac{\langle\eta|\mathcal{T}\left(-\frac{i}{\hbar}E_h + \frac{\varepsilon}{\hbar}\right)\left[a_h\right]a_r^\dagger|\lambda\rangle}{\left[-\frac{i}{\hbar}\left(E_h + E_\eta - E_r - E_\lambda\right) - \frac{\varepsilon}{\hbar}\right]}\langle\lambda|$$

$$= 2\varepsilon \sum_{\substack{\alpha\lambda\\ \eta h}} |\alpha\rangle\langle\alpha, s|\mathcal{T}\left(\frac{i}{\hbar}E_h + \frac{\varepsilon}{\hbar}\right)\left[a_h^\dagger\right]|\eta\rangle\langle\eta|\mathcal{T}\left(-\frac{i}{\hbar}E_h + \frac{\varepsilon}{\hbar}\right)\left[a_h\right]|\lambda, r\rangle\langle\lambda|$$

$$\times\left[-2\frac{\varepsilon}{\hbar} + \frac{i}{\hbar}\left(E_r + E_\lambda - E_s - E_\alpha\right)\right]^{-1}$$

$$\times\left[\frac{1}{\frac{i}{\hbar}E_h - \frac{\varepsilon}{\hbar} + \frac{i}{\hbar}\left(E_\eta - E_s - E_\alpha\right)} + \frac{1}{-\frac{i}{\hbar}E_h - \frac{\varepsilon}{\hbar} - \frac{i}{\hbar}\left(E_\eta - E_r - E_\lambda\right)}\right]$$

and exploiting (3.2.20)

$$\approx -\hbar \sum_{\substack{\alpha\lambda \\ \eta h}} \left[|\alpha\rangle\langle\alpha, s| \frac{1}{\frac{i}{\hbar}E_h - \frac{\varepsilon}{\hbar} - \mathcal{H}_0'} \mathcal{T}\left(\frac{i}{\hbar}E_h + \frac{\varepsilon}{\hbar}\right) [a_h^\dagger] \, |\eta\rangle\langle\eta| \mathcal{T}\left(-\frac{i}{\hbar}E_h + \frac{\varepsilon}{\hbar}\right) [a_h] \, |\lambda, r\rangle\langle\lambda| \right.$$

$$\left. + |\alpha\rangle\langle\alpha, s| \mathcal{T}\left(\frac{i}{\hbar}E_h + \frac{\varepsilon}{\hbar}\right) [a_h^\dagger] \, |\eta\rangle\langle\eta| \frac{1}{-\frac{i}{\hbar}E_h - \frac{\varepsilon}{\hbar} - \mathcal{H}_0'} \mathcal{T}\left(-\frac{i}{\hbar}E_h + \frac{\varepsilon}{\hbar}\right) [a_h] \, |\lambda, r\rangle\langle\lambda| \right].$$

To proceed further we use the identity

$$\frac{1}{z - \eta - \mathcal{H}_0'} \mathcal{T}(z + \eta) = \left[1 + \frac{2\eta}{z - \eta - \mathcal{H}_0'}\right] \frac{1}{z + \eta - \mathcal{H}'} \mathcal{V}',$$

obtained starting from $(z - \mathcal{H}_0')^{-1} \mathcal{T}(z) = (z - \mathcal{H}')^{-1} \mathcal{V}'$; in particular we have

$$\frac{1}{\frac{i}{\hbar}E_h - \frac{\varepsilon}{\hbar} - \mathcal{H}_0'} \mathcal{T}\left(\frac{i}{\hbar}E_h + \frac{\varepsilon}{\hbar}\right) [a_h^\dagger] =$$

$$= \left[1 + \frac{2(\varepsilon/\hbar)}{\frac{i}{\hbar}E_h - \frac{\varepsilon}{\hbar} - \mathcal{H}_0'}\right] \frac{1}{\frac{i}{\hbar}E_h + \frac{\varepsilon}{\hbar} - \mathcal{H}'} \left(\mathcal{H}' - \frac{i}{\hbar}E_h\right) a_h^\dagger$$

$$= a_h^\dagger + \frac{\varepsilon/\hbar}{\frac{i}{\hbar}E_h + \frac{\varepsilon}{\hbar} - \mathcal{H}'} a_h^\dagger + 2\left(\frac{\varepsilon}{\hbar}\right)^2 \frac{1}{\frac{i}{\hbar}E_h - \frac{\varepsilon}{\hbar} - \mathcal{H}_0'} \frac{1}{\frac{i}{\hbar}E_h + \frac{\varepsilon}{\hbar} - \mathcal{H}'} a_h^\dagger$$

$$\approx a_h^\dagger.$$

As a result

$$\sum_{h\lambda} R_{h\lambda s}^\dagger R_{h\lambda r} \approx -\hbar \sum_{\substack{\alpha\lambda \\ \eta h}} \left[|\alpha\rangle\langle\alpha, s| a_h^\dagger |\eta\rangle\langle\eta| \frac{1}{i\hbar} T_r^h(E_h + i\varepsilon) |\lambda\rangle\langle\lambda| \right.$$

$$\left. + |\alpha\rangle\langle\alpha| \frac{-1}{i\hbar} T_s^{h\dagger}(E_h + i\varepsilon) |\eta\rangle\langle\eta| a_h |\lambda, r\rangle\langle\lambda| \right]$$

$$= i \left[T_r^s(E_s + i\varepsilon) - T_s^{r\dagger}(E_r + i\varepsilon) \right],$$

so that (3.2.25) is satisfied.

The structure of (3.2.24) is such that $\mathcal{U}'(t)$ satisfies a property analogous to complete positivity [16, 17, 30] when applied to a couple of creation and annihilation operators, in fact we will show that

$$\sum_{i,j=1}^{n} \langle\psi_i| \mathcal{U}'(t) \left[\sum_{hk} a_h^\dagger \langle h| \hat{\mathsf{B}}_i^\dagger \hat{\mathsf{B}}_j |k\rangle a_k \right] |\psi_j\rangle \geq 0$$

with $n \in \mathbf{N}$, $\{\psi_i\}$ vectors in Fock-space, $\{\hat{\mathsf{B}}_i\}$ operators in the one-particle Hilbert space $\mathcal{H}^{(1)}$. Setting

$$\left[\Gamma^{[1]}, a_k\right] = -F_k, \qquad \left[\Gamma^{[1]}, a_h^\dagger\right] = F_h^\dagger, \qquad H_0 + V^{[1]} = C$$

we have in fact, at first order in t

$$\sum_{i,j=1}^{n} \langle\psi_i|\mathcal{U}'(t)\left[\sum_{hk} a_h^\dagger \langle h|\hat{\mathsf{B}}_i^\dagger \hat{\mathsf{B}}_j|k\rangle a_k\right]|\psi_j\rangle =$$

$$\begin{aligned}
&= \sum_{i,j=1}^{n}\sum_{hk}\langle h|\hat{\mathsf{B}}_i^\dagger \hat{\mathsf{B}}_j|k\rangle\langle\psi_i|a_h^\dagger a_k + t\mathcal{L}'(a_h^\dagger a_k)|\psi_j\rangle \\
&= \sum_{i,j=1}^{n}\sum_{hk}\langle h|\hat{\mathsf{B}}_i^\dagger \hat{\mathsf{B}}_j|k\rangle\langle\psi_i|\left[a_h + t\frac{i}{\hbar}\left[C,a_h\right] - \frac{t}{\hbar}F_h\right]^\dagger \\
&\qquad \times\left[a_k + t\frac{i}{\hbar}\left[C,a_k\right] - \frac{t}{\hbar}F_k\right] + \frac{t}{\hbar}\sum_{\lambda} R_{h\lambda}^{[1]\dagger} R_{k\lambda}^{[1]}|\psi_j\rangle \\
&= \sum_{g}\left(\sum_{i=1}^{n}\sum_{h}\langle h|\hat{\mathsf{B}}_i^\dagger|g\rangle\langle\psi_i|\left[a_h + t\frac{i}{\hbar}\left[C,a_h\right] - \frac{t}{\hbar}F_h\right]^\dagger\right) \\
&\qquad \times\left(\sum_{j=1}^{n}\sum_{k}\langle g|\hat{\mathsf{B}}_j|k\rangle\left[a_k + t\frac{i}{\hbar}\left[C,a_k\right] - \frac{t}{\hbar}F_k\right]|\psi_j\rangle\right) \\
&\quad +\frac{t}{\hbar}\sum_{g\lambda}\left(\sum_{i=1}^{n}\sum_{h}\langle h|\hat{\mathsf{B}}_i^\dagger|g\rangle\langle\psi_i|R_{h\lambda}^{[1]\dagger}\right)\left(\sum_{j=1}^{n}\sum_{k}\langle g|\hat{\mathsf{B}}_j|k\rangle R_{k\lambda}^{[1]}|\psi_j\rangle\right) \\
&= \sum_{g}\left\|\sum_{j=1}^{n}\sum_{k}\langle g|\hat{\mathsf{B}}_j|k\rangle\left[a_k + t\frac{i}{\hbar}\left[C,a_k\right] - \frac{t}{\hbar}F_k\right]|\psi_j\rangle\right\|_{\mathcal{H}_F}^2 \\
&\quad + \frac{t}{\hbar}\sum_{g\lambda}\left\|\sum_{j=1}^{n}\sum_{k}\langle g|\hat{\mathsf{B}}_j|k\rangle R_{k\lambda}^{[1]}|\psi_j\rangle\right\|_{\mathcal{H}_F}^2 \geq 0 \qquad \text{for } t\geq 0.
\end{aligned}$$

3.2.3 The Master Equation

Exploiting the reduction formulas (3.2.11) and (3.2.12), together with (3.2.21), we come to the master equation for the statistical operator describing the microsystem

$$\begin{aligned}
\frac{d}{dt}\varrho_{kh} &= \mathrm{Tr}_{\mathcal{H}_F}\left(\mathcal{L}'\left(a_h^\dagger a_k\right)\rho\right) \\
&= +\frac{i}{\hbar}(E_h - E_k)\sum_{pq}\mathrm{Tr}_{\mathcal{H}_F}\left(a_h^\dagger a_k a_p^\dagger \varrho_{\mathrm{m}} a_q \varrho_{pq}\right) \\
&\quad -\frac{i}{\hbar}\sum_{pqf}\mathrm{Tr}_{\mathcal{H}_F}\left(a_h^\dagger T_f^k(E_k + i\varepsilon) a_f a_p^\dagger \varrho_{\mathrm{m}} a_q \varrho_{pq}\right)
\end{aligned}$$

$$+\frac{i}{\hbar}\sum_{pqg}\mathrm{Tr}_{\mathcal{H}_F}\left(a_g^\dagger T_g^{h\dagger}(E_h+i\varepsilon)a_k a_p^\dagger \varrho_{\mathrm{m}} a_q \varrho_{pq}\right)$$

$$+2\frac{\varepsilon}{\hbar}\sum_{\substack{\lambda\alpha\alpha'\\pqgf}}\mathrm{Tr}_{\mathcal{H}_F}\left(a_g^\dagger|\alpha\rangle\frac{\langle\alpha|T_g^{h\dagger}(E_h+i\varepsilon)|\alpha'\rangle}{E_g+E_\alpha-E_h-E_{\alpha'}-i\varepsilon}\right.$$

$$\left.\times\frac{\langle\alpha'|T_f^k(E_k+i\varepsilon)|\lambda\rangle}{E_f+E_\lambda-E_k-E_{\alpha'}+i\varepsilon}\langle\lambda|a_f a_p^\dagger\varrho_{\mathrm{m}}a_q\varrho_{pq}\right)$$

which due to (3.2.9) and using the decomposition $\varrho_{\mathrm{m}}=\sum_\xi \pi_\xi|\xi\rangle\langle\xi|$ becomes

$$\begin{aligned}\frac{d}{dt}\varrho_{kh} &= -\frac{i}{\hbar}(E_k-E_h)\varrho_{kh}\\ &-\frac{i}{\hbar}\sum_f \mathrm{Tr}_{\mathcal{H}_F}\left[T_f^k(E_k+i\varepsilon)\varrho_{\mathrm{m}}\right]\varrho_{fh}\\ &+\frac{i}{\hbar}\sum_g \varrho_{kg}\mathrm{Tr}_{\mathcal{H}_F}\left[T_g^{h\dagger}(E_h+i\varepsilon)\varrho_{\mathrm{m}}\right]\\ &+2\frac{\varepsilon}{\hbar}\sum_{\substack{\eta\xi\\gf}}\frac{\langle\eta|T_f^k(E_k+i\varepsilon)|\xi\rangle}{E_f+E_\xi-E_k-E_\eta+i\varepsilon}\pi_\xi\varrho_{fg}\frac{\langle\xi|T_g^{h\dagger}(E_h+i\varepsilon)|\eta\rangle}{E_g+E_\xi-E_h-E_\eta-i\varepsilon}.\end{aligned}$$

The master equation describing the irreversible time evolution of the statistical operator on the chosen time scale can also be written:

$$\frac{d}{dt}\varrho_{kh}=-\frac{i}{\hbar}\left(E_k-E_h\right)\varrho_{kh}-\frac{i}{\hbar}\sum_f Q_{kf}\varrho_{fh}+\frac{i}{\hbar}\sum_g\varrho_{kg}Q^*_{hg}+\frac{1}{\hbar}\sum_{\substack{gf\\\lambda\xi}}\left(L_{\lambda\xi}\right)_{kf}\varrho_{fg}\left(L_{\lambda\xi}\right)^*_{hg}, \quad (3.2.26)$$

the quantities appearing in (3.2.26) being defined in the following way:

$$\begin{aligned}Q_{kf} &= \mathrm{Tr}_{\mathcal{H}_F}\left[T_f^k(E_k+i\varepsilon)\varrho_{\mathrm{m}}(t)\right]\\ Q^*_{hg} &= \mathrm{Tr}_{\mathcal{H}_F}\left[T_g^{h\dagger}(E_h+i\varepsilon)\varrho_{\mathrm{m}}(t)\right] \quad (3.2.27)\\ \left(L_{\lambda\xi}\right)_{kf} &= \sqrt{2\varepsilon\pi_\xi}\frac{\langle\lambda|T_f^k(E_k+i\varepsilon)|\xi(t)\rangle}{E_f+E_\xi-E_k-E_\lambda+i\varepsilon}.\end{aligned}$$

If we now introduce in $\mathcal{H}^{(1)}$ the operators $\hat{\mathsf{H}}_0,\hat{\mathsf{Q}},\hat{\mathsf{L}}_{\lambda\xi}$ and $\hat{\varrho}$

$$\langle g|\hat{\mathsf{H}}_0|f\rangle=E_f\delta_{gf},\quad\langle g|\hat{\mathsf{Q}}|f\rangle=Q_{gf},\quad\langle g|\hat{\mathsf{L}}_{\lambda\xi}|f\rangle=\left(L_{\lambda\xi}\right)_{gf},\quad\langle g|\hat{\varrho}|f\rangle=\varrho_{gf}, \quad (3.2.28)$$

eq. (3.2.26) becomes:

$$\frac{d\hat{\varrho}}{dt}=-\frac{i}{\hbar}\left[\hat{\mathsf{H}}_0+\hat{\mathsf{V}},\hat{\varrho}\right]-\frac{1}{\hbar}\left\{\hat{\Gamma},\hat{\varrho}\right\}+\frac{1}{\hbar}\sum_{\xi\lambda}\hat{\mathsf{L}}_{\lambda\xi}\hat{\varrho}\hat{\mathsf{L}}^\dagger_{\lambda\xi}\ , \quad (3.2.29)$$

where

$$\hat{\mathsf{V}} = \frac{\hat{\mathsf{Q}} + \hat{\mathsf{Q}}^\dagger}{2}, \qquad \hat{\mathsf{\Gamma}} = i\frac{\hat{\mathsf{Q}} - \hat{\mathsf{Q}}^\dagger}{2}. \tag{3.2.30}$$

Verification of the conservation of the trace of the statistical operator within the adopted approximations leads to the following relationship

$$\hat{\mathsf{\Gamma}} \approx \frac{1}{2}\sum_{\xi\lambda} \hat{\mathsf{L}}^\dagger_{\lambda\xi}\hat{\mathsf{L}}_{\lambda\xi},$$

and therefore to:

$$\frac{d\hat{\varrho}}{dt} = -\frac{i}{\hbar}\left[\hat{\mathsf{H}}_0 + \hat{\mathsf{V}}, \hat{\varrho}\right] - \frac{1}{\hbar}\left\{\frac{1}{2}\sum_{\xi\lambda}\hat{\mathsf{L}}^\dagger_{\lambda\xi}\hat{\mathsf{L}}_{\lambda\xi}, \hat{\varrho}\right\} + \frac{1}{\hbar}\sum_{\xi\lambda}\hat{\mathsf{L}}_{\lambda\xi}\hat{\varrho}\hat{\mathsf{L}}^\dagger_{\lambda\xi}\ . \tag{3.2.31}$$

In particular we have the relations

$$\langle k|\hat{\mathsf{V}}|f\rangle = \mathrm{Tr}_{\mathcal{H}_F}\left(V_{kf}\varrho_{\mathrm{m}}\right) \qquad \langle k|\hat{\mathsf{\Gamma}}|f\rangle = \mathrm{Tr}_{\mathcal{H}_F}\left(\Gamma_{kf}\varrho_{\mathrm{m}}\right)$$

$$\langle k|\hat{\mathsf{L}}_{\lambda\xi}|f\rangle = \sqrt{\pi_\xi}R_{k\lambda f}|\xi\rangle \qquad \langle k|\hat{\mathsf{L}}^\dagger_{\lambda\xi}|f\rangle = \sqrt{\pi_\xi}\langle\xi|R^\dagger_{k\lambda f}$$

3.2.4 Structure of the Generator

Our formalism points to the matrix $T^k_h(z)$ given in (3.2.18), whose entries are operators on the Hilbert space of the macrosystem, as the basic mathematical tool to describe the physics of the microsystem: we will show that it yields all relevant quantities and, in our opinion, could be a sound starting point for phenomenological assumptions. $T^k_h(z)$ bears a connection to scattering theory, as it is clear from (3.2.16); it is also related to the thermodynamics of the macrosystem being an operator on $\mathcal{H}^0_F$. To help clarifying this connection we consider a simple case in which $T^k_h(z)$ can be explicitly calculated. Let the macrosystem be composed of non-interacting particles

$$H_{\mathrm{m}} = \sum_\eta E_\eta b^\dagger_\eta b_\eta,$$

where $b^\dagger_\eta$ is the creation operator of a particle in an eigenstate v_η with energy E_η (either a Bose or a Fermi particle), and let us make for the potential the following natural choice

$$V = \sum_{p\xi q\eta} a^\dagger_p b^\dagger_\xi V_{p\xi q\eta} a_q b_\eta.$$

Recalling that we are describing a single particle and exploiting the superoperators introduced in (3.2.13) and (3.2.15) we can calculate $T^k_h(z)$ as defined by (3.2.17). To do this we bring to normal order the creation and annihilation operators associated with the macrosystem and restrict ourselves to a one mode dynamics, in which, apart from statistical corrections, only one creation and one annihilation operator of the type b appear: that is to say we neglect three particle collisions. Then one obtains:

$$T_f^k(E_k + i\varepsilon) = \sum_{\xi\eta} b_\xi^\dagger \langle k, \xi | V^{(2)} + V^{(2)} \frac{1}{E_\xi + E_k + i\varepsilon - \left(H_0^{(2)} + V_L\right)} V_L | f, \eta \rangle b_\eta,$$

where ε is a positive quantity and the following relationships hold ($+, -$ signs stand for Bose and Fermi statistics respectively),

$$\begin{aligned} \langle k, \xi | H_0^{(2)} | f, \eta \rangle &= (E_f + E_\eta)\delta_{kf}\delta_{\xi\eta} \\ \langle k, \xi | V_L | f, \eta \rangle &= (1 \pm b_\xi^\dagger b_\xi)\langle k, \xi | V^{(2)} | f, \eta \rangle = (1 \pm b_\xi^\dagger b_\xi) V_{k\xi f\eta}; \end{aligned} \tag{3.2.32}$$

here the superscript (2) denotes operators in the two-particle Hilbert space and statistical corrections for scattering in the medium are taken into account in the potential term V_L, implicitly defined by (3.2.32) and by the usual resolvent series (see Chap. 5). The connection to the familiar T-matrix is evident. A formally similar result holds if we make no restrictive hypothesis on H_m but assume an interaction potential of the form:

$$\mathsf{V} = \sum_{p\zeta q\lambda} a_p^\dagger a_q |\zeta\rangle\langle\lambda| V_{p\zeta q\lambda},$$

where $|\zeta\rangle$ and $|\lambda\rangle$ are eigenstates of H_m. In this case one has:

$$T_f^k(E_k + i\varepsilon) = \sum_{\zeta\lambda} |\zeta\rangle\langle k, \zeta | \mathsf{V} + \mathsf{V} \frac{1}{E_\zeta + E_k + i\varepsilon - (H_0 + H_\mathrm{m} + \mathsf{V})} \mathsf{V} | f, \lambda\rangle\langle\lambda|,$$

where:

$$\langle k, \zeta | H_0 + H_\mathrm{m} | f, \eta \rangle = (E_f + E_\eta)\delta_{kf}\delta_{\zeta\eta} \qquad \langle p, \zeta | \mathsf{V} | q, \lambda \rangle = V_{p\zeta q\lambda}.$$

In the general case the exact evaluation of $T_h^k(z)$ is a very difficult task, if feasible at all, like the treatment of scattering of a microsystem off a macroscopic system. In this context phenomenological or approximate expressions can be usefully introduced, as is usual practice in the description of real systems; an opportunity suggested by the very formalism. Formulas (3.2.14) and (3.2.15) are clearly reminiscent of the usual identities satisfied by the resolvent operator in the theory of scattering. The mathematical framework is however quite different, since we are now dealing with superoperators. The quantity to be related with the usual T-matrix is the operator $T_h^k(z)$ of (3.2.18), acting in the subspace $\mathcal{H}_F^0$, that is to say a second-quantized operator for the macrosystem.

Before applying (3.2.31) to a concrete physical situation it can be useful to gain some further insight into the structure of the operators appearing in it. As already said the quantity that the formalism suggests as a natural candidate where to put in suitable phenomenological expressions is the operator $T_f^k(z)$, an operator whose trace over the Fock-space for the macrosystem calculated with $\varrho_{\rm m}$ gives the value of the T-matrix for scattering from state u_f to state u_k averaged over the state of the macroscopic system. A quite general phenomenological expression can be obtained in the following way. Suppose that $\mathcal{T}(z)$ has the form

$$\mathcal{T}(z) = \frac{i}{\hbar}\left[T(i\hbar z), \cdot\right], \qquad T(z) = \sum_{k\lambda f\mu} a_k^\dagger b_\lambda^\dagger T_{k\lambda f\mu}(z) a_f b_\mu,$$

with $b^\dagger$, b creation and annihilation operators in the Fock-space for the macrosystem. We thus have

$$i\hbar\mathcal{T}(z)[a_k] = \sum_{\lambda f\mu} b_\lambda^\dagger T_{k\lambda f\mu}(i\hbar z) a_f b_\mu = \sum_f T_f^k(i\hbar z)\, a_f,$$

and supposing translation invariance in the interaction kernel:

$$T_f^k(z) = \sum_{\lambda\mu} b_\lambda^\dagger T_{k\lambda f\mu}(z) b_\mu = \int d^3\mathbf{x} \int d^3\mathbf{y}\, \psi^\dagger(\mathbf{x}) u_k^*(\mathbf{y}) t(z, \mathbf{x}-\mathbf{y}) u_f(\mathbf{y}) \psi(\mathbf{x}). \tag{3.2.33}$$

Such an Ansatz amounts to introducing an effective potential which should give in Born approximation the full scattering amplitude. As a result the potential term in (3.2.31) is linked to the scattering amplitude, as we shall see in Sect. 4.2.1, while the incoherent contribution is generally connected to the scattering cross section. To realize this let us consider the last term of (3.2.26), keeping the proposed Ansatz into account:

$$\frac{2\varepsilon}{\hbar} \sum_{\substack{\lambda\lambda' \\ \lambda''}} \sum_{fg} \int d^3\mathbf{x} \int d^3\mathbf{y}\, u_k^*(\mathbf{y}) \frac{t\left(E_k + i\varepsilon, \mathbf{x}-\mathbf{y}\right)}{E_f + E_\lambda - E_k - E_{\lambda''} + i\varepsilon} u_f(\mathbf{y}) \langle\lambda''|\psi^\dagger(\mathbf{x})\psi(\mathbf{x})|\lambda\rangle\langle\lambda|\varrho_{\rm m}(t)|\lambda'\rangle$$

$$\times \varrho_{fg}(t) \int d^3\mathbf{x}' \int d^3\mathbf{y}'\, \langle\lambda'|\psi^\dagger(\mathbf{x}')\psi(\mathbf{x}')|\lambda''\rangle u_g^*(\mathbf{y}') \frac{t^*\left(E_h + i\varepsilon, \mathbf{x}'-\mathbf{y}'\right)}{E_g + E_{\lambda'} - E_h - E_{\lambda''} - i\varepsilon} u_h(\mathbf{y}'), \tag{3.2.34}$$

and let us specialize to the case of a diagonal matrix element. Supposing the statistical operator for the microsystem is quasi-diagonal and the macrosystem is at equilibrium, so that $\varrho_{\rm m}|\lambda\rangle = \varrho_{\rm m}^\lambda|\lambda\rangle$, we exploit the usual representation for the delta function, thus obtaining:

$$\sum_f \sum_{\lambda\lambda'} \frac{2\pi}{\hbar} \delta\left(E_k + E_\lambda - E_f - E_{\lambda'}\right)$$

$$\times \left| \int d^3\mathbf{x} \int d^3\mathbf{y}\, u_k^*(\mathbf{y}) \langle\lambda|\psi^\dagger(\mathbf{x}) t\left(E_k + i\varepsilon, \mathbf{x}-\mathbf{y}\right)\psi(\mathbf{x})|\lambda'\rangle u_f(\mathbf{y}) \right|^2 \varrho_{\rm m}^{\lambda'} \varrho_{ff}(t).$$

In this formula one has the typical transition probability between an initial state f, λ' and a final state k, λ, averaged over all possible initial configurations and summed over all possible final states for the macrosystem, that is to say contributions from both coherent and diffuse scattering are included. It might be instructive to show in a different way the connection between the last term of (3.2.26) and the total scattering cross section, referring to a famous paper by van Hove [40]. Taking for concreteness the Fermi pseudopotential (see Sect. 4.2.1 or [41, 42]), whose Fourier transform is simply the constant $\tilde{V} = \frac{2\pi\hbar^2}{m} b$, we evaluate the diagonal element of (3.2.34) assuming that the u_f are given by plane waves (the indexes f, g, h, k becoming momenta), thus obtaining $[N(\mathbf{x}) = \psi^\dagger(\mathbf{x})\psi(\mathbf{x})]$:

$$\frac{2\varepsilon}{\hbar}\left|\tilde{V}\right|^2 \sum_{\lambda\lambda'} \int \frac{d^3\mathbf{P}}{(2\pi\hbar)^3} \int \frac{d^3\mathbf{q}}{(2\pi\hbar)^3} \int d^3\mathbf{x} \int d^3\mathbf{y}$$

$$\times\, e^{-\frac{i}{\hbar}\left[\mathbf{k}-\left(\mathbf{P}+\frac{\mathbf{q}}{2}\right)\right]\cdot\mathbf{x}} \frac{\langle\lambda'|N(\mathbf{x})|\lambda\rangle}{\frac{1}{2m}\left(\mathbf{P}+\frac{1}{2}\mathbf{q}\right)^2 + E_\lambda - E_k - E_{\lambda'} + i\varepsilon} \langle \mathbf{P}+\tfrac{1}{2}\mathbf{q}|\hat{\varrho}|\mathbf{P}-\tfrac{1}{2}\mathbf{q}\rangle$$

$$\times\, \langle\lambda\left|\varrho_{\mathrm{m}}(t)\right|\lambda\rangle \frac{\langle\lambda|N(\mathbf{y})|\lambda'\rangle}{\frac{1}{2m}\left(\mathbf{P}-\frac{1}{2}\mathbf{q}\right)^2 + E_\lambda - E_k - E_{\lambda'} - i\varepsilon} e^{\frac{i}{\hbar}\left[\mathbf{k}-\left(\mathbf{P}-\frac{\mathbf{q}}{2}\right)\right]\cdot\mathbf{y}},$$

and supposing $\hat{\varrho}$ such that the energies in the denominators may be considered approximately equal, introducing the Wigner function for the neutron

$$f_{\mathrm{w}}(\mathbf{x},\mathbf{p}) = \int \frac{d^3\mathbf{q}}{(2\pi\hbar)^3} e^{\frac{i}{\hbar}\mathbf{x}\cdot\mathbf{q}} \langle \mathbf{p}+\tfrac{1}{2}\mathbf{q}|\hat{\varrho}|\mathbf{p}-\tfrac{1}{2}\mathbf{q}\rangle$$

one easily has

$$\frac{2\pi}{\hbar}\left(\frac{1}{2\pi\hbar}\right)^4 \left|\tilde{V}\right|^2 \int d^3\mathbf{P} \int dt \int d^3\mathbf{r}\, e^{-\frac{i}{\hbar}\left(\frac{P^2}{2m}-E_k\right)t + \frac{i}{\hbar}(\mathbf{P}-\mathbf{k})\cdot\mathbf{r}}$$

$$\times \int d^3\mathbf{X} f_{\mathrm{w}}(\mathbf{X},\mathbf{P}) \langle N\left(\mathbf{X}-\frac{\mathbf{r}}{2}\right) N\left(\mathbf{X}+\frac{\mathbf{r}}{2}, t\right)\rangle, \quad (3.2.35)$$

where $\langle \ldots \rangle \equiv \mathrm{Tr}_{\mathcal{H}_F}(\ldots \varrho_{\mathrm{m}})$, and $N(\mathbf{x}, t)$ denotes the operator in the Heisenberg picture. We have thus recovered the typical factorized structure appearing in the expression for the scattering cross section of a neutron off a macroscopic system: square modulus of the Fourier transform of the interaction potential times the dynamic structure function depending on transferred momentum and energy, with the refinement that it is here weighted according to position and momentum distribution of the incoming particle. For the non-diagonal matrix element one can expect to obtain analogous results if the quantities appearing in (3.2.34) are sufficiently slowly varying functions of their arguments, so that, in the continuous limit, an interpolation formula of the form

$$\varepsilon \int d\xi \frac{g(\xi)}{(\alpha+\xi+i\varepsilon)(\beta+\xi-i\varepsilon)} \approx \pi \int d\xi\, g(\xi)\delta(\beta+\xi) \approx \pi \int d\xi\, g(\xi)\delta(\alpha+\xi), \qquad |\alpha-\beta| \ll \varepsilon$$

with $g(\xi)$ a suitably smooth function may be used. The failure of such an approximation and thus the relevance of the actual value of the parameter ε in the final expression might be traced back to the breakdown of the approximations that have led to the Markovian evolution generated by the master-equation (3.2.26).

3.2.5 Physical Discussion

To elucidate how an equation of the form (3.2.29) or equivalently (3.2.26) may be well suited to describe an interplay between a *purely optical* (that is wavelike) dynamics and an interaction with a measuring character let us introduce the reversible mappings $\mathcal{A}_{t''t'} = U_{t''t'} \cdot U^{\dagger}_{t''t'}$, where

$$U_{t''t'} = T\left(e^{-\frac{i}{\hbar}\int_{t'}^{t''} d\tau\, \left(\hat{\mathsf{H}}_0 + i\hat{\mathsf{Q}}(\tau)\right)}\right), \tag{3.2.36}$$

corresponding to a coherent contractive evolution of the microsystem during the time interval $[t', t'']$, and the completely positive mappings

$$\mathcal{L}_{\lambda\xi} = \hat{\mathsf{L}}_{\lambda\xi}(t) \cdot \hat{\mathsf{L}}^{\dagger}_{\lambda\xi}(t)\pi_{\xi(t)}, \tag{3.2.37}$$

whose measuring character may be inferred from the discussion following (3.2.7). The structure of the operators $\hat{\mathsf{L}}_{\lambda\xi}$ [see (3.2.27)] further shows that these mappings may be linked with a transition inside the macrosystem specified by the pair of indexes ξ, λ, as a result of scattering with the microsystem. Under very particular conditions, strongly enhancing the measuring character of the interaction (as would be the case for a detector), these transitions could be macroscopically detectable, thus leading to a localization of the particle. To indicate such interactions we will therefore use the word "event".

The solution of (3.2.29) can be written as:

$$\begin{aligned}\hat{\varrho}_t &= \mathcal{A}_{tt_0}\hat{\varrho}_{t_0} + \sum_{\lambda_1\xi_1}\int_{t_0}^{t} dt_1\, \mathcal{A}_{tt_1}\mathcal{L}_{\lambda_1\xi_1}(t_1)\mathcal{A}_{t_1t_0}\hat{\varrho}_{t_0} + \\ &+ \sum_{\substack{\lambda_1\xi_1\\ \lambda_2\xi_2}}\int_{t_0}^{t} dt_2 \int_{t_0}^{t_2} dt_1\, \mathcal{A}_{tt_2}\mathcal{L}_{\lambda_2\xi_2}(t_2)\mathcal{A}_{t_2t_1}\mathcal{L}_{\lambda_1\xi_1}(t_1)\mathcal{A}_{t_1t_0}\hat{\varrho}_{t_0} + \ldots\end{aligned} \tag{3.2.38}$$

which can be interpreted as a sum over subcollections corresponding to the realization of no event, one event, two events and so on. To see this let us perform some measurement on the microsystem at time t, associated with an eigenstate u_α of some observable $\hat{\mathsf{A}}$. Then by (3.2.37) and (3.2.38) the probability $p_\alpha(t)$ of the result α for this observable at time t has the following structure:

$$\begin{aligned}p_\alpha(t) &= \langle u_\alpha|\mathcal{A}_{tt_0}\hat{\varrho}_{t_0}|u_\alpha\rangle + \sum_{\lambda_1\xi_1}\int_{t_0}^{t} dt_1\, \langle u_\alpha|\mathcal{A}_{tt_1}\mathcal{L}_{\lambda_1\xi_1}(t_1)\mathcal{A}_{t_1t_0}\hat{\varrho}_{t_0}|u_\alpha\rangle + \\ &+ \sum_{\substack{\lambda_1\xi_1\\ \lambda_2\xi_2}}\int_{t_0}^{t} dt_2 \int_{t_0}^{t_2} dt_1\, \langle u_\alpha|\mathcal{A}_{tt_2}\mathcal{L}_{\lambda_2\xi_2}(t_2)\mathcal{A}_{t_2t_1}\mathcal{L}_{\lambda_1\xi_1}(t_1)\mathcal{A}_{t_1t_0}\hat{\varrho}_{t_0}|u_\alpha\rangle + \ldots\end{aligned} \tag{3.2.39}$$

Let us assume for simplicity that the initial preparation $\hat{\varrho}_{t_0}$ is a pure state $\hat{\varrho}_{t_0} = |\psi_{t_0}\rangle\langle\psi_{t_0}|$, then the first term in the r.h.s. of (3.2.39) has by (3.2.36) the form:

$$\langle u_\alpha | \mathcal{A}_{tt_0} \hat{\varrho}_{t_0} | u_\alpha \rangle = |\langle u_\alpha | \psi(t) \rangle|^2, \quad \psi(t) = T\left(e^{-\frac{i}{\hbar}\int_{t_0}^t d\tau\, (\hat{\mathsf{H}}_0 + i\hat{\mathsf{Q}}(\tau))} \right) \psi_{t_0},$$

and it gives the probability of measuring $\hat{\mathsf{A}}$ equal to α at time t when no event is produced in between the preparation of the state ψ_{t_0} at time t_0 and the measurement of $\hat{\mathsf{A}}$ at time t; the trace of the first subcollection $p_t^0 = \mathrm{Tr}_{\mathcal{H}^{(1)}} \mathcal{A}_{tt_0} \hat{\varrho}_{t_0} = \|\psi(t)\|^2$ gives the probability that no event happens in the time interval $[t_0, t]$; then apart from the fact that $p_t^0 \leq 1$ (p_t^0 is a non-increasing function) the usual statistical interpretation of the wave-function is recovered. The integrand of the second term $\langle u_\alpha | \mathcal{A}_{tt_1} \mathcal{L}_{\lambda_1 \xi_1}(t_1) \mathcal{A}_{t_1 t_0} \hat{\varrho}_{t_0} | u_\alpha \rangle$ can be interpreted as the probability of detecting $\hat{\mathsf{A}}$ equal to α at time t, when the transition $\lambda_1 \xi_1$ happens in the time interval $[t', t' + dt']$, while no transition $\lambda\xi$ happens in the time intervals $[t_0, t']$, $[t' + dt', t]$; in other words the expression

$$\int_{t_0}^t dt_1\, \langle u_\alpha | \mathcal{A}_{tt_1} \mathcal{L}_{\lambda_1 \xi_1}(t_1) \mathcal{A}_{t_1 t_0} \hat{\varrho}_{t_0} | u_\alpha \rangle$$

gives the probability of $\hat{\mathsf{A}}$ equal to α at time t when one and only one event linked to the transition $\lambda_1 \xi_1$ happens in the time interval $[t_0, t]$, while

$$p_t^1 = \mathrm{Tr}_{\mathcal{H}^{(1)}} \left(\int_{t_0}^t dt_1\, \mathcal{A}_{tt_1} \mathcal{L}_{\lambda_1 \xi_1}(t_1) \mathcal{A}_{t_1 t_0} \hat{\varrho}_{t_0} \right)$$

is just the probability for this sole event in the time interval $[t_0, t]$. While the first term in the r.h.s. of (3.2.38) is a pure state, provided $\hat{\varrho}_{t_0}$ is, the second one, due to different transition times, is a mixture. The other terms of (3.2.38) provide the almost obvious generalization describing repeated production of events $\lambda\xi$.

If the macrosystem is an interferometer, the role of the first term is enhanced by the experimental situation, nevertheless if one can monitor the path followed by the microsystem inside the interferometer, then the other terms also become relevant. If at the output of the interferometer an interference pattern is observed, some disturbance by an incoherent background due to these terms is unavoidable. Obviously such disturbance can be made negligible if the experimental setup is such as to "automatically" select only coherent contributions. This is the case if the disturbance originates in scattering and the acceptance along the whole path is small enough as in neutron interferometry, however, forward scattering cannot be eliminated, so, even simply relying on the present general theoretical framework, one should expect that the first term of (3.2.39) cannot account for the whole experimental evidence (see also Sect. 4.2.3), and this could explain some difficulties that have been reported in the interpretation of neutron interference experiments, without resorting to a reformulation of quantum mechanics, as proposed by [27]. A more precise insight into the structure of the operators $\hat{\mathsf{Q}}$ and $\hat{\mathsf{L}}$ can be obtained introducing the field operator

$$\psi(\mathbf{x}) = \sum_f a_f u_f(\mathbf{x}), \quad a_f = \int d^3x\, u_f^*(\mathbf{x})\psi(\mathbf{x}),$$

and writing instead of (3.2.17):

$$i\hbar \left(\mathcal{T}(z)\psi\right)(\mathbf{x}) = \int d^3x' \,\mathrm{T}\left(\mathbf{x}, \mathbf{x}', i\hbar z\right) \psi(\mathbf{x}').$$

Then (3.2.18) becomes, assuming also translation invariance

$$\begin{aligned} T_l^k\,(z) &= \int d^3x\, d^3x'\, u_k^*(\mathbf{x})\mathrm{T}\left(\mathbf{x}-\mathbf{x}', z\right) u_l(\mathbf{x}') = \int d^3X\, T_l^k\left(\mathbf{X}, z\right), \\ T_l^k\left(\mathbf{X}, z\right) &= \int d^3r\, u_k^*\left(\mathbf{X}+\frac{\mathbf{r}}{2}\right) \mathrm{T}\left(\mathbf{r}, z\right) u_l\left(\mathbf{X}-\frac{\mathbf{r}}{2}\right). \end{aligned} \tag{3.2.40}$$

In correspondence with the representation (3.2.40) of $T_l^k\,(z)$ one has a similar representation for $(\hat{\mathsf{L}}_{\lambda\xi})_{kf}$:

$$(\hat{\mathsf{L}}_{\lambda\xi})_{kf} = \int d^3X\, [\hat{\mathsf{L}}_{\lambda\xi}(\mathbf{X})]_{kf},$$

simply obtained substituting (3.2.40) inside (3.2.27). Now one can expect that the transition $\lambda\xi$ can be in some way "localized", i.e., a region $\omega_{\lambda\xi} \subset \mathbf{R}^3$ can be specified such that $[\hat{\mathsf{L}}_{\lambda\xi}(\mathbf{X})]_{kf}$ is practically negligible $\forall\, k, f$ if $\mathbf{X}$ is outside $\omega_{\lambda\xi}$; then the last term of (3.2.29) becomes

$$\frac{1}{\hbar}\sum_{\xi\lambda} \int_{\omega_{\lambda\xi}} d^3X\, \hat{\mathsf{L}}_{\lambda\xi}(\mathbf{X})\hat{\varrho}(t) \int_{\omega_{\lambda\xi}} d^3X'\, \hat{\mathsf{L}}^\dagger_{\lambda\xi}(\mathbf{X}'),$$

thus providing an association of the event $\lambda\xi$ to the region $\omega_{\lambda\xi}$.

The set of variables $N_{\lambda\xi}(\tau)$, $\tau \geq t_0$, $N_{\lambda\xi}(\tau)$ being the number of transitions $\lambda\xi$ up to time τ, define a multicomponent classical stochastic process for which probability distributions and description of statistical subcollections at times τ, conditioned by the values $N_{\lambda\xi}(\tau)$, can be given. This is a straightforward generalization of the typical *counting process* considered by Srinivas and Davies [33]; e.g., the probability that in a time interval $[\tau_1, \tau_2]$ there are N events related to transitions $\lambda_1\xi_1, \lambda_2\xi_2, \ldots, \lambda_N\xi_N(\boldsymbol{\lambda\xi})$, belonging respectively to certain subsets $\sigma_1 \in \Gamma_{t_1}, \sigma_2 \in \Gamma_{t_2}, \ldots \sigma_N \in \Gamma_{t_N}$ (λ and $\xi(t)$ belong respectively to the spectra Λ of H_m and $\Xi(t)$ of $\varrho_\mathrm{m}(t)$, which are practically a continuum, and Γ_t is a σ-algebra on $\Lambda \times \Xi(t)$), when no event happens before τ_1, is given by:

$$P_{\tau_1,\tau_2}(N, \boldsymbol{\sigma}) = \mathrm{Tr}\left(\mathcal{F}_{\tau_1,\tau_2}(N, \boldsymbol{\sigma})\mathcal{A}_{\tau_1 t_0}\hat{\varrho}_{t_0}\right)$$

where $\mathcal{F}_{\tau_1,\tau_2}(N, \boldsymbol{\sigma})$ is an operation, i.e., a contractive positive mapping on $\mathcal{T}(\mathcal{H}^{(1)})$:

$$\mathcal{F}_{\tau_1,\tau_2}(N, \boldsymbol{\sigma}) = \sum_{(\boldsymbol{\lambda\xi})\in\boldsymbol{\sigma}} \int_{\tau_1}^{\tau_2} dt_N \ldots \int_{\tau_1}^{t_2} dt_1 \mathcal{A}_{\tau_2 t_N}\mathcal{L}_{\lambda_N\xi_N}(t_N)\mathcal{A}_{t_N t_{N-1}} \ldots \mathcal{L}_{\lambda_1\xi_1}(t_1)\mathcal{A}_{t_1\tau_1}.$$

This flow of transitions accompanying in the medium the propagation of the microsystem could prime a measurement inside some suitable measuring device, then $P_{\tau_1,\tau_2}(N, \boldsymbol{\sigma})$ would be the probability for this device to be affected by the microsystem. In fact writing $F_{\tau_2\tau_1}(\boldsymbol{\sigma}) = \mathcal{F}'_{\tau_1,\tau_2}(N, \boldsymbol{\sigma})\mathbf{1}$, with $\mathcal{F}'$ the adjoint mapping on $\mathcal{B}(\mathcal{H}^{(1)})$, (the set of bounded operators on $\mathcal{H}^{(1)}$) one has:

$$P_{\tau_1,\tau_2}(N, \boldsymbol{\sigma}) = \mathrm{Tr}_{\mathcal{H}^{(1)}} \left(F_{\tau_2\tau_1}(\boldsymbol{\sigma}) \mathcal{A}_{\tau_1 t_0} \hat{\varrho}_{t_0} \right),$$

$F_{\tau_2\tau_1}(\boldsymbol{\sigma})$ being a positive operator, $F_{\tau_2\tau_1}(\boldsymbol{\sigma}) \leq \mathbf{1}$. This equation gives the typical probability rule of modern quantum mechanics in which the notion of an *effect valued measure* $F_{\tau_2\tau_1}(\boldsymbol{\sigma})$ on some σ-algebra of subsets generalizes the customary concept of a projection valued measure, or equivalently of a self-adjoint operator, associated to an observable; these observables present an idealization that is very useful to understand the basic structure of quantum mechanics, but is too strong for representing real measuring devices [12, 16, 17, 18]. A similar situation is met if one considers the statistical operator

$$\hat{\varrho}_{\tau_2} = \frac{\mathcal{F}_{\tau_1,\tau_2}(N, \boldsymbol{\sigma}) \mathcal{A}_{\tau_1 t_0} \hat{\varrho}_{t_0}}{P_{\tau_1,\tau_2}(N, \boldsymbol{\sigma})},$$

which represents the repreparation at time τ_2 of the statistical collection $\hat{\varrho}_{t_0}$ under the condition that the aforementioned effect happens in the time interval $[\tau_1, \tau_2]$. Taking (3.2.37) into account $\hat{\varrho}_{\tau_2}$ is seen to bear an analogy with the highly idealized von Neumann state reduction rule

$$\hat{\varrho}^{(+)}_{\tau_2} = \frac{\hat{\mathsf{P}} \hat{\varrho}^{(-)}_{\tau_2} \hat{\mathsf{P}}}{\mathrm{Tr} \left(\hat{\mathsf{P}} \hat{\varrho}^{(-)}_{\tau_2} \right)}$$

for the statistical operator $\hat{\varrho}^{(-)}_{\tau_2}$, when it is reprepared at time τ_2 taking a measurement into account, associated with the projection operator $\hat{\mathsf{P}}$.

Actually by (3.2.38) a decomposition of $\hat{\varrho}_t$ is given into subcollections related to all possible detection patterns of events primed by the elementary transitions $\lambda\xi$; mathematically this means that a decomposition of the evolution mapping $\mathrm{T} \left(\exp \int_{t_0}^{t} dt' \, \mathcal{L}(t') \right)$ has been given on the space of the jump processes $N_{\lambda\xi}(\tau)$. In different physical contexts more general decompositions of an evolution mapping can be given, as it has been shown in the aforementioned theory of continuous measurement: then the variables involved are not only $N_{\lambda\xi}(\tau)$, but also the values of continuously measured variables related to the system.

3.3 Summary and outlook

In this chapter we have considered the problem of the description of the dynamics of a microsystem interacting with a system having many degrees of freedom. After discussing the typical features of modern single particle experiments, together with their interpretation and relevance for the foundations of quantum mechanics, in Sect. 3.2.1 we have constructed the generator of the time evolution for the microsystem. In order to obtain this result we have worked in Heisenberg picture, on a time scale much longer than the typical relaxation time for the macrosystem, calculating the time evolution of couples of field operators $a_h^\dagger a_k$ corresponding to creation and annihilation operators for the particle and acting in the Fock-space of the whole system. This has been done exploiting techniques of scattering theory in the superoperator formalism. The expression for the generator defined on such couples of operators and ensuring complete positivity appears in (3.2.24)

$$\mathcal{L}'\left(a_h^\dagger a_k\right) = \frac{i}{\hbar}\left[H_0 + V^{[1]}, a_h^\dagger a_k\right] - \frac{1}{\hbar}\left\{\left[\Gamma^{[1]}, a_h^\dagger\right] a_k - a_h^\dagger\left[\Gamma^{[1]}, a_k\right]\right\} + \frac{1}{\hbar}\sum_\lambda R_{h\lambda}^{[1]\dagger} R_{k\lambda}^{[1]},$$

and the different operators are explicitly given in Sect. 3.2.1. The aim is to obtain a general structure for the description of subdynamics in nonrelativistic quantum field theory and as we shall see in Chap. 5 an expression having the same structure can be obtained studying the problem of the description of the dynamics of reduced degrees of freedom for a macrosystem. Exploiting the simple formulas (3.2.8), (3.2.10) and (3.2.11)

$$\rho = \sum_{gf} a_g^\dagger \varrho_{\mathrm{m}} a_f \langle u_g|\hat{\varrho}|u_f\rangle, \qquad A = \sum_{hk} a_h^\dagger \langle h|\hat{\mathsf{A}}|k\rangle a_k$$

$$\mathrm{Tr}_{\mathcal{H}_F}\left(A\rho\right) = \mathrm{Tr}_{\mathcal{H}^{(1)}}\left(\hat{\mathsf{A}}\hat{\varrho}\right),$$

connecting the expectation values of observables in the Fock-space with expectation values in the one particle Hilbert space, a master equation of the Lindblad form for the statistical operator describing the microsystem is obtained in (3.2.29)

$$\frac{d\hat{\varrho}}{dt} = -\frac{i}{\hbar}\left[\hat{\mathsf{H}}_0 + \hat{\mathsf{V}}, \hat{\varrho}\right] - \frac{1}{\hbar}\left\{\hat{\Gamma}, \hat{\varrho}\right\} + \frac{1}{\hbar}\sum_{\xi\lambda} \hat{\mathsf{L}}_{\lambda\xi}\hat{\varrho}\hat{\mathsf{L}}_{\lambda\xi}^\dagger.$$

The structure of the operators appearing in this master equation, linked to the T-matrix describing scattering between the particle and the macroscopic system, is considered in Sect. 3.2.4, where possible useful phenomenological Ansatz are indicated and the connection between the mixture term and the scattering cross-section is explored. Finally in Sect. 3.2.5 we consider the general physical meaning of the obtained master equation and its capability to describe both an optical, wavelike dynamics and an interaction with a measuring character, linked to transitions taking place inside the macrosystem as a consequence of the interaction. This is done making reference to the theory of counting processes.

The formal scheme we have developed in this chapter should serve as a preliminary step towards the description of slowly varying degrees of freedom in Heisenberg picture inside a field theoretical formalism. In fact a microsystem interacting with matter can be seen as the simplest case of reduced dynamics. The result is however relevant by itself, both because of the importance that single particle experiments have assumed in the last few years and because the obtained master equation can describe both coherent and incoherent interactions, while usual treatments are often restricted to only one type of interaction. This will become clearer considering the applications to neutron optics and quantum Brownian motion in Chap. 4.

Chapter 4

Neutron-Matter Interaction and Brownian Motion

4.1 Introduction

The formalism developed in Chap. 3, that has led to the master equation (3.2.31) for the time evolution of the statistical operator describing the microsystem, will now be tested in the specific case of neutron-matter interaction and Brownian motion. This test will allow us to better understand the role and the relevance of the different contributions in (3.2.31), with reference to concrete physical examples. Furthermore we shall see the differences with respect to other approaches to the same physical situations. One expects that the major differences should come from the two terms

$$-\frac{1}{\hbar}\left\{\frac{1}{2}\sum_{\xi\lambda}\hat{\mathsf{L}}^{\dagger}_{\lambda\xi}\hat{\mathsf{L}}_{\lambda\xi},\hat{\varrho}\right\}+\frac{1}{\hbar}\sum_{\xi\lambda}\hat{\mathsf{L}}_{\lambda\xi}\hat{\varrho}\hat{\mathsf{L}}^{\dagger}_{\lambda\xi}\ ,$$

which are peculiar to the formalism of the statistical operator, as clarified in Sect. 3.2.1. This is indeed the case, both for neutron-matter interaction and for Brownian motion. Moreover, in both cases, the balance between the two contributions is of utmost importance and their influence on the dynamics becomes clear only when they are studied jointly.

Considering neutron optics, the commutator term is the most important physical contribution, being responsible for the wavelike behavior. A correction to this behavior according to (3.2.31) has been tentatively estimated in Sect. 4.2.3 in order to give a simple example of possible experimental implications.

In the case of Brownian motion the connection to actual physical experiments is for the moment not so straightforward, even though the study of quantum dissipation is of tremendous importance: it suffices to think of the relevance of friction and dissipative effects in atom cooling and trapping or with reference to the problem of decoherence, which affects both applications, being decisive with respect to the feasibility of quantum computing, and fundamental questions, especially the still much debated transition from quantum to classical [6].

4.2 Neutron-Matter Interaction

In recent years there has been a rapidly growing interest in the field of particle optics, especially neutron and atom optics (for a recent review see [20, 8, 41, 43, 44] and [45] respectively, and references quoted therein), due to a spectacular improvement of the experimental techniques, connected to the introduction of the single crystal interferometer in the first case, and to progress in microfabrication technology and development of intense tunable lasers in the second one. Such new achievements provide very important tests verifying the validity of quantum mechanics, especially in that it predicts wavelike behaviors even for single microsystems.

At the same time a new challenge arises, linked to the accuracy required in the description of the interaction between the microsystem and the apparatus acting as optical device. The question of the description of the dynamics of a microsystem interacting with a system having many degrees of freedom (e.g., matter seen as an optical medium characterized by an index of refraction) has been extensively studied and contains some typical quantum mechanical features, such as quantum correlations between the two systems, by which a reduced description of the microsystem's degrees of freedom can arise only by suitable approximations. This subtle point is particularly important in the case of particle optics, where the main interest is devoted to the coherent wavelike behavior of particles, as can be justified on the basis of the similarity between a Schrödinger equation with an optical potential and the Helmholtz wave equation [41, 45]. The very existence of such an optical description of the interaction is far from trivial and strongly depends on the experimental conditions. The attention has been mostly devoted to exploiting the optical analogies, while little has been said on the borderline between the optical regime, in which coherent effects are predominant and a classical wavelike description plays a major role, and an incoherent regime, where incoherent effects, caused by the interaction between the microsystem and the apparatus and showing typical particle-like features, should not be neglected. This attitude is exemplified in neutron optics by the use of the *coherent wave* formalism (see for example [46]), instead of a reduced density matrix description, as usually adopted in quantum optics.

In this chapter we want to address the question of how to consistently describe both regimes applying the approach to the description of irreversible subdynamics in quantum mechanics exposed in Chap. 3 to the specific case of neutron-matter interaction. The expressions appearing in the generator of the time evolution are linked to particle-particle interactions, like the Fermi pseudopotential, and to properties of the macroscopic system, like the dynamic structure function, first introduced by van Hove [40]. The first part of the generator accounts for the description of the coherent interaction in terms of optical potential and index of refraction well-known in neutron optics [41, 47, 48]. The remaining part is shown to be related to the dynamic structure function or, equivalently, to the density correlation function and leads in a straightforward way to results obtained in the so called *rigorous theory of dispersion* [41].

4.2.1 Optical Behavior

The field of neutron-matter interaction is well suited to test our formalism both because of the very refined experiments that have been carried out in neutron interferometry [8, 49] and because of the very well studied description of neutron optics phenomena, as developed for example in the book by Sears [41], that we will take as basic reference. As a first step we want to consider the coherent interaction of neutrons with matter and therefore we neglect in (3.2.26) the last contribution, linked to incoherent processes. As we will see later this term implies indeed a smaller correction in the case of neutron scattering. We are left with:

$$\frac{d\varrho_{kh}}{dt} = -\frac{i}{\hbar}\left(E_k - E_h\right)\varrho_{kh} - \frac{i}{\hbar}\sum_f Q_{kf}\varrho_{fh} + \frac{i}{\hbar}\sum_g \varrho_{kg}Q^*_{hg}, \tag{4.2.1}$$

and we need a suitable expression for the operator

$$Q_{kf} = \mathrm{Tr}_{\mathcal{H}_F}\left[T^k_f(E_k + i\varepsilon)\varrho_{\mathrm{m}}(t)\right].$$

Following Sears we adopt the Fermi pseudopotential to describe the neutron nucleus interaction in impulse approximation; let us recall the form of the T-matrix in the context of the elementary theory of dispersion:

$$T = \frac{2\pi\hbar^2}{m}\sum_\alpha b_\alpha \sum_{i=1}^{N_\alpha}\delta^3(\hat{\mathsf{x}} - \mathbf{R}_i), \tag{4.2.2}$$

where $\hat{\mathsf{x}}$ is the position operator for the neutron, $\mathbf{R}_i$ the position operator for the i-th nucleus of type α, b_α the bound scattering length, depending on isotope and spin orientation, m the neutron mass, N_α the number of nuclei of type α. An operator of the form (4.2.2), that is to say a sum over one-particle operators, is expressed in second quantization by:

$$T = \frac{2\pi\hbar^2}{m}\sum_\alpha b_\alpha \int d^3\mathbf{x}\,\psi^\dagger_\alpha(\mathbf{x})\delta^3(\hat{\mathsf{x}} - \mathbf{x})\psi_\alpha(\mathbf{x}), \tag{4.2.3}$$

where $\psi_\alpha(\mathbf{x})$ is the field operator, acting in the Fock-space of the macrosystem, corresponding to particles of type α. For the sake of simplicity from now on we will consider one kind of particles, thus dropping the subscript α. Furthermore we will assume that b is a real quantity, since we are not going to deal with absorption phenomena. As we shall see in the next section we concentrate on non-hermiticity of the potential connected with incoherent processes and not with net absorption. A phenomenological description as given by (4.2.3) falls within the class of effective potentials considered in the previous paragraph and corresponds to the following interaction kernel:

$$t(z, \mathbf{x} - \mathbf{y}) = \frac{2\pi\hbar^2}{m} b\, \delta^3(\mathbf{x} - \mathbf{y}), \tag{4.2.4}$$

leading to

$$T^k_f(E_k + i\varepsilon) = \frac{2\pi\hbar^2}{m} b \int d^3\mathbf{x} \int d^3\mathbf{y}\, \psi^\dagger(\mathbf{x}) u^*_k(\mathbf{y}) \delta^3(\mathbf{x} - \mathbf{y}) u_f(\mathbf{y}) \psi(\mathbf{x}).$$

Eq. (4.2.1) thus becomes, in operator form:

$$\begin{aligned} \frac{d\hat{\varrho}(t)}{dt} = &- \frac{i}{\hbar} \left[\hat{\mathsf{H}}_0, \hat{\varrho}(t)\right] - \frac{i}{\hbar} \frac{2\pi\hbar^2}{m} b \int d^3\mathbf{x}\, \langle \psi^\dagger(\mathbf{x}) \psi(\mathbf{x}) \rangle_t\, \delta^3(\hat{\mathsf{x}} - \mathbf{x}) \hat{\varrho}(t) \\ &+ \frac{i}{\hbar} \frac{2\pi\hbar^2}{m} b \int d^3\mathbf{x}\, \langle \psi^\dagger(\mathbf{x}) \psi(\mathbf{x}) \rangle_t\, \hat{\varrho}(t) \delta^3(\hat{\mathsf{x}} - \mathbf{x}), \end{aligned} \tag{4.2.5}$$

where $\hat{\mathsf{x}}$ is the position operator for the neutron and $\langle A \rangle_t \equiv \mathrm{Tr}_{\mathcal{H}_F}(\varrho_{\mathrm{m}}(t) A)$. If we consider only pure states and assume the macrosystem to be at equilibrium ($\langle \ldots \rangle_t \equiv \langle \ldots \rangle$), eq. (4.2.5) is equivalent to the following stationary Schrödinger equation

$$\left\{ -\frac{\hbar^2}{2m} \Delta_x + \frac{2\pi\hbar^2}{m} b \langle \psi^\dagger(\mathbf{x}) \psi(\mathbf{x}) \rangle \right\} \phi(\mathbf{x}) = E \phi(\mathbf{x}), \tag{4.2.6}$$

which, remembering that the average particle density $\langle \sum_i \delta^3(\mathbf{x} - \mathbf{R}_i) \rangle$ is given in second quantization by $\langle \psi^\dagger(\mathbf{x}) \psi(\mathbf{x}) \rangle$, is exactly the equation used by Sears to describe all coherent neutron optical phenomena, here recovered in a straightforward, alternative way, though in a very different framework. The term

$$\frac{2\pi\hbar^2}{m} b \langle \psi^\dagger(\mathbf{x}) \psi(\mathbf{x}) \rangle$$

is called optical potential and assumes different expressions according to the structure of the system. If the medium can be considered homogeneous, with density n_{o}, eq. (4.2.6) describes propagation of matter waves with an index of refraction given by

$$n = \left(1 - \frac{2\pi\hbar^2}{mE} b n_{\mathrm{o}}\right)^{\frac{1}{2}} \simeq 1 - \frac{\lambda^2}{2\pi} b n_{\mathrm{o}}\ , \tag{4.2.7}$$

as first obtained by Goldberger and Seitz [48] in the absence of absorption. This is the formula currently used to calculate phase shifts in neutron interferometry experiments [8]:

$$e^{i\chi} = e^{i(n-1)\frac{2\pi}{\lambda} D} = e^{-i n_{\mathrm{o}} b \lambda D}, \tag{4.2.8}$$

where D is the thickness of the sample.

In a similar way we can obtain from (4.2.1) a more general formula for the refractive index introduced for the first time by Lax [47]. Starting from the general expression (3.2.33) the potential term in (4.2.1) becomes

$$\sum_f Q_{kf}\varrho_{fh} = \sum_f \mathrm{Tr}_{\mathcal{H}_F} \int d^3\mathbf{x} \int d^3\mathbf{y}\, \psi^\dagger(\mathbf{x}) u_k^*(\mathbf{y}) t(E_k + i\varepsilon, \mathbf{x}-\mathbf{y}) u_f(\mathbf{y}) \psi(\mathbf{x}) \varrho_{\mathrm{m}}(t) \varrho_{fh}.$$

Following Lax we suppose that the system is homogeneous, so that

$$\mathrm{Tr}_{\mathcal{H}_F} \left[\psi^\dagger(\mathbf{x})\psi(\mathbf{x})\varrho_{\mathrm{m}}(t)\right] = n_{\mathrm{o}}.$$

We have

$$\begin{aligned} \sum_f Q_{kf}\varrho_{fh} &= n_{\mathrm{o}} \sum_f \int d^3\mathbf{x}\, t(E_k + i\varepsilon, \mathbf{x}) \int d^3\mathbf{y}\, u_k^*(\mathbf{y}) u_f(\mathbf{y}) \varrho_{fh} \\ &= n_{\mathrm{o}} \int d^3\mathbf{x}\, t(E_k + i\varepsilon, \mathbf{x}) \varrho_{kh}, \end{aligned}$$

where we have exploited the orthogonality between the states $\{u_f\}$, thus obtaining the matrix element of the T-operator for forward scattering, averaged over the possible states of the macrosystem. Keeping the relation between T-operator and scattering amplitude into account we come to

$$-n_{\mathrm{o}} \frac{2\pi\hbar^2}{m} f(0, E_k) \varrho_{kh}. \tag{4.2.9}$$

Inserted in the Schrödinger equation this term is equivalent to an index of refraction of the form:

$$n = \left(1 + \frac{2\pi\hbar^2}{mE_k} n_{\mathrm{o}} f(0, E_k)\right)^{\frac{1}{2}} \simeq 1 + \frac{\lambda^2}{2\pi} n_{\mathrm{o}} f(0, E_k), \tag{4.2.10}$$

simply linked to the forward scattering amplitude. An analogous result holds for electromagnetic waves propagating in a material with low density [50]. A similar treatment has been proposed [51] and adopted (see for example [52]) in the description of the propagation of atoms through a dilute medium, showing the interest of similar descriptions also for atom optics. In the case of thermal neutrons the scattering amplitude is isotropic within a very good approximation and is given in terms of the scattering length by the simple formula $f = -b$ which reduces (4.2.10) to (4.2.7).

So far we have shown how, starting from (3.2.26) and neglecting the incoherent term, we can recover some important results obtained within the framework of multiple scattering theory and used to describe the coherent interaction of neutrons with matter. Our formalism puts into evidence the statistical operator of the macrosystem, the T-matrix and the scattering amplitude, so that phenomenological inputs are rather direct. Further improvements of the formulas obtained are allowed by the presence of $\varrho_{\rm m}(t)$ and depend on its evaluation. The correction factor c that Lax includes in (4.2.10) to obtain the index of refraction

$$n \simeq 1 + \frac{\lambda^2}{2\pi} n_{\rm o} c f(0, E_k),$$

is connected to fulfillment of the optical theorem, which in our formalism, as we will see in the next section, is related to the presence of the incoherent contribution.

4.2.2 The Incoherent Contribution

We now come to the main result of this investigation, the connection between the contributions other than the commutator in (3.2.31) and the dynamic structure function, together with the relevance of this relationship to the optical theorem. As observed by Sears an expression of the form (4.2.7) or (4.2.10) for the refractive index *doesn't include the contribution to the attenuation of the coherent wave in the medium due to diffuse scattering and, hence, violates the "optical theorem" of scattering theory* [44, 41, 53]. To overcome this difficulty he refrains from ad hoc assumptions as in [54], which amount to introduce a suitable imaginary contribution to the potential, and considers a rigorous theory of dispersion. In this more accurate treatment (4.2.2) is replaced by

$$T = \frac{2\pi\hbar^2}{m} \sum_{\alpha} f_\alpha \sum_{i=1}^{N_\alpha} \delta^3(\hat{\mathsf{x}} - \mathbf{R}_i),$$

and f_α has the general expression ($\mathbf{k}$ is the incident neutron momentum)

$$f_\alpha = -b_\alpha + \frac{i}{\hbar} k b_\alpha^2 + O(k^2),$$

where the second term had been previously omitted because of its smallness, since typically $\frac{1}{\hbar} kb \leq 10^{-4}$. Furthermore the scattering amplitude is to be multiplied by a constant c which should take local field corrections into account and whose value depends only on the temperature, density and chemical composition of the medium. Sears obtains an estimate for this constant in terms of the structure function of the macroscopic scatterer in the case of an homogeneous medium, applying a multiple wave formalism to solve the scattering problem, and drawing strong analogies to the usual descriptions of propagation of electromagnetic waves. In this way he recovers a correspondence between attenuation of the coherent wave in the medium and diffuse scattering. In the following we shall set $f_\alpha = f$ for all α and consider only real b, in order to concentrate upon diffuse scattering, neglecting absorption. By diffuse scattering we intend all scattering that is not coherent in the absolute sense, that is elastic and coherent (for the distinction between absolute and relative incoherence see for example [41, 47]). To compare with these more refined results we have to consider all contributions in (3.2.31). Let us stress from the very beginning some general features of this expression, thanks to which it can describe more general physical situations than those arising in an evolution driven by a Schrödinger-like equation. The last two terms

$$-\frac{1}{\hbar}\left\{\frac{1}{2}\sum_{\xi,\lambda}\hat{\mathsf{L}}^{\dagger}_{\lambda\xi}\hat{\mathsf{L}}_{\lambda\xi},\hat{\varrho}\right\}+\frac{1}{\hbar}\sum_{\xi,\lambda}\hat{\mathsf{L}}_{\lambda\xi}\hat{\varrho}\hat{\mathsf{L}}^{\dagger}_{\lambda\xi} \qquad (4.2.11)$$

allow for the presence of a non-self-adjoint potential which is nevertheless not linked to real absorption (sse Sect. 3.2). This is the case for the present treatment, in which the imaginary part of the optical potential is to be traced back to the existence of diffuse scattering, as opposed to the coherent wavelike behavior. Attenuation of the *coherent wave* is due to the presence of the anticommutator term, responsible for the imaginary potential, balanced by the last contribution, typically incoherent in that it leads from a pure state to a mixture. This last term is given by a sum over subcollections, formally similar to the expression that we would obtain for the statistical operator after the measurement of a given observable. The subcollections are denoted by the indexes $\lambda\xi$, which specify a change of the state of the macroscopic system, caused by interaction with the microsystem, thus making this contribution to the dynamics incoherent (see Sect. 3.2.5). In fact we will see in the case of neutron-matter interaction that the trace of this term gives all the contributions to incoherent scattering, that is to say the total diffusion cross section. The balance between the two terms of (4.2.11) accounts for fulfilment of the optical theorem.

To see this let us now consider (4.2.11) in more detail. Starting from (3.2.27) and (3.2.33), introducing a Laplace transform for the energy dependence of the effective T-matrix

$$t(E,\mathbf{x})=\int_0^\infty d\sigma\, e^{\frac{i}{\hbar}E\sigma}\bar{t}(\sigma,\mathbf{x}),$$

together with the following expression for the density number operator in terms of creation and annihilation operators with specified momentum

$$N(\mathbf{x})=\psi^\dagger(\mathbf{x})\psi(\mathbf{x})=\frac{1}{\mathsf{V}}\sum_{\kappa,P}e^{-\frac{i}{\hbar}\boldsymbol{\kappa}\cdot\mathbf{x}}b^\dagger_{P+\frac{\kappa}{2}}b_{P-\frac{\kappa}{2}},$$

we obtain

$$\begin{aligned}\hat{\mathsf{L}}_{\lambda\xi} \;=\; & \frac{i}{\hbar}\sqrt{2\varepsilon\pi_\xi}\frac{1}{\mathsf{V}}\sum_{\kappa,P}\int_0^\infty d\tau\, e^{-\frac{\varepsilon}{\hbar}\tau}\int_0^\infty d\sigma\int d^3\mathbf{x}''\, e^{-\frac{\varepsilon}{\hbar}\sigma}e^{-\frac{i}{\hbar}\hat{\mathsf{H}}_0(\tau-\sigma)}\bar{t}(\sigma,\mathbf{x}''-\hat{\mathsf{x}})e^{\frac{i}{\hbar}\hat{\mathsf{H}}_0\tau}e^{-\frac{i}{\hbar}\boldsymbol{\kappa}\cdot\mathbf{x}''}\\ & \times\langle\lambda|e^{-\frac{i}{\hbar}H_{\mathrm{m}}\tau}b^\dagger_{P+\frac{\kappa}{2}}b_{P-\frac{\kappa}{2}}e^{\frac{i}{\hbar}H_{\mathrm{m}}\tau}|\xi\rangle,\end{aligned}$$

where V is the volume of the region in which the system is supposed to be confined. Indicating by $\tilde{t}(E,\boldsymbol{\kappa})$ the Fourier transform of the potential with respect to space

$$\tilde{t}(E,\boldsymbol{\kappa})=\int d^3\mathbf{x}\, t(E,\mathbf{x})e^{-\frac{i}{\hbar}\boldsymbol{\kappa}\cdot\mathbf{x}}$$

and after some simple manipulations one comes to

$$\hat{\mathsf{L}}_{\lambda\xi} = \frac{i}{\hbar}\sqrt{2\varepsilon\pi_\xi}\frac{1}{\mathsf{V}}\sum_{\kappa,P}\int_0^\infty d\tau\, e^{-\frac{\varepsilon}{\hbar}\tau}\,\tilde{t}(\hat{\mathsf{H}}_0+i\varepsilon,\boldsymbol{\kappa})e^{\frac{i}{\hbar}\frac{\boldsymbol{\kappa}^2}{2m}\tau}e^{\frac{i}{\hbar}\frac{\boldsymbol{\kappa}\cdot\hat{\mathsf{p}}}{m}\tau}e^{-\frac{i}{\hbar}\boldsymbol{\kappa}\cdot\hat{\mathsf{x}}}\langle\lambda|e^{-\frac{i}{\hbar}H_{\mathrm{m}}\tau}b^\dagger_{P+\frac{\kappa}{2}}b_{P-\frac{\kappa}{2}}e^{\frac{i}{\hbar}H_{\mathrm{m}}\tau}|\xi\rangle,$$

to be inserted in (4.2.11). Before doing this let us introduce the useful notation

$$e^{-\frac{i}{\hbar}H_{\mathrm{m}}\tau}Ae^{\frac{i}{\hbar}H_{\mathrm{m}}\tau}=\sum_\Delta e^{-\frac{i}{\hbar}\Delta t}(A)_\Delta,\quad (A)_\Delta=\sum_E|E+\Delta\rangle\langle E+\Delta|A|E\rangle\langle E|,\quad (A)^\dagger_\Delta=(A^\dagger)_{-\Delta}.$$

We have

$$\begin{aligned}\frac{1}{\hbar}\sum_{\xi,\lambda}\hat{\mathsf{L}}_{\lambda\xi}\hat{\varrho}\hat{\mathsf{L}}^\dagger_{\lambda\xi} &= \frac{2\varepsilon}{\hbar^3\mathsf{V}^2}\sum_{\kappa,P}\sum_{\kappa',P'}\int_0^\infty d\tau\, e^{-\frac{\varepsilon}{\hbar}\tau}e^{\frac{i}{\hbar}\frac{\boldsymbol{\kappa}^2}{2m}\tau}e^{\frac{i}{\hbar}\frac{\boldsymbol{\kappa}\cdot\hat{\mathsf{p}}}{m}\tau}\,\tilde{t}(\hat{\mathsf{H}}_0+i\varepsilon,\boldsymbol{\kappa})\\ &\times e^{-\frac{i}{\hbar}\boldsymbol{\kappa}\cdot\hat{\mathsf{x}}}\,\hat{\varrho}\,e^{\frac{i}{\hbar}\boldsymbol{\kappa}'\cdot\hat{\mathsf{x}}}\,\tilde{t}^\dagger(\hat{\mathsf{H}}_0+i\varepsilon,\boldsymbol{\kappa}')\int_0^\infty d\tau'\,e^{-\frac{\varepsilon}{\hbar}\tau'}e^{-\frac{i}{\hbar}\frac{\boldsymbol{\kappa}'^2}{2m}\tau'}e^{-\frac{i}{\hbar}\frac{\boldsymbol{\kappa}'\cdot\hat{\mathsf{p}}}{m}\tau'}\\ &\times\sum_{\Delta,\Delta'}e^{-\frac{i}{\hbar}\Delta\tau}\mathrm{Tr}_{\mathcal{H}_F}\left[\left(b^\dagger_{P+\frac{\kappa}{2}}b_{P-\frac{\kappa}{2}}\right)_\Delta\varrho_{\mathrm{m}}\left(b^\dagger_{P'-\frac{\kappa'}{2}}b_{P'+\frac{\kappa'}{2}}\right)_{-\Delta'}\right]e^{\frac{i}{\hbar}\Delta'\tau'},\end{aligned}$$

and similarly for the anticommutator part. An important simplification takes place if one can use symmetry under time and space translations. Time translation invariance occurs if, at least with reference to the interaction with the microsystem, matter can be considered at equilibrium, then:

$$\mathrm{Tr}_{\mathcal{H}_F}\left(A_\Delta\varrho_{\mathrm{m}}B_{-\Delta'}\right)=\delta_{\Delta,\Delta'}\mathrm{Tr}_{\mathcal{H}_F}\left(A_\Delta\varrho_{\mathrm{m}}B_{-\Delta}\right).$$

Similarly space translation invariance implies

$$\begin{aligned}&\mathrm{Tr}_{\mathcal{H}_F}\left[\left(b^\dagger_{P+\frac{\kappa}{2}}b_{P-\frac{\kappa}{2}}\right)_\Delta\varrho_{\mathrm{m}}\left(b^\dagger_{P'-\frac{\kappa'}{2}}b_{P'+\frac{\kappa'}{2}}\right)_{-\Delta'}\right]=\\ &\qquad=\delta_{\Delta,\Delta'}\delta_{\kappa,\kappa'}\mathrm{Tr}_{\mathcal{H}_F}\left[\left(b^\dagger_{P+\frac{\kappa}{2}}b_{P-\frac{\kappa}{2}}\right)_\Delta\varrho_{\mathrm{m}}\left(b^\dagger_{P'-\frac{\kappa}{2}}b_{P'+\frac{\kappa}{2}}\right)_{-\Delta}\right],\end{aligned}$$

such a symmetry can be implemented at equilibrium in the thermodynamic limit and can be practically assumed for a microsystem interacting with a homogeneous portion of a macrosystem. Then one has, performing also the τ, τ' integrals:

$$\begin{aligned}&-\frac{1}{\hbar}\left\{\frac{1}{2}\sum_{\xi,\lambda}\hat{\mathsf{L}}^\dagger_{\lambda\xi}\hat{\mathsf{L}}_{\lambda\xi},\hat{\varrho}\right\}+\frac{1}{\hbar}\sum_{\xi,\lambda}\hat{\mathsf{L}}_{\lambda\xi}\hat{\varrho}\hat{\mathsf{L}}^\dagger_{\lambda\xi}=\\ &=-\frac{\varepsilon}{\hbar\mathsf{V}^2}\sum_{\kappa,\Delta}\Bigg(\Bigg\{\hat{\varrho},e^{\frac{i}{\hbar}\boldsymbol{\kappa}\cdot\hat{\mathsf{x}}}\frac{1}{\frac{\boldsymbol{\kappa}\cdot\hat{\mathsf{p}}}{m}+\frac{\boldsymbol{\kappa}^2}{2m}-\Delta-i\varepsilon}\tilde{t}^\dagger(\hat{\mathsf{H}}_0+i\varepsilon,\boldsymbol{\kappa})\\ &\qquad\times\tilde{t}(\hat{\mathsf{H}}_0+i\varepsilon,\boldsymbol{\kappa})\frac{1}{\frac{\boldsymbol{\kappa}\cdot\hat{\mathsf{p}}}{m}+\frac{\boldsymbol{\kappa}^2}{2m}-\Delta+i\varepsilon}e^{-\frac{i}{\hbar}\boldsymbol{\kappa}\cdot\hat{\mathsf{x}}}\Bigg\}\end{aligned}$$

$$- 2\frac{1}{\frac{\boldsymbol{\kappa}\cdot\hat{\mathsf{p}}}{m}+\frac{\boldsymbol{\kappa}^2}{2m}-\Delta+i\varepsilon}\tilde{t}(\hat{\mathsf{H}}_0+i\varepsilon,\boldsymbol{\kappa})e^{-\frac{i}{\hbar}\boldsymbol{\kappa}\cdot\hat{\mathsf{x}}}\,\hat{\varrho}\,e^{\frac{i}{\hbar}\boldsymbol{\kappa}\cdot\hat{\mathsf{x}}}\tilde{t}^\dagger(\hat{\mathsf{H}}_0+i\varepsilon,\boldsymbol{\kappa})$$

$$\times\frac{1}{\frac{\boldsymbol{\kappa}\cdot\hat{\mathsf{p}}}{m}+\frac{\boldsymbol{\kappa}^2}{2m}-\Delta-i\varepsilon}\Bigg)\varrho^M(\kappa,\Delta),$$

where

$$\varrho^M(\kappa,\Delta)\equiv\mathrm{Tr}_{\mathcal{H}_F}\left[\left(\sum_P b^\dagger_{P+\frac{\kappa}{2}}b_{P-\frac{\kappa}{2}}\right)_\Delta\varrho_{\mathrm{m}}\left(\sum_P b^\dagger_{P-\frac{\kappa}{2}}b_{P+\frac{\kappa}{2}}\right)_{-\Delta}\right],$$

or equivalently, introducing the $\hat{\mathsf{x}},\hat{\mathsf{p}}$ dependent amplitude

$$\check{t}(\hat{\mathsf{H}}_0+i\varepsilon,\boldsymbol{\kappa},\hat{\mathsf{x}})=e^{\frac{i}{\hbar}\boldsymbol{\kappa}\cdot\hat{\mathsf{x}}}\,t(\hat{\mathsf{H}}_0+i\varepsilon,\boldsymbol{\kappa})\,e^{-\frac{i}{\hbar}\boldsymbol{\kappa}\cdot\hat{\mathsf{x}}},$$

in the form:

$$-\frac{1}{\hbar\mathsf{V}^2}\sum_{\kappa,\Delta}\Bigg(\left\{\hat{\varrho},\check{t}^\dagger(\hat{\mathsf{H}}_0+i\varepsilon,\boldsymbol{\kappa},\hat{\mathsf{x}})\frac{\varepsilon}{\left(\frac{\boldsymbol{\kappa}\cdot\hat{\mathsf{p}}}{m}-\frac{\boldsymbol{\kappa}^2}{2m}-\Delta\right)^2+\varepsilon^2}\check{t}(\hat{\mathsf{H}}_0+i\varepsilon,\boldsymbol{\kappa},\hat{\mathsf{x}})\right\}$$

$$-2\varepsilon\,e^{-\frac{i}{\hbar}\boldsymbol{\kappa}\cdot\hat{\mathsf{x}}}\,\check{t}(\hat{\mathsf{H}}_0+i\varepsilon,\boldsymbol{\kappa},\hat{\mathsf{x}})\frac{1}{\frac{\boldsymbol{\kappa}\cdot\hat{\mathsf{p}}}{m}-\frac{\boldsymbol{\kappa}^2}{2m}-\Delta+i\varepsilon}\hat{\varrho}$$

$$\times\frac{1}{\frac{\boldsymbol{\kappa}\cdot\hat{\mathsf{p}}}{m}-\frac{\boldsymbol{\kappa}^2}{2m}-\Delta-i\varepsilon}\check{t}^\dagger(\hat{\mathsf{H}}_0+i\varepsilon,\boldsymbol{\kappa},\hat{\mathsf{x}})e^{\frac{i}{\hbar}\boldsymbol{\kappa}\cdot\hat{\mathsf{x}}}\Bigg)\varrho^M(\kappa,\Delta). \qquad (4.2.12)$$

Exploiting the fact that $\varrho^M(0,\Delta)$ contains a $\delta_{\Delta,0}$ factor, one can immediately see by inspection that the $\kappa=0$ contributions cancel each other provided the effective T-matrix is a slow function of energy,

$$\langle\mathbf{k}\,|\hat{\varrho}|\,\mathbf{f}\rangle\,\tilde{t}(E_k,0)\tilde{t}^\dagger(E_f,0)\approx\langle\mathbf{k}\,|\hat{\varrho}|\,\mathbf{f}\rangle\,\frac{1}{2}\left[\tilde{t}^\dagger(E_k,0)\tilde{t}(E_k,0)+\tilde{t}^\dagger(E_f,0)\tilde{t}(E_f,0)\right];$$

on the other hand for a homogeneous medium the $\kappa=0$ contributions are equal to those obtained writing the correlation function as a factorized product

$$\mathrm{Tr}_{\mathcal{H}_F}\left[\left(\sum_P b^\dagger_{P+\frac{\kappa}{2}}b_{P-\frac{\kappa}{2}}\right)_\Delta\varrho_{\mathrm{m}}\left(\sum_P b^\dagger_{P-\frac{\kappa}{2}}b_{P+\frac{\kappa}{2}}\right)_{-\Delta}\right]\longrightarrow$$

$$\mathrm{Tr}_{\mathcal{H}_F}\left[\left(\sum_P b^\dagger_{P+\frac{\kappa}{2}}b_{P-\frac{\kappa}{2}}\right)_\Delta\varrho_{\mathrm{m}}\right]\mathrm{Tr}_{\mathcal{H}_F}\left[\left(\sum_P b^\dagger_{P-\frac{\kappa}{2}}b_{P+\frac{\kappa}{2}}\right)_{-\Delta}\varrho_{\mathrm{m}}\right],$$

provided we assume the condition of *normal density fluctuations*, $(\langle N^2\rangle-\langle N\rangle^2)/\mathsf{V}^2\ll n_{\mathrm{o}}^2$. Instead of restricting the sum to the $\kappa\neq 0$ contributions we can therefore subtract from the correlation function its factorized part. After straightforward manipulations, using

$$\sum_P b^\dagger_{P+\frac{\kappa}{2}}b_{P-\frac{\kappa}{2}}=\int d^3\mathbf{x}\,\psi^\dagger(\mathbf{x})\psi(\mathbf{x})e^{\frac{i}{\hbar}\boldsymbol{\kappa}\cdot\mathbf{x}},\qquad \mathrm{Tr}_{\mathcal{H}_F}\left[(A)_\Delta\varrho_{\mathrm{m}}(B)_{-\Delta}\right]=\int\frac{dt}{2\pi\hbar}e^{-\frac{i}{\hbar}\Delta t}\,\langle BA(t)\rangle$$

we come to

$$\mathrm{Tr}_{\mathcal{H}_F}\left[\left(\sum_P b^\dagger_{P+\frac{\kappa}{2}} b_{P-\frac{\kappa}{2}}\right)_\Delta \varrho_{\mathrm{m}} \left(\sum_P b^\dagger_{P-\frac{\kappa}{2}} b_{P+\frac{\kappa}{2}}\right)_{-\Delta}\right]$$

$$-\mathrm{Tr}_{\mathcal{H}_F}\left[\left(\sum_P b^\dagger_{P+\frac{\kappa}{2}} b_{P-\frac{\kappa}{2}}\right)_\Delta \varrho_{\mathrm{m}}\right] \mathrm{Tr}_{\mathcal{H}_F}\left[\left(\sum_P b^\dagger_{P-\frac{\kappa}{2}} b_{P+\frac{\kappa}{2}}\right)_{-\Delta} \varrho_{\mathrm{m}}\right] =$$

$$= \int \frac{dt}{2\pi\hbar} e^{-\frac{i}{\hbar}\Delta t} \int d^3\mathbf{x} \int d^3\mathbf{y}\, e^{\frac{i}{\hbar}\boldsymbol{\kappa}\cdot(\mathbf{x}-\mathbf{y})} \left\langle \delta N(\mathbf{y}) \delta N(\mathbf{x},t)\right\rangle$$

where

$$\langle N(\mathbf{x})\rangle = \mathrm{Tr}_{\mathcal{H}_F}\left[N(\mathbf{x})\varrho_{\mathrm{m}}\right], \qquad \delta N(\mathbf{x}) = N(\mathbf{x}) - \langle N(\mathbf{x})\rangle,$$

and finally:

$$-\frac{1}{\hbar}\left\{\frac{1}{2}\sum_{\xi,\lambda} \hat{\mathsf{L}}^\dagger_{\lambda\xi}\hat{\mathsf{L}}_{\lambda\xi}, \hat{\varrho}\right\} + \frac{1}{\hbar}\sum_{\xi,\lambda}\hat{\mathsf{L}}_{\lambda\xi}\hat{\varrho}\hat{\mathsf{L}}^\dagger_{\lambda\xi} =$$

$$= -\frac{\varepsilon}{\hbar \mathsf{V}^2}\sum_{\kappa,\Delta}\left(\left\{\hat{\varrho}, e^{\frac{i}{\hbar}\boldsymbol{\kappa}\cdot\hat{\mathsf{x}}} \frac{1}{\frac{\boldsymbol{\kappa}\cdot\hat{\mathsf{p}}}{m} + \frac{\boldsymbol{\kappa}^2}{2m} - \Delta - i\varepsilon} \tilde{t}^\dagger(\hat{\mathsf{H}}_0 + i\varepsilon, \boldsymbol{\kappa})\right.\right.$$

$$\left. \times\, \tilde{t}(\hat{\mathsf{H}}_0 + i\varepsilon, \boldsymbol{\kappa}) \frac{1}{\frac{\boldsymbol{\kappa}\cdot\hat{\mathsf{p}}}{m} + \frac{\boldsymbol{\kappa}^2}{2m} - \Delta + i\varepsilon} e^{-\frac{i}{\hbar}\boldsymbol{\kappa}\cdot\hat{\mathsf{x}}}\right\}$$

$$-\, 2\frac{1}{\frac{\boldsymbol{\kappa}\cdot\hat{\mathsf{p}}}{m} + \frac{\boldsymbol{\kappa}^2}{2m} - \Delta + i\varepsilon} \tilde{t}(\hat{\mathsf{H}}_0 + i\varepsilon, \boldsymbol{\kappa}) e^{-\frac{i}{\hbar}\boldsymbol{\kappa}\cdot\hat{\mathsf{x}}}\, \hat{\varrho}$$

$$\left. \times\, e^{\frac{i}{\hbar}\boldsymbol{\kappa}\cdot\hat{\mathsf{x}}}\, \tilde{t}^\dagger(\hat{\mathsf{H}}_0 + i\varepsilon, \boldsymbol{\kappa}) \frac{1}{\frac{\boldsymbol{\kappa}\cdot\hat{\mathsf{p}}}{m} + \frac{\boldsymbol{\kappa}^2}{2m} - \Delta - i\varepsilon}\right)$$

$$\times \int \frac{dt}{2\pi\hbar} e^{-\frac{i}{\hbar}\Delta t} \int d^3\mathbf{x} \int d^3\mathbf{y}\, e^{\frac{i}{\hbar}\boldsymbol{\kappa}\cdot\mathbf{x}} \left\langle \delta N(\mathbf{y}) \delta N(\mathbf{x}+\mathbf{y},t)\right\rangle. \tag{4.2.13}$$

Thanks to the last term of (3.2.31) it is possible to take into account collisions that modify the state of the macroscopic system (see Sect. 3.2.5). The probability per unit time of such collisions is given by the trace of $\frac{1}{\hbar}\sum_{\xi,\lambda}\hat{\mathsf{L}}_{\lambda\xi}\hat{\varrho}\hat{\mathsf{L}}^\dagger_{\lambda\xi}$ as seen in Sect. 3.2.4. In the case considered this trace may be written as

$$\frac{2\pi}{\hbar}\frac{n_{\mathrm{o}}}{(2\pi\hbar)^4}\int d^3\mathbf{k}\int d^3\boldsymbol{\kappa}\, \langle \boldsymbol{\kappa}|\hat{\varrho}|\boldsymbol{\kappa}\rangle \left|\tilde{t}(E_k, \boldsymbol{\kappa}-\mathbf{k})\right|^2 \tag{4.2.14}$$

$$\times \int dt \int d^3\mathbf{x}\, e^{-\frac{i}{\hbar}\left(\frac{\boldsymbol{\kappa}^2}{2m} - \frac{\mathbf{k}^2}{2m}\right)t + \frac{i}{\hbar}(\boldsymbol{\kappa}-\mathbf{k})\cdot\mathbf{x}} \int d^3\mathbf{y}\, \frac{1}{N}\left\langle \delta N(\mathbf{y}) \delta N(\mathbf{x}+\mathbf{y},t)\right\rangle,$$

thus recovering again the van Hove structure for the scattering cross section [compare (3.2.35)], with the difference that now the system is considered to be homogeneous, so that only the momentum distribution of the incoming microsystem is of relevance. Let us observe that subtraction of the uncorrelated part of the response function accounts for the fact that only diffuse scattering, that is scattering that does not leave the macroscopic system unchanged [41], contributes to this term. We now specialize to the case of neutrons, adopting the Fermi pseudopotential given by (4.2.4), so that (4.2.14) becomes

$$\frac{1}{\hbar} n_{\mathrm{o}} \frac{b^2}{m^2} \int d^3\mathbf{k} \int d^3\boldsymbol{\kappa} \, \langle \boldsymbol{\kappa} | \hat{\varrho} | \boldsymbol{\kappa} \rangle \, S_{\mathrm{c}} \left(\frac{1}{\hbar} [\boldsymbol{\kappa} - \mathbf{k}] , \frac{1}{\hbar} \left[\frac{\boldsymbol{\kappa}^2}{2m} - \frac{\mathbf{k}^2}{2m} \right] \right), \tag{4.2.15}$$

where, denoting by ω and $\mathbf{q}$ energy and momentum transfer respectively,

$$S_{\mathrm{c}}(\mathbf{q}, \omega) = \frac{1}{2\pi N} \int dt \int d^3\mathbf{x} \, e^{-i(\omega t - \mathbf{q} \cdot \mathbf{x})} \int d^3\mathbf{y} \, \langle \delta N(\mathbf{y}) \delta N(\mathbf{x} + \mathbf{y}, t) \rangle \, . \tag{4.2.16}$$

If the momentum distribution of the incoming particle is suitably peaked around $\mathbf{p}_0$ with respect to the momentum dependence of S_{c} we have from (4.2.15)

$$\frac{n_{\mathrm{o}} b^2}{\hbar m^2} \int d^3\mathbf{k} \int d^3\boldsymbol{\kappa} \, \langle \boldsymbol{\kappa} | \hat{\varrho} | \boldsymbol{\kappa} \rangle \, S_{\mathrm{c}} \left(\frac{1}{\hbar} [\mathbf{p}_0 - \mathbf{k}] , \omega_{p_0} - \omega_k \right) = \frac{n_{\mathrm{o}} b^2}{\hbar m^2} \int d^3\mathbf{k} \, S_{\mathrm{c}} \left(\frac{1}{\hbar} [\mathbf{p}_0 - \mathbf{k}] , \omega_{p_0} - \omega_k \right)$$

in particular, in the static limit expression (4.2.15) becomes:

$$n_{\mathrm{o}} b^2 \frac{p_0}{m} \int d\Omega_q \, S_{\mathrm{c}}(\mathbf{q}) = n_{\mathrm{o}} \frac{p_0}{m} \sigma_{\mathrm{d}}$$

where

$$S_{\mathrm{c}}(\mathbf{q}) = \frac{1}{N} \int d^3\mathbf{x} \, e^{i\mathbf{q} \cdot \mathbf{x}} \int d^3\mathbf{y} \, \langle \delta N(\mathbf{y}) \delta N(\mathbf{x} + \mathbf{y}) \rangle \, ,$$

and we have denoted by $\mathbf{q}$ the momentum transfer and by σ_{d} the total diffusion cross section per particle. This is the result derived by Sears for the attenuation of the coherent beam due to incoherent scattering, which he obtains by an evaluation of the local field effects, neglected in the equation giving the optical neutron dynamics (4.2.6) (see [41, 44, 53]). In our approach, however, the incoherent contribution is already present in the equation giving the dynamics of the microsystem, being connected to the thermodynamic properties of the macrosystem through the response function $S_{\mathrm{c}}(\mathbf{q}, \omega)$. This new feature is obtained by means of the more general formalism adopted, leading to a master-equation of the Lindblad type for the statistical operator, in which due to the optical theorem a close correlation exists between the incoherent contribution and the imaginary part of the optical potential which is not connected to absorption. To see this correction to the optical potential let us exploit the simple relation

$$\hat{\mathsf{A}} = \hat{\mathsf{A}}^\dagger, \quad \hat{\mathsf{B}} = \hat{\mathsf{B}}^\dagger, \quad \hat{\mathsf{U}} = \hat{\mathsf{A}} + i\hat{\mathsf{B}} \qquad \Rightarrow \qquad \hat{\mathsf{U}}\hat{\varrho} - \hat{\varrho}\hat{\mathsf{U}}^\dagger = \left[\hat{\mathsf{A}}, \hat{\varrho}\right] + i\left\{\hat{\mathsf{B}}, \hat{\varrho}\right\}$$

and write the commutator and anticommutator term of (3.2.31) in the form $-\frac{i}{\hbar}\left(\hat{\mathsf{U}}\hat{\varrho}-\hat{\varrho}\hat{\mathsf{U}}^{\dagger}\right)$. The calculation of $\hat{\mathsf{U}}$ is essentially given by the anticommutator at the r.h.s. of (4.2.13) and the commutator in (4.2.5). In the case of the Fermi pseudopotential, using (4.2.16) one has:

$$\hat{\mathsf{U}}=\frac{2\pi\hbar^2}{m}n_{\rm o}\left[b-i\frac{b^2}{4\pi}\int d^3\mathbf{k}\,|\mathbf{k}\rangle\langle\mathbf{k}|\int d\omega_\kappa\int d\Omega_\kappa\,\frac{\kappa}{\hbar}\,S_{\rm c}\left(\frac{1}{\hbar}\left[\boldsymbol{\kappa}-\mathbf{k}\right],\frac{1}{\hbar}\left[\frac{\boldsymbol{\kappa}^2}{2m}-\frac{\mathbf{k}^2}{2m}\right]\right)\right],$$

or in the static limit

$$\hat{\mathsf{U}}=\frac{2\pi\hbar^2}{m}n_{\rm o}\left[b-i\frac{b^2}{4\pi}\int d^3\mathbf{k}\,|\mathbf{k}\rangle\langle\mathbf{k}|\,\frac{k}{\hbar}\int d\Omega_q\,S_{\rm c}(\mathbf{q})\right], \tag{4.2.17}$$

where $\mathbf{q}$ denotes as usual the momentum transfer. Neglecting diffuse scattering we would have $\hat{\mathsf{U}}=\frac{2\pi\hbar^2}{m}n_{\rm o}b$, simply a c-number giving the usual refractive index; the remaining part is, in a sense, induced by the optical theorem. To compare with the results derived by Sears we have to consider the expression obtained for the static limit (4.2.17) applied to a plane wave of momentum $\mathbf{p}_0$, which gives an idealized description of the preparation of the incoming microsystem, thus leading to

$$\hat{\mathsf{U}}=\frac{2\pi\hbar^2}{m}n_{\rm o}\left[b-i\frac{b^2}{4\pi}\frac{p_0}{\hbar}\int d\Omega_q\,S_{\rm c}(\mathbf{q})\right]; \tag{4.2.18}$$

this expression agrees with the results obtained relying on the idea of local field corrections (see [41], Ch. 4), however here (4.2.17) is a direct consequence of the equation driving the dynamics and of the Ansatz (3.2.33). The analysis that we have put forward relies on the assumption that the main contribution to the dynamics is given by the commutator term in (3.2.31), while the terms in (4.2.11) may, as a first approximation, be neglected. This leads to an optical description, as for the case of neutrons, in which, considering the dimensionless parameter $\frac{2\pi\hbar^2}{mE}n_{\rm o}b$, the terms other than the commutator are of second order. The opposite situation takes place if the interaction is such that the main contribution is given by (4.2.11), while the commutator may be neglected. This happens when dissipative effects are predominant, as in the case of Brownian motion mentioned below (4.2.12), where incoherent interactions through collisions involving energy and momentum transfer play the main role.

4.2.3 Experimental Implications

We now address our attention to potential experimental implications of the above introduced description of neutron-matter interaction. Of course possible new features in the dynamics are linked to the presence of the last two terms in the r.h.s. of (3.2.31), as given by (4.2.13), and such corrections will be generally small, being of second order in $\frac{2\pi\hbar^2}{mE}n_{\rm o}b$ (typically $\frac{2\pi\hbar^2}{mE}n_{\rm o}b\leq 10^{-5}$ at thermal neutron energies). In this respect interferometric experiments, in which the experimental setup is conceived in order to enhance the coherent behavior, should be particularly relevant: think for example of the beautiful experiments realized by the Rauch group in Wien exploiting the perfect crystal neutron interferometer [8, 20, 49].

Consider now eq.(3.2.31): the map on the r.h.s. is affine and trace preserving, and therefore clearly predicts neutron conservation. Nevertheless the last contribution which offsets the anticommutator term is linked to diffuse scattering: one has neutron conservation if also diffuse particles contribute to the experimental observation. This is not so for interferometric experiments. In such cases only the wavelike behavior affects the observed dynamics, and thus only the commutator part of the evolution map is of relevance: the net result is an imaginary correction to the coherent scattering length as in (4.2.18), that is to say a reduction of the neutron flux responsible for the interference pattern. This fact is usually taken into account adding an imaginary part proportional to the total scattering cross-section $\sigma_{\rm t}$ to the phase shift calculated as in (4.2.8), thus including both absorption and diffuse scattering (see [20, 21]) according to the formula:

$$\chi = \chi' + i\chi'' = -n_{\rm o} b\lambda D + i n_{\rm o}\sigma_{\rm t}\frac{D}{2}, \qquad \exp(i\chi) = \exp\left(-i n_{\rm o} b\lambda D - n_{\rm o}\sigma_{\rm t}\frac{D}{2}\right).$$

In the absence of absorption this correction is considered negligible and the relevant incident flux is often evaluated simply closing one of the two beam paths. This attitude is, however, at least in principle incorrect, as it appears taking the whole dynamics as given by (3.2.31) into account. In fact when one closes the path without the sample also diffuse neutrons, which are lost for the interference pattern, having their path "labeled" by scattering with the sample, may contribute to the transmitted intensity. The experimental device is no more acting as an interferometer and therefore cannot select only those neutrons that have undergone coherent interactions. This additional contribution to the transmitted neutron flux is given by the trace of the last term of (3.2.31), that is to say by (4.2.15). In calculating the amplitude of the interference pattern one should therefore rely not simply on the measured transmitted flux, but on this quantity minus the additional incoherent contribution given by (4.2.15), thus obtaining a reduction of this amplitude: the purely *optical* treatment leads in principle to an overestimate of the visibility of the interference pattern. This is normally not the case in real experiments, since the angle of acceptance of diffuse neutrons is very small, as for the perfect crystal neutron interferometer. Let us give some quantitative estimate of the aforementioned effect.

In order to evaluate (4.2.15) we have to make a definite choice for the structure function $S_{\rm c}(\mathbf{q},\omega)$, in fact (4.2.15) is given by:

$$\mathcal{A} \equiv \frac{1}{\hbar}{\rm Tr}_{\mathcal{H}^{(1)}} \sum_{\xi,\lambda} \hat{\mathsf{L}}_{\lambda\xi}\hat{\varrho}\hat{\mathsf{L}}^{\dagger}_{\lambda\xi} = \frac{n_{\rm o} b^2}{\hbar m^2}\int d^3\mathbf{k} \int d^3\boldsymbol{\kappa}\; \langle \boldsymbol{\kappa}\,|\hat{\varrho}|\,\boldsymbol{\kappa}\rangle\, S_{\rm c}\left(\frac{1}{\hbar}\left[\boldsymbol{\kappa}-\mathbf{k}\right], \frac{1}{\hbar}\left[\frac{\boldsymbol{\kappa}^2}{2m}-\frac{\mathbf{k}^2}{2m}\right]\right),$$

where the quantity $\mathcal{A}$ takes diffusion at any angle into account. In the static approximation, for a homogeneous and isotropic medium, such as a liquid or a gas, one has [41]:

$$S_{\mathrm{c}}(\mathbf{q},\omega) = S_{\mathrm{c}}(\mathbf{q})\delta(\omega) \qquad\qquad S_{\mathrm{c}}(\mathbf{q}) = 1 + n_{\mathrm{o}} \int d^3\mathbf{r}\, e^{i\mathbf{q}\cdot\mathbf{r}}[g(r)-1], \tag{4.2.19}$$

where $g(r)$ is the pair correlation function. A possible choice for $g(r)$, allowing $S_{\mathrm{c}}(\mathbf{q})$ to be evaluated analytically, is the following, valid for a dilute hard sphere gas with atomic diameter a:

$$g(r) = \begin{cases} 0 & r < a \\ 1 & r > a \end{cases} .$$

The quantity of interest for us is $\mathcal{A}$ in its dependence from the maximal angular acceptance φ, determined by the experimental apparatus, multiplied by the time the neutron takes to go through the sample. Supposing the momentum distribution of the incoming particle sufficiently well peaked around $\mathbf{p}_0$ we rewrite $\mathcal{A}$ introducing the expression given by (4.2.19) and multiplying by the time interval, thus coming to:

$$\begin{aligned}\mathcal{A}(\varphi) &= 2\pi n_{\mathrm{o}} b^2 D \int_0^{\varphi} d\theta \sin\theta \\ &\quad \times \left\{ 1 - \frac{2\pi n_{\mathrm{o}} a^3}{(1-\cos\theta)} \left(\frac{\hbar}{ap_0}\right)^2 \left[\frac{\sin\left(\frac{ap_0}{\hbar}\sqrt{2(1-\cos\theta)}\right)}{\frac{ap_0}{\hbar}\sqrt{2(1-\cos\theta)}} - \cos\left(\frac{ap_0}{\hbar}\sqrt{2(1-\cos\theta)}\right)\right]\right\},\end{aligned}$$

where $\cos\theta = (\mathbf{p}_0 \cdot \mathbf{k})/p_0^2$. The primitive of this integral can be straightforwardly evaluated by a change of variables, and exploiting the fact that in our model $S_{\mathrm{c}}(0) = 1 - \frac{4}{3}\pi a^3 n_{\mathrm{o}}$, we have an explicit representation of diffuse scattering at any angle φ:

$$\mathcal{A}(\varphi) = 2\pi n_{\mathrm{o}} b^2 D \left\{ (1-\cos\varphi) + 3[1-S_{\mathrm{c}}(0)]\left(\frac{\hbar}{ap_0}\right)^2 \left[\frac{\sin\left(\frac{ap_0}{\hbar}\sqrt{2(1-\cos\varphi)}\right)}{\frac{ap_0}{\hbar}\sqrt{2(1-\cos\varphi)}} - 1 \right]\right\};$$

considering in particular small φ the expression may be approximated as:

$$\mathcal{A}(\varphi) \simeq \pi n_{\mathrm{o}} b^2 D \left\{ \varphi^2 S_{\mathrm{c}}(0) + \varphi^4 \left(\frac{1}{20}[1-S_{\mathrm{c}}(0)]\left(\frac{ap_0}{\hbar}\right)^2 - \frac{1}{12} S_{\mathrm{c}}(0) \right) + O(\varphi^6) \right\}.$$

Let us now consider the experiments performed using the perfect crystal interferometer. The angular acceptance is very small, only a few microradians for thermal neutrons [55]. Taking for instance a gaseous sample, an order of magnitude estimate gives $\mathcal{A}(\varphi) \simeq 10^{-14}$, that is to say an extremely small quantity, in agreement with the accuracy obtained using this interferometer based on Bragg diffraction. An interferometer based on a different physical principle could possibly lead to a higher angular acceptance, thus enhancing this effect connected to diffusion. In view of the next equation (4.2.20) a completely different situation arises if one considers systems with abnormally large density fluctuations, as would be the case near a first order phase-transition.

Another point of interest is the linear dependence on $S_c(0)$ of the leading term in $\mathcal{A}(\varphi)$. The quantity $S_c(0)$ is particularly relevant from the physical point of view, being connected to the isothermal compressibility χ_T and to the fluctuations in the number of particles in the sample [56]:

$$S_c(0) = n_o k_B T \chi_T = \frac{\overline{(\Delta N)^2}}{N}. \qquad (4.2.20)$$

The actual value of $S_c(0)$ cannot be measured experimentally from scattering experiments, and has to be obtained by an analytical continuation. The analysis we propose could provide an independent way to measure S_c at $\mathbf{q} = 0$. In fact in the static approximation, independently of the particular form of $S_c(\mathbf{q})$, for very small $|\mathbf{q}|$, that is to say for very small φ, one has in good approximation:

$$\mathcal{A}(\varphi) \simeq \pi n_o b^2 D\, S_c(0)\varphi^2.$$

The value of $S_c(0)$ could then be obtained, at least in principle, comparing the amplitude of the interference pattern with the measured transmitted intensity.

4.2.4 Final Remarks

The example of neutron interaction with matter has been discussed inside the approach outlined in Chap. 3 for the description of the subdynamics of a microsystem interacting with a system having many degrees of freedom. The formal scheme leads to a generator for the irreversible time evolution of the Lindblad form, whose expression relies on suitable choices for the potential term related to the T-matrix and the statistical operator describing the thermodynamic state of the system. In the example considered the main ingredient is given by the Fermi pseudopotential adopted to describe the neutron-nucleus interaction in impulse approximation. Then we obtain from (3.2.26), neglecting the incoherent contribution, the equation used by Sears to describe all neutron optical phenomena, as well as known expressions for the index of refraction. The incoherent contribution is necessary to fulfill the optical theorem and take diffuse scattering, that attenuates the coherent beam, into account. We have also shown how it may be connected to properties of the macrosystem, as expressed by the dynamic structure function.

Even though it introduces a smaller correction the incoherent contribution is very important from the theoretical point of view. We expect that it will help studying the tricky borderline between a pure optical wavelike behavior and the fully incoherent particle-like one, based on a diffusion equation: in fact (3.2.31) leads in a direct way to the theory of Brownian motion, as we shall see in Sect. 4.3. It is not surprising that the incoherent contribution to the dynamics has grown out of a thoroughly quantum mechanical treatment, as shown by the typical quantum structure of the Lindblad equation, relying on non-commutating operators, in which an essential role is played by the statistical operator ϱ, rather then by the wave function ψ. This point is of central relevance, since the terms which describe the incoherent dynamics cannot be introduced in the formalism of the wave function and are therefore unavoidably absent in an optical-like treatment, simply reminiscent of classical optical descriptions.

We hope that this study of the emergence of incoherence in neutron-matter interaction will lead to a better understanding of the general problem of irreversibility and of description of non-equilibrium systems. Typically coexistence of an incoherent particle-like behavior, described by a quantum Boltzmann equation, and a wavefunction description by means of Gross-Pitaevskii equation, is important for understanding Bose-Einstein condensation [10], as we shall see in Chap. 5.

4.3 Brownian Motion

The problem of irreversibility, which automatically sets in when one considers the phenomenology of a system composed of many particles, has been historically first tackled in an intuitive, semi-phenomenological way in a few simple cases, which have however provided us with important physical insights. Among these a classical problem of non-equilibrium statistical mechanics is Brownian motion, that is to say the study of the motion of a heavy particle immersed in a fluid made up of light particles, interacting with these lighter particles through collisions. Considering Brownian motion as a stationary Markov process, the classical phenomenological theory leads to the celebrated Fokker-Planck equation for the momentum distribution function of the Brownian particle $f(\mathbf{p})$

$$\frac{\partial f(\mathbf{p},t)}{\partial t} = \zeta \nabla (\mathbf{p} f(\mathbf{p},t)) + D_{pp} \Delta f(\mathbf{p},t) \tag{4.3.1}$$

where ζ is the friction constant and D_{pp} the coefficient of momentum diffusion, given by $D_{pp} = \zeta(k_{\mathrm{B}}T/M)$, M being the mass of the Brownian particle, provided the environment can be considered in equilibrium at temperature T. The physical mechanism described by this equation is quite intuitive, and can be understood by starting at time zero with a momentum distribution sharply peaked at $\mathbf{p} = \mathbf{p}_0$. As time passes, the maximum of this distribution is shifted toward smaller momenta, as a result of the systematic friction undergone by the particles. Moreover, the peak broadens progressively as a result of diffusion in velocity space: a finite dispersion of the velocities sets in. The final, time-independent distribution reached by the Brownian particles is nothing other than the Maxwell distribution:

$$f(\mathbf{p},\infty) = \frac{1}{(2\pi M k_{\mathrm{B}} T)^{3/2}} \exp\left(-\frac{\mathbf{p}^2}{2M k_{\mathrm{B}} T}\right).$$

If one tries to obtain a quantum counterpart of the Fokker-Planck equation (4.3.1) by intuitively resorting to the correspondence principle, thus obtaining

$$\frac{d\hat{\varrho}}{dt} = -\frac{i}{2}\zeta\,[\hat{\mathsf{x}},\{\hat{\mathsf{p}},\hat{\varrho}\}] - D_{pp}\,[\hat{\mathsf{x}},[\hat{\mathsf{x}},\hat{\varrho}]]\,, \tag{4.3.2}$$

where $\hat{\mathsf{x}}, \hat{\mathsf{p}}$ denote position and momentum operators, one does not obtain a generator of the Lindblad form, corresponding to a completely positive time evolution, so that this equation may violate the positivity of the statistical operator. In order to improve this situation, a thorough quantum mechanical treatment is needed. We will therefore approach this problem starting from the master equation (3.2.31), which we have obtained working in a fully quantum mechanical framework, already having the Lindblad structure and therefore preserving positivity.

4.3.1 Dissipative Behavior

We now consider (3.2.31) for the case of a particle of mass M interacting with homogeneous portions of a system supposed to be at equilibrium. Being interested in the local dissipative behavior, we neglect the influence of the actual boundary conditions, and suppose that the system may be considered locally homogeneous within a very good approximation, thus analyzing the interaction in momentum space. The relevant contribution, as far as the dissipative behavior is concerned, comes from

$$-\frac{1}{\hbar}\left\{\frac{1}{2}\sum_{\xi\lambda}\hat{\mathsf{L}}^{\dagger}_{\lambda\xi}\hat{\mathsf{L}}_{\lambda\xi},\hat{\varrho}\right\} + \frac{1}{\hbar}\sum_{\xi\lambda}\hat{\mathsf{L}}_{\lambda\xi}\hat{\varrho}\hat{\mathsf{L}}^{\dagger}_{\lambda\xi}\ , \tag{4.3.3}$$

where the two expressions have to be evaluated jointly, due to cancellations and compensations which take place between them. We will therefore momentarily neglect the commutator term in (3.2.31) and concentrate first on the mixture term at the r.h.s. of (4.3.3). First of all we have to specify the structure of the $\hat{\mathsf{L}}_{\lambda\xi}$ operators given by (3.2.27) and (3.2.28)

$$\hat{\mathsf{L}}_{\lambda\xi} = \sqrt{2\varepsilon\pi_\xi}\sum_{kf}|k\rangle\frac{\langle\lambda|T^k_f(E_k+i\varepsilon)|\xi(t)\rangle}{E_f+E_\xi-E_k-E_\lambda+i\varepsilon}\langle f|. \tag{4.3.4}$$

Analogously to (3.2.33) we suppose

$$T^k_f\,(z) = \sum_{\eta\mu} b^{\dagger}_{\eta}T_{k\eta f\mu}(z)b_\mu = \int d^3\mathbf{x}\int d^3\mathbf{y}\,\psi^{\dagger}(\mathbf{x})u^*_k(\mathbf{y})t(z,|\mathbf{x}-\mathbf{y}|)u_f(\mathbf{y})\psi(\mathbf{x})$$

where $b^{\dagger}_{\eta}, b_\mu$ are creation and annihilation operators in the Fock-space for the macrosystem, the indexes η,μ correspond to the momenta $\mathbf{p}_\eta, \mathbf{p}_\mu$, and the collision kernel t depends only on the modulus of the relative distance. If also the microsystem is analyzed in momentum space, so that the indexes k, f correspond to $\mathbf{p}_k, \mathbf{p}_f$, we have

$$\psi(\mathbf{x}) = \sum_\eta b_\eta\frac{1}{\sqrt{\mathsf{V}}}e^{\frac{i}{\hbar}\mathbf{p}_\eta\cdot\mathbf{x}}, \qquad u^*_k(\mathbf{y}) = \frac{1}{\sqrt{\mathsf{V}}}e^{-\frac{i}{\hbar}\mathbf{p}_k\cdot\mathbf{y}}$$

and consequently

$$T_{k\eta f\mu}(z) = \delta_{p_\eta+p_k,p_f+p_\mu}\left[\frac{1}{\mathsf{V}}\int d^3\mathbf{x}\, t(z,|\mathbf{x}|)e^{\frac{i}{\hbar}(\mathbf{p}_\mu-\mathbf{p}_\eta)\cdot\mathbf{x}}\right];$$

setting

$$\tilde{t}(z,|\mathbf{p}_\mu-\mathbf{p}_\eta|) \equiv \frac{1}{\mathsf{V}}\int d^3\mathbf{x}\, t(z,|\mathbf{x}|)e^{\frac{i}{\hbar}(\mathbf{p}_\mu-\mathbf{p}_\eta)\cdot\mathbf{x}}$$

we come to

$$T^k_f(E_k+i\varepsilon) = \sum_{\eta\mu}\delta_{p_\eta+p_k,p_f+p_\mu}b^\dagger_\eta\tilde{t}(E_k+i\varepsilon,|\mathbf{p}_\mu-\mathbf{p}_\eta|)b_\mu. \tag{4.3.5}$$

The mixture term thus becomes

$$\begin{aligned}
\frac{1}{\hbar}\sum_{\xi\lambda}\hat{\mathsf{L}}_{\lambda\xi}\hat{\varrho}\hat{\mathsf{L}}^\dagger_{\lambda\xi} &= \frac{1}{\hbar}\sum_{\xi\lambda}\sum_{\substack{kf\\hg}}2\varepsilon\pi_\xi|\mathbf{p}_k\rangle\frac{\langle\lambda|T^k_f(E_k+i\varepsilon)|\xi\rangle}{E_f+E_\xi-E_k-E_\lambda+i\varepsilon}\langle\mathbf{p}_f|\hat{\varrho}|\mathbf{p}_g\rangle\frac{\langle\xi|T^{h\dagger}_g(E_h+i\varepsilon)|\lambda\rangle}{E_g+E_\xi-E_h-E_\lambda-i\varepsilon}\langle\mathbf{p}_h| \\
&= \frac{2\varepsilon}{\hbar}\sum_{\xi\lambda}\sum_{\substack{kf\\hg}}\sum_{\substack{\eta\mu\\\eta'\mu'}}\langle\lambda|b^\dagger_\eta b_\mu|\xi\rangle\pi_\xi\langle\xi|b^\dagger_{\mu'}b_{\eta'}|\lambda\rangle|\mathbf{p}_k\rangle\langle\mathbf{p}_f|\hat{\varrho}|\mathbf{p}_g\rangle\langle\mathbf{p}_h| \qquad (4.3.6) \\
&\quad\times\delta_{p_\eta+p_k,p_f+p_\mu}\frac{\tilde{t}(E_k+i\varepsilon,|\mathbf{p}_\mu-\mathbf{p}_\eta|)}{E_f+E_\xi-E_k-E_\lambda+i\varepsilon}\delta_{p_{\eta'}+p_h,p_g+p_{\mu'}}\frac{\tilde{t}^*(E_h+i\varepsilon,|\mathbf{p}_{\mu'}-\mathbf{p}_{\eta'}|)}{E_g+E_\xi-E_h-E_\lambda-i\varepsilon}
\end{aligned}$$

If the Brownian particle interacts with a locally homogeneous system at equilibrium so that both the eigenstates $|\lambda\rangle$ of H_{m} and the eigenstates $|\xi\rangle$ of ϱ_{m} may be obtained by the repeated action of creation operators $b^\dagger_\nu$ on the vacuum, we may write

$$|\lambda\rangle = |\{n^\lambda_\nu\}\rangle, \qquad |\xi\rangle = |\{n^\xi_\nu\}\rangle$$

where n^λ_ν is the occupation number relative to the momentum ν in the state $|\lambda\rangle$. Consider first the case $\lambda=\xi$, we then have

$$\langle\lambda|b^\dagger_\eta b_\mu|\lambda\rangle = \delta_{\eta,\mu}n^\lambda_\mu$$

and in particular, from (4.3.4) and (4.3.5):

$$\hat{\mathsf{L}}_{\lambda\lambda} = \sqrt{2\varepsilon\pi_\lambda}\sum_k\sum_\mu\frac{i}{\varepsilon}n^\lambda_\nu\,\tilde{t}(E_k+i\varepsilon,0)|\mathbf{p}_k\rangle\langle\mathbf{p}_k|, \tag{4.3.7}$$

so that, neglecting the energy dependence in $\tilde{t}$, (4.3.7) is a c-number and therefore the $\lambda=\xi$ contributions in the mixture and anticommutator term of (4.3.3) cancel each other. We see here how important it is to contemporaneously consider both contributions to (4.3.3). Considering the collision kernel $\tilde{t}$ slowly energy dependent we will replace the sum over λ and ξ by a primed sum, in which $\lambda\neq\xi$. In the case $\lambda\neq\xi$ we have

$$\begin{aligned}
\langle\lambda|b^\dagger_\eta b_\mu|\xi\rangle &= \langle\{n^\lambda_\nu\}|b^\dagger_\eta b_\mu|\{n^\xi_\nu\}\rangle = \langle\{n^\lambda_\nu-\delta_{\nu\eta}\}|\{n^\xi_\nu-\delta_{\nu\mu}\}\rangle\sqrt{n^\xi_\mu}\sqrt{n^\lambda_\eta} \\
&= \Big(\prod_{\nu\neq\mu,\eta}\delta_{n^\lambda_\nu,n^\xi_\nu}\Big)\delta_{(n^\lambda_\eta-1),n^\xi_\eta}\delta_{n^\lambda_\mu,(n^\xi_\mu-1)}(1-\delta_{\eta,\mu})\sqrt{n^\xi_\mu}\sqrt{n^\lambda_\eta},
\end{aligned}$$

so that the expectation value is different from zero only if $n_\nu^\lambda = n_\nu^\xi$ for every ν different from either η or μ, together with $n_\eta^\lambda = n_\eta^\xi + 1$ and $n_\mu^\lambda = n_\mu^\xi - 1$. Similarly

$$\langle\xi|b^\dagger_{\mu'}b_{\eta'}|\lambda\rangle = \Big(\prod_{\nu\neq\mu',\eta'}\delta_{n_\nu^\lambda,n_\nu^\xi}\Big)\delta_{(n^\xi_{\mu'}-1),n^\lambda_{\mu'}}\delta_{n^\xi_{\eta'},(n^\lambda_{\eta'}-1)}(1-\delta_{\eta',\mu'})\sqrt{n^\xi_{\mu'}}\sqrt{n^\lambda_{\eta'}},$$

so that the factor

$$\langle\lambda|b^\dagger_\eta b_\mu|\xi\rangle\pi_\xi\langle\xi|b^\dagger_{\mu'}b_{\eta'}|\lambda\rangle$$

with $\lambda \neq \xi$ gives a non vanishing contribution only if $\mu = \mu'$, $\eta = \eta'$ but $\eta \neq \mu$, and moreover $n_\nu^\lambda = n_\nu^\xi$ for every $\nu \neq \mu, \nu$ together with $n_\eta^\lambda = n_\eta^\xi + 1$ and $n_\mu^\lambda = n_\mu^\xi - 1$; in particular

$$E_\lambda - E_\xi = \frac{\mathbf{p}_\eta{}^2}{2m} - \frac{\mathbf{p}_\mu{}^2}{2m} \equiv E_\eta - E_\mu,$$

m being the mass of particles in the medium. For a generic function $F(\mathbf{p}_\mu - \mathbf{p}_\eta, \mathbf{p}_{\mu'} - \mathbf{p}_{\eta'}, E_\lambda - E_\xi)$ we have

$$\sum_{\xi\lambda}{}'\sum_{\substack{\eta\mu\\ \eta'\mu'}}\langle\lambda|b^\dagger_\eta b_\mu|\xi\rangle\pi_\xi\langle\xi|b^\dagger_{\mu'}b_{\eta'}|\lambda\rangle F(\mathbf{p}_\mu - \mathbf{p}_\eta, \mathbf{p}_{\mu'} - \mathbf{p}_{\eta'}, E_\lambda - E_\xi)$$

$$= \sum_\xi\sum_{\eta\mu}{}'\pi_\xi n^\xi_\mu(n^\xi_\eta+1)F(\mathbf{p}_\mu - \mathbf{p}_\eta, \mathbf{p}_\mu - \mathbf{p}_\eta, E_\eta - E_\mu)$$

$$= \sum_{\eta\mu}{}'\,\langle n_\mu(n_\eta+1)\rangle\, F(\mathbf{p}_\mu - \mathbf{p}_\eta, \mathbf{p}_\mu - \mathbf{p}_\eta, E_\eta - E_\mu), \tag{4.3.8}$$

where $\langle\ldots\rangle$ denotes the average with the statistical operator $\varrho_{\rm m}$ associated to the macrosystem. If we now go back to (4.3.6), exploiting (4.3.8) and momentum conservation as expressed by the two Kronecker's delta, we obtain the following expression

$$\frac{2\varepsilon}{\hbar}\sum_{pp'}\sum_{\eta\mu}{}'\,\langle n_\mu(n_\eta+1)\rangle\frac{\tilde{t}\left(\frac{[\mathbf{p}+(\mathbf{p}_\mu-\mathbf{p}_\eta)]^2}{2M}+i\varepsilon, |\mathbf{p}_\mu-\mathbf{p}_\eta|\right)}{E_\mu-E_\eta+i\varepsilon-\frac{(\mathbf{p}_\mu-\mathbf{p}_\eta)^2}{2M}-\frac{\mathbf{p}}{M}\cdot(\mathbf{p}_\mu-\mathbf{p}_\eta)}e^{\frac{i}{\hbar}(\mathbf{p}_\mu-\mathbf{p}_\eta)\cdot\hat{\mathsf{x}}}|\mathbf{p}\rangle\langle\mathbf{p}|\hat{\varrho}|\mathbf{p}'\rangle$$

$$\times\,\langle\mathbf{p}'|e^{-\frac{i}{\hbar}(\mathbf{p}_\mu-\mathbf{p}_\eta)\cdot\hat{\mathsf{x}}}\frac{\tilde{t}^*\left(\frac{[\mathbf{p}'+(\mathbf{p}_\mu-\mathbf{p}_\eta)]^2}{2M}+i\varepsilon, |\mathbf{p}_\mu-\mathbf{p}_\eta|\right)}{E_\mu-E_\eta-i\varepsilon-\frac{(\mathbf{p}_\mu-\mathbf{p}_\eta)^2}{2M}-\frac{\mathbf{p}'}{M}\cdot(\mathbf{p}_\mu-\mathbf{p}_\eta)},$$

which we rewrite going over to the center of mass coordinates

$$\mathbf{P} = \frac{1}{2}(\mathbf{p}+\mathbf{p}') \qquad \mathbf{q} = \mathbf{p}-\mathbf{p}',$$

coming to

$$\frac{2\varepsilon}{\hbar}\sum_{Pq}\sum_{\eta\mu}{}'\,\langle n_\mu(n_\eta+1)\rangle\,\frac{\tilde{t}\left(\frac{\left[\mathbf{P}+\frac{\mathbf{q}}{2}+(\mathbf{p}_\mu-\mathbf{p}_\eta)\right]^2}{2M}+i\varepsilon, |\mathbf{p}_\mu-\mathbf{p}_\eta|\right)}{E_\mu-E_\eta+i\varepsilon-\frac{(\mathbf{p}_\mu-\mathbf{p}_\eta)^2}{2M}-\frac{\mathbf{P}}{M}\cdot(\mathbf{p}_\mu-\mathbf{p}_\eta)-\frac{\mathbf{q}}{2M}\cdot(\mathbf{p}_\mu-\mathbf{p}_\eta)}$$

$$\times e^{\frac{i}{\hbar}(\mathbf{p}_\mu-\mathbf{p}_\eta)\cdot\hat{\mathsf{x}}}|\mathbf{P}+\mathbf{q}/2\rangle\langle\mathbf{P}+\mathbf{q}/2|\hat{\varrho}|\mathbf{P}-\mathbf{q}/2\rangle\langle\mathbf{P}-\mathbf{q}/2|e^{-\frac{i}{\hbar}(\mathbf{p}_\mu-\mathbf{p}_\eta)\cdot\hat{\mathsf{x}}}$$

$$\times\frac{\tilde{t}^*\left(\frac{\left[\mathbf{P}-\frac{\mathbf{q}}{2}+(\mathbf{p}_\mu-\mathbf{p}_\eta)\right]^2}{2M}+i\varepsilon,|\mathbf{p}_\mu-\mathbf{p}_\eta|\right)}{E_\mu-E_\eta-i\varepsilon-\frac{(\mathbf{p}_\mu-\mathbf{p}_\eta)^2}{2M}-\frac{\mathbf{P}}{M}\cdot(\mathbf{p}_\mu-\mathbf{p}_\eta)+\frac{\mathbf{q}}{2M}\cdot(\mathbf{p}_\mu-\mathbf{p}_\eta)}.$$

This expression may undergo a major simplification if we assume that $\hat{\varrho}$ is quasi-diagonal in momentum space, describing a particle which is not well localized, so that

$$\left|\frac{\mathbf{q}}{M}\cdot(\mathbf{p}_\mu-\mathbf{p}_\eta)\right|\ll\left|E_\eta-E_\mu+\frac{\mathbf{P}}{M}\cdot(\mathbf{p}_\mu-\mathbf{p}_\eta)+\frac{(\mathbf{p}_\mu-\mathbf{p}_\eta)^2}{2M}\right|$$

and we may extract a delta accounting for energy conservation, so that, exploiting also the slow energy dependence of $\tilde{t}$ we finally obtain

$$\frac{2\pi}{\hbar}\sum_{pp'}\sum_{\eta\mu}{}'\langle n_\mu(n_\eta+1)\rangle\,\delta\left[E_\eta-E_\mu+\frac{(\mathbf{p}_\mu-\mathbf{p}_\eta)^2}{2M}+\frac{(\mathbf{p}+\mathbf{p}')}{2M}\cdot(\mathbf{p}_\mu-\mathbf{p}_\eta)\right]$$

$$\times\left|\tilde{t}\left(\frac{\left[\frac{\mathbf{p}+\mathbf{p}'}{2}+(\mathbf{p}_\mu-\mathbf{p}_\eta)\right]^2}{2M}+i\varepsilon,|\mathbf{p}_\mu-\mathbf{p}_\eta|\right)\right|^2 e^{\frac{i}{\hbar}(\mathbf{p}_\mu-\mathbf{p}_\eta)\cdot\hat{\mathsf{x}}}|\mathbf{p}\rangle\langle\mathbf{p}|\hat{\varrho}|\mathbf{p}'\rangle\langle\mathbf{p}'|e^{-\frac{i}{\hbar}(\mathbf{p}_\mu-\mathbf{p}_\eta)\cdot\hat{\mathsf{x}}}.$$

The anticommutator term in (4.3.3) may be evaluated in an analogous way. Using (4.3.5) we have

$$\begin{aligned}-\frac{1}{\hbar}\left\{\frac{1}{2}\sum_{\xi\lambda}\hat{\mathsf{L}}^\dagger_{\lambda\xi}\hat{\mathsf{L}}_{\lambda\xi},\hat{\varrho}\right\} &= -\frac{\varepsilon}{\hbar}\left\{\sum_{\xi\lambda}\sum_{\substack{gh\\f}}\pi_\xi|\mathbf{p}_g\rangle\frac{\langle\xi|T^{h\dagger}_g(E_h+i\varepsilon)|\lambda\rangle}{E_g+E_\xi-E_h-E_\lambda-i\varepsilon}\right.\\
&\qquad\left.\times\frac{\langle\lambda|T^h_f(E_h+i\varepsilon)|\xi\rangle}{E_f+E_\xi-E_h-E_\lambda+i\varepsilon}\langle\mathbf{p}_f|,\hat{\varrho}\right\}\\
&= -\frac{\varepsilon}{\hbar}\sum_{\xi\lambda}\sum_{\substack{gh\\f}}\sum_{\substack{\eta\mu\\\eta'\mu'}}\pi_\xi\langle\xi|b^\dagger_{\mu'}b_{\eta'}|\lambda\rangle\langle\lambda|b^\dagger_\eta b_\mu|\xi\rangle\\
&\qquad\times\delta_{p_\eta+p_h,p_f+p_\mu}\frac{\tilde{t}(E_h+i\varepsilon,|\mathbf{p}_\mu-\mathbf{p}_\eta|)}{E_h+E_\lambda-E_f-E_\xi-i\varepsilon}\\
&\qquad\times\delta_{p_{\eta'}+p_h,p_g+p_{\mu'}}\frac{\tilde{t}^*(E_h+i\varepsilon,|\mathbf{p}_{\mu'}-\mathbf{p}_{\eta'}|)}{E_h+E_\lambda-E_g-E_\xi+i\varepsilon}\{|\mathbf{p}_g\rangle\langle\mathbf{p}_f|,\hat{\varrho}\}\end{aligned}$$

and recalling the cancellation between the $\lambda=\xi$ contributions, thanks to (4.3.5) we have

$$-\frac{1}{\hbar}\sum_{p}\sum_{\eta\mu}{}'\langle n_\mu(n_\eta+1)\rangle\frac{\varepsilon}{\left[E_\eta-E_\mu+\frac{(\mathbf{p}_\mu-\mathbf{p}_\eta)^2}{2M}+\frac{\mathbf{p}}{M}\cdot(\mathbf{p}_\mu-\mathbf{p}_\eta)\right]}$$

$$\times\left|\tilde{t}\left(\frac{[\mathbf{p}+(\mathbf{p}_\mu-\mathbf{p}_\eta)]^2}{2M}+i\varepsilon,|\mathbf{p}_\mu-\mathbf{p}_\eta|\right)\right|^2\{|\mathbf{p}\rangle\langle\mathbf{p}|,\hat{\varrho}\}.$$

The final expression is therefore

$$
-\frac{1}{\hbar}\left\{\frac{1}{2}\sum_{\xi\lambda}\hat{\mathsf{L}}^{\dagger}_{\lambda\xi}\hat{\mathsf{L}}_{\lambda\xi},\hat{\varrho}\right\}+\frac{1}{\hbar}\sum_{\xi\lambda}\hat{\mathsf{L}}_{\lambda\xi}\hat{\varrho}\hat{\mathsf{L}}^{\dagger}_{\lambda\xi}=
$$

$$
\frac{2\pi}{\hbar}\sum_{\eta\mu}{}'\,\langle n_\mu(n_\eta+1)\rangle\left\{\sum_{pp'}\delta\left[E_\eta-E_\mu+\frac{(\mathbf{p}_\mu-\mathbf{p}_\eta)^2}{2M}+\frac{(\mathbf{p}+\mathbf{p}')}{2M}\cdot(\mathbf{p}_\mu-\mathbf{p}_\eta)\right]\right.
$$

$$
\times\left|\tilde{t}\left(\frac{\left[\frac{\mathbf{p}+\mathbf{p}'}{2}+(\mathbf{p}_\mu-\mathbf{p}_\eta)\right]^2}{2M}+i\varepsilon,|\mathbf{p}_\mu-\mathbf{p}_\eta|\right)\right|^2
$$

$$
\times\, e^{\frac{i}{\hbar}(\mathbf{p}_\mu-\mathbf{p}_\eta)\cdot\hat{\mathsf{x}}}|\mathbf{p}\rangle\langle\mathbf{p}|\hat{\varrho}|\mathbf{p}'\rangle\langle\mathbf{p}'|e^{-\frac{i}{\hbar}(\mathbf{p}_\mu-\mathbf{p}_\eta)\cdot\hat{\mathsf{x}}}
$$

$$
-\frac{1}{2}\sum_{p}\delta\left[E_\eta-E_\mu+\frac{(\mathbf{p}_\mu-\mathbf{p}_\eta)^2}{2M}+\frac{\mathbf{p}}{M}\cdot(\mathbf{p}_\mu-\mathbf{p}_\eta)\right]
$$

$$
\left.\times\left|\tilde{t}\left(\frac{[\mathbf{p}+(\mathbf{p}_\mu-\mathbf{p}_\eta)]^2}{2M}+i\varepsilon,|\mathbf{p}_\mu-\mathbf{p}_\eta|\right)\right|^2\{|\mathbf{p}\rangle\langle\mathbf{p}|,\hat{\varrho}\}\right\} \quad (4.3.9)
$$

Even if it plays a minor role in the description of a dissipative dynamics such as Brownian motion, we will consider for completeness the commutator term, whose relevant contribution according to (3.2.30) is given by

$$
\hat{\mathsf{V}}=\frac{\hat{\mathsf{Q}}+\hat{\mathsf{Q}}^{\dagger}}{2}.
$$

In our case, due to (4.3.5) and (3.2.27) we have

$$
\begin{aligned}
\hat{\mathsf{Q}} &= \sum_{kf}\sum_{\mu\eta}\delta_{p_\eta+p_k,p_f+p_\mu}\mathrm{Tr}_{\mathcal{H}_F}\left(b^{\dagger}_{\eta}b_\mu\varrho_{\mathrm{m}}\right)\tilde{t}(E_k+i\varepsilon,|\mathbf{p}_\mu-\mathbf{p}_\eta|)|\mathbf{p}_k\rangle\langle\mathbf{p}_k| \\
&= \sum_{\mu}\langle n_\mu\rangle\sum_{k}\tilde{t}(E_k+i\varepsilon,0)|\mathbf{p}_k\rangle\langle\mathbf{p}_k|
\end{aligned}
$$

so that keeping the relation between T-matrix and scattering amplitude into account, we obtain in the continuum limit

$$
\hat{\mathsf{V}}=-n_{\mathrm{o}}\frac{2\pi\hbar^2}{m}\int d^3\mathbf{p}|\mathbf{p}\rangle\langle\mathbf{p}|\,\mathrm{Re}f(E_p,\theta=0), \quad (4.3.10)
$$

analogously to (4.2.9) so that the commutator term is simply linked to the forward scattering amplitude, corresponding to a coherent interaction.

4.3.2 Quantum Master Equations for Local Dissipation

We will now show how, starting from (4.3.9), one can derive, under suitable hypothesis, equations which have already been obtained in the literature in order to describe quantum Brownian motion and more generally local quantum dissipation, based both on fundamental and phenomenological treatments [57, 58, 59, 60, 61, 62]. In order to do this let us neglect in (4.3.9) the energy dependence of the collision kernel $\tilde{t}$ and let us denote by $\mathbf{Q}_{\mu\eta} \equiv \mathbf{p}_\mu - \mathbf{p}_\eta$ the momentum transfer undergone by the macroscopic system, thus writing more compactly

$$-\frac{1}{\hbar}\left\{\frac{1}{2}\sum_{\xi\lambda}\hat{\mathsf{L}}^\dagger_{\lambda\xi}\hat{\mathsf{L}}_{\lambda\xi},\hat{\varrho}\right\}+\frac{1}{\hbar}\sum_{\xi\lambda}\hat{\mathsf{L}}_{\lambda\xi}\hat{\varrho}\hat{\mathsf{L}}^\dagger_{\lambda\xi} \;=\; \frac{2\pi}{\hbar}\sum_{\eta\mu}{}'\,\langle n_\mu(n_\eta+1)\rangle\left|\tilde{t}\,(|\mathbf{Q}_{\mu\eta}|)\right|^2$$

$$\left\{\sum_{pp'}\delta\!\left[E_\eta - E_\mu + \frac{{\mathbf{Q}_{\mu\eta}}^2}{2M}+\frac{(\mathbf{p}+\mathbf{p}')}{2M}\cdot\mathbf{Q}_{\mu\eta}\right]\right.$$

$$\times\, e^{\frac{i}{\hbar}\mathbf{Q}_{\mu\eta}\cdot\hat{\mathsf{x}}}|\mathbf{p}\rangle\langle\mathbf{p}|\hat{\varrho}|\mathbf{p}'\rangle\langle\mathbf{p}'|e^{-\frac{i}{\hbar}\mathbf{Q}_{\mu\eta}\cdot\hat{\mathsf{x}}}$$

$$\left.-\frac{1}{2}\sum_{p}\delta\!\left[E_\eta - E_\mu + \frac{{\mathbf{Q}_{\mu\eta}}^2}{2M}+\frac{\mathbf{p}}{M}\cdot\mathbf{Q}_{\mu\eta}\right]\{|\mathbf{p}\rangle\langle\mathbf{p}|,\hat{\varrho}\}\right\}.$$

In the hypothesis of small momentum transfer $|\mathbf{Q}_{\mu\eta}|$ we write the Taylor series for the δ distribution

$$\frac{2\pi}{\hbar}\sum_{\eta\mu}{}'\,\langle n_\mu(n_\eta+1)\rangle\left|\tilde{t}\,(|\mathbf{Q}_{\mu\eta}|)\right|^2$$

$$\times\left\{\sum_{pp'}\left(\delta(E_\eta-E_\mu)+\left[\frac{{\mathbf{Q}_{\mu\eta}}^2}{2M}+\frac{(\mathbf{p}+\mathbf{p}')}{2M}\cdot\mathbf{Q}_{\mu\eta}\right]\delta'(E_\eta-E_\mu)\right.\right.$$

$$\left.+\frac{1}{2}\left[\frac{{\mathbf{Q}_{\mu\eta}}^2}{2M}+\frac{(\mathbf{p}+\mathbf{p}')}{2M}\cdot\mathbf{Q}_{\mu\eta}\right]^2\delta''(E_\eta-E_\mu)\right)e^{\frac{i}{\hbar}\mathbf{Q}_{\mu\eta}\cdot\hat{\mathsf{x}}}|\mathbf{p}\rangle\langle\mathbf{p}|\hat{\varrho}|\mathbf{p}'\rangle\langle\mathbf{p}'|e^{-\frac{i}{\hbar}\mathbf{Q}_{\mu\eta}\cdot\hat{\mathsf{x}}}$$

$$-\frac{1}{2}\sum_{p}\left(\delta(E_\eta-E_\mu)+\left[\frac{{\mathbf{Q}_{\mu\eta}}^2}{2M}+\frac{\mathbf{p}}{2M}\cdot\mathbf{Q}_{\mu\eta}\right]\delta'(E_\eta-E_\mu)\right.$$

$$\left.\left.+\frac{1}{2}\left[\frac{{\mathbf{Q}_{\mu\eta}}^2}{2M}+\frac{\mathbf{p}}{2M}\cdot\mathbf{Q}_{\mu\eta}\right]^2\delta''(E_\eta-E_\mu)\right)\{|\mathbf{p}\rangle\langle\mathbf{p}|,\hat{\varrho}\}\right\}.$$

We then expand the exponentials, keeping terms up to second order in $|\mathbf{Q}_{\mu\eta}|$, thus obtaining terms which are at most bilinear in the operators $\hat{\mathsf{x}}$ and $\hat{\mathsf{p}}$; supposing also $\langle n_\mu(n_\eta+1)\rangle$ dependent only on the modulus of $\mathbf{p}_\mu$ and $\mathbf{p}_\eta$ we neglect in the expansion the contributions linear in $\mathbf{Q}_{\mu\eta}$. We have

$$\approx\frac{2\pi}{\hbar}\sum_{\eta\mu}{}'\,\langle n_\mu(n_\eta+1)\rangle\left|\tilde{t}\,(|\mathbf{Q}_{\mu\eta}|)\right|^2\sum_{i,j=1}^{3}Q^i_{\mu\eta}Q^j_{\mu\eta}$$

$$\left\{-\delta(E_\eta-E_\mu)\frac{1}{2\hbar^2}\left[\hat{\mathsf{x}}_i,\left[\hat{\mathsf{x}}_j,\hat{\varrho}\right]\right]+\delta'(E_\eta-E_\mu)\frac{1}{2M}\frac{i}{\hbar}\left[\hat{\mathsf{x}}_j,\{\hat{\mathsf{p}}_i,\hat{\varrho}\}\right]\right.$$

$$+ \delta''(E_\eta - E_\mu)\frac{1}{8M^2}\left(\hat{\mathsf{p}}_i\hat{\mathsf{p}}_j\hat{\varrho} + 2\hat{\mathsf{p}}_i\hat{\varrho}\hat{\mathsf{p}}_j + \hat{\varrho}\hat{\mathsf{p}}_i\hat{\mathsf{p}}_j\right) - \delta''(E_\eta - E_\mu)\frac{1}{4M^2}\left(\hat{\mathsf{p}}_i\hat{\mathsf{p}}_j\hat{\varrho} + \hat{\varrho}\hat{\mathsf{p}}_i\hat{\mathsf{p}}_j\right)\Big\}$$

and exploiting again the dependence of $\langle n_\mu(n_\eta+1)\rangle$ on the modulus of the momentum we have $Q^i_{\mu\eta}Q^j_{\mu\eta} = \delta_{ij}Q^i_{\mu\eta}$ and therefore

$$\frac{2\pi}{\hbar}\sum_{\eta\mu}{}' \langle n_\mu(n_\eta+1)\rangle \left|\tilde{t}\left(|\mathbf{Q}_{\mu\eta}|\right)\right|^2 \sum_{i=1}^{3} {Q^i_{\mu\eta}}^2$$

$$\left\{ -\frac{1}{2\hbar^2}\delta(E_\eta - E_\mu)\left[\hat{\mathsf{x}}_i,\left[\hat{\mathsf{x}}_i,\hat{\varrho}\right]\right] + \frac{i}{\hbar}\delta'(E_\eta - E_\mu)\frac{1}{2M}\left[\hat{\mathsf{x}}_i,\{\hat{\mathsf{p}}_i,\hat{\varrho}\}\right] - \delta''(E_\eta - E_\mu)\frac{1}{8M^2}\left[\hat{\mathsf{p}}_i,\left[\hat{\mathsf{p}}_i,\hat{\varrho}\right]\right]\right\}.$$

If momentum transfers are isotropically distributed we have in particular ${Q^i_{\mu\eta}}^2 = \frac{1}{3}\mathbf{Q}^2_{\mu\eta}$. Considering a gas at equilibrium at temperature T, in case of low degeneracy, assuming the Boltzmann distribution we have

$$\langle n_\mu(n_\eta+1)\rangle \approx \langle n_\mu\rangle = \frac{N}{\mathsf{V}}\left(\frac{2\pi\hbar^2}{m}\beta\right)^{3/2} e^{-\beta\frac{\mathbf{p}_\mu^2}{2m}} \equiv \frac{e^{-\beta E_\mu}}{\mathcal{Z}} \tag{4.3.11}$$

with $\beta = 1/(k_\mathrm{B}T)$ and m the mass of the gas molecules, and therefore, in the continuum limit

$$\frac{2\pi}{\hbar}\int d^3\mathbf{p}_\mu \int d^3\mathbf{p}_\eta\ \langle n_\mu\rangle \left|\tilde{t}\left(|\mathbf{p}_\mu - \mathbf{p}_\eta|\right)\right|^2 \frac{|\mathbf{p}_\mu - \mathbf{p}_\eta|^2}{3}\left(-\frac{1}{2}\right)\sum_{i=1}^{3}$$

$$\left\{\frac{1}{\hbar^2}\delta(E_\eta - E_\mu)\left[\hat{\mathsf{x}}_i,\left[\hat{\mathsf{x}}_i,\hat{\varrho}\right]\right] - \frac{i}{\hbar}\delta'(E_\eta - E_\mu)\frac{1}{M}\left[\hat{\mathsf{x}}_i,\{\hat{\mathsf{p}}_i,\hat{\varrho}\}\right] + \delta''(E_\eta - E_\mu)\left(\frac{1}{2M}\right)^2\left[\hat{\mathsf{p}}_i,\left[\hat{\mathsf{p}}_i,\hat{\varrho}\right]\right]\right\},$$

and considering the terms coming from the action of the derivative on (4.3.11)

$$\frac{2\pi}{\hbar}\int d\Omega_\mu \int d\Omega_\eta \int_0^\infty dE_\mu \int_0^\infty dE_\eta\, m^2\,|\mathbf{p}_\mu|\,|\mathbf{p}_\eta|\,\langle n_\mu\rangle \left|\tilde{t}\left(|\mathbf{p}_\mu - \mathbf{p}_\eta|\right)\right|^2 \frac{|\mathbf{p}_\mu - \mathbf{p}_\eta|^2}{3}\delta(E_\eta - E_\mu)$$

$$\times\left(-\frac{1}{2}\right)\sum_{i=1}^{3}\left\{\frac{1}{\hbar^2}\left[\hat{\mathsf{x}}_i,\left[\hat{\mathsf{x}}_i,\hat{\varrho}\right]\right] + \frac{i}{\hbar}\frac{\beta}{M}\left[\hat{\mathsf{x}}_i,\{\hat{\mathsf{p}}_i,\hat{\varrho}\}\right] + \left(\frac{\beta}{2M}\right)^2\left[\hat{\mathsf{p}}_i,\left[\hat{\mathsf{p}}_i,\hat{\varrho}\right]\right]\right\},$$

but the presence of the delta of energy conservation implies

$$|\mathbf{p}_\mu - \mathbf{p}_\eta|^2 = 4p^2\sin^2\frac{\theta}{2}$$

with $|\mathbf{p}_\mu| = |\mathbf{p}_\eta| = p$ and θ the angle between the two vectors. We further have

$$\left|\tilde{t}\left(|\mathbf{p}_\mu - \mathbf{p}_\eta|\right)\right|^2 = \frac{1}{(2\pi)^4\hbar^2\mu^2}\frac{d\sigma}{d\Omega_\eta}$$

with $\mu = (mM)/(m+M) \approx m$, being $m \ll M$ because the Brownian particle is supposed to be much heavier than the particles in the medium. We finally have

$$-\frac{2}{3}\frac{1}{(2\pi\hbar)^3}\int d\Omega_\mu \int d\Omega_\eta \int_0^\infty dE\, p^4 \frac{d\sigma}{d\Omega_\eta}\langle n_\mu\rangle \sin^2\frac{\theta}{2}$$

$$\times\sum_{i=1}^{3}\left\{\frac{1}{\hbar^2}\left[\hat{\mathsf{x}}_i,\left[\hat{\mathsf{x}}_i,\hat{\varrho}\right]\right] + 2\frac{i}{\hbar}\left(\frac{\beta}{2M}\right)\left[\hat{\mathsf{x}}_i,\{\hat{\mathsf{p}}_i,\hat{\varrho}\}\right] + \left(\frac{\beta}{2M}\right)^2\left[\hat{\mathsf{p}}_i,\left[\hat{\mathsf{p}}_i,\hat{\varrho}\right]\right]\right\},$$

so that our master equation takes the form

$$\frac{d\hat{\varrho}}{dt} = -\frac{i}{\hbar}\left[\hat{\mathsf{H}}_0 + \hat{\mathsf{V}}, \hat{\varrho}\right] - \frac{1}{\hbar^2} D_{pp} \sum_{i=1}^{3} [\hat{\mathsf{x}}_i, [\hat{\mathsf{x}}_i, \hat{\varrho}]] - D_{qq} \sum_{i=1}^{3} [\hat{\mathsf{p}}_i, [\hat{\mathsf{p}}_i, \hat{\varrho}]] - \frac{i}{\hbar} D_{qp} \sum_{i=1}^{3} [\hat{\mathsf{x}}_i, \{\hat{\mathsf{p}}_i, \hat{\varrho}\}] \quad (4.3.12)$$

where the coefficients connected to diffusion in phase space are given by

$$\begin{aligned} D_{pp} &= \frac{2}{3}\frac{1}{(2\pi\hbar)^3} \int d\Omega_\mu \int d\Omega_\eta \int_0^\infty dE\, p^4 \frac{d\sigma}{d\Omega_\eta} \langle n_\mu \rangle \sin^2\frac{\theta}{2} \\ D_{qq} &= \left(\frac{\beta}{2M}\right)^2 D_{pp} \qquad (4.3.13) \\ D_{qp} &= 2\left(\frac{\beta}{2M}\right) D_{pp}, \end{aligned}$$

and the potential $\hat{\mathsf{V}}$ is given by (4.3.10)

$$\hat{\mathsf{V}} = -n_{\rm o}\frac{2\pi\hbar^2}{m} \int d^3\mathbf{p} |\mathbf{p}\rangle\langle\mathbf{p}| \,\mathrm{Re} f(E_p, \theta = 0).$$

In the limit of small momentum transfer we have thus recovered the master equation obtained by Dekker [59], apart from the double commutator with $\hat{\mathsf{x}}$ and $\hat{\mathsf{p}}$, giving a definite expression for the coefficients appearing in it, which depend on the features of the collision cross section between the Brownian particle and the medium. A similar result has recently been obtained by Diósi [57]. He obtains an equation with the same structure, so that a direct comparison of the coefficients is feasible. Apart from an overall $(2\pi\hbar)^3$ factor due to a different normalization of the momentum eigenstates, our expression for D_{pp}, D_{qq} and D_{qp} given in (4.3.13) coincide with Diósi's results provided in his "$\hat{\mathsf{L}}$" operator $\mathbf{k}_i \cdot \mathbf{p}$ is substituted by $(\mathbf{k}_i - \mathbf{k}_f) \cdot \mathbf{p}$, so that the whole expression in analyzed in terms of momentum transfers, thus avoiding his somewhat asymmetric choice. The difference amounts however only to a small numerical coefficient.

4.3.3 Final Remarks

In the preceding paragraphs we have shown how the formalism developed in Chap. 3 and in particular the master equation (3.2.31) can cope with the description of quantum Brownian motion, a typical example of irreversible behavior. The dissipative behavior is naturally linked to the contributions other than the commutator, peculiar to the formalism of the statistical operator, whose structure is thoroughly quantum mechanical and cannot be simply guessed on the basis of a correspondence principle. This explains the richness of (4.3.12) with respect to (4.3.2), which is a kind of naive counterpart of the classical Fokker-Planck equation. The result has been obtained introducing a translation invariant interaction kernel and analyzing the whole expression in terms of the momentum transfer between microsystem and environment. Further simplifications, such as low degeneracy and the neglect of the energy dependence in the collision kernel, have been adopted only in order to recover results already obtained in the literature.

4.4 Summary and outlook

This chapter has been devoted to the application of the master equation (3.2.31) obtained in Chap. 3 to some concrete physical situation. In Sect. 4.2 we consider the case of neutron optics, that is to say the description of the interaction of neutrons with homogeneous samples, usually performed reducing the quantum dynamics to a simple wavelike dynamics describable in terms of a refractive index, on the basis of the similarity between the stationary Schrödinger equation and the Helmoltz wave equation. The importance of this field is linked to recent single particle neutron interferometry experiments, performed by different experimental groups in order to verify some fundamental laws of quantum mechanics, which heavily rely upon this optical description for the interaction between neutrons and blocks of matter inducing the phase-shifts. In Sect. 4.2.1 we see how exploiting as phenomenological Ansatz for the T-matrix the Fermi pseudopotential (4.2.4)

$$t(\mathbf{x}) = \frac{2\pi\hbar^2}{m} b\,\delta^3(\mathbf{x})$$

and leaving out the incoherent contributions typical of the formalism of the statistical operator the usual stationary Schrödinger equation (4.2.6) describing a wavelike behavior is recovered

$$\left\{-\frac{\hbar^2}{2m}\Delta_x + \frac{2\pi\hbar^2}{m} b\langle\psi^\dagger(\mathbf{x})\psi(\mathbf{x})\rangle\right\}\phi(\mathbf{x}) = E\phi(\mathbf{x}),$$

equivalent to an index of refraction of the form (4.2.7)

$$n \simeq 1 - \frac{\lambda^2}{2\pi} b n_{\mathrm{o}}.$$

In Sect. 4.2.2 we have considered the contribution given by the terms linked to an incoherent interaction, showing their connection with the dynamic structure function of the medium S_{c}. The result is an imaginary correction to the optical potential (4.2.18)

$$\hat{\mathsf{U}} = \frac{2\pi\hbar^2}{m} n_{\mathrm{o}} \left[b - i\frac{b^2}{4\pi}\frac{p_0}{\hbar}\int d\Omega_q\, S_{\mathrm{c}}(\mathbf{q}) \right],$$

together with a non-vanishing mixture term which accounts for fulfillment of the optical theorem keeping also diffuse scattering into account. The relevance of this contribution in actual experiments has been estimated in Sect. 4.2.3 with the help of a simple model for the dynamic structure function.

The case in which a dissipative dynamics is predominant has been analyzed in Sect. 4.3, considering a particle interacting through collisions with a homogeneous gas supposed to be at equilibrium. In the hypothesis of small momentum transfers we recover the master equation (4.3.12) for the description of quantum Brownian motion, giving a quantum generalization of the Fokker-Planck equation

$$\frac{d\hat{\varrho}}{dt} = -\frac{i}{\hbar}\left[\hat{\mathsf{H}}_0 + \hat{\mathsf{V}}, \hat{\varrho}\right] - \frac{1}{\hbar^2} D_{pp} \sum_{i=1}^{3} [\hat{\mathsf{x}}_i, [\hat{\mathsf{x}}_i, \hat{\varrho}]] - D_{qq} \sum_{i=1}^{3} [\hat{\mathsf{p}}_i, [\hat{\mathsf{p}}_i, \hat{\varrho}]] - \frac{i}{\hbar} D_{qp} \sum_{i=1}^{3} [\hat{\mathsf{x}}_i, \{\hat{\mathsf{p}}_i, \hat{\varrho}\}]$$

$$D_{pp} = \frac{(2/3)}{(2\pi\hbar)^3} \int d\Omega_\mu \int d\Omega_\eta \int_0^\infty dE \, p^4 \frac{d\sigma}{d\Omega_\eta} \langle n_\mu \rangle \sin^2 \frac{\theta}{2} \qquad D_{qq} = \frac{\beta^2}{4M^2} D_{pp} \qquad D_{qp} = \frac{\beta}{M} D_{pp},$$

where the potential term is linked to the forward scattering amplitude. Contrary to most results obtained in the literature starting at a fundamental level this equation has the property of complete positivity and therefore in particular preserves positivity of the statistical operator.

The fact that the very same equation (3.2.31)

$$\frac{d\hat{\varrho}}{dt} = -\frac{i}{\hbar}\left[\hat{\mathsf{H}}_0 + \hat{\mathsf{V}}, \hat{\varrho}\right] - \frac{1}{\hbar}\left\{\frac{1}{2}\sum_{\xi\lambda} \hat{\mathsf{L}}^\dagger_{\lambda\xi}\hat{\mathsf{L}}_{\lambda\xi}, \hat{\varrho}\right\} + \frac{1}{\hbar}\sum_{\xi\lambda} \hat{\mathsf{L}}_{\lambda\xi}\hat{\varrho}\hat{\mathsf{L}}^\dagger_{\lambda\xi}$$

can be successfully applied to two quite different physical situations, such as neutron-matter interaction near the optical regime and Brownian motion, shows how fundamental the treatment developed in Chap. 3 actually is. The key point lies in the choice of the features of the interaction between microsystem and macrosystem, which actually determine the structure of the "$\hat{\mathsf{L}}$" operators in (3.2.31) and therefore of the dissipative or incoherent contributions, and also the relevance of the commutator term to the dynamics. One might therefore hope that (3.2.31), also thanks to the by now canonical Lindblad structure, has really caught some general feature of the intrinsically irreversible interaction of a microsystem with a macroscopic system and might therefore also be applied to other physical situations. Let us stress that the whole treatment in Chap. 3 has been based on the introduction of a time scale and the choice of suitably slowly varying degrees of freedom, which determine the range of validity of the whole description. This conceptual scheme is of general validity and may also be applied to the case of macroscopic systems, as we shall see in Chap. 5.

Chapter 5

Time Scale and Macroscopic Systems

5.1 Introduction

Quantum mechanics has non-separability as its most striking feature, i.e., one cannot attribute "properties" to parts of a system and therefore typical problems like the measurement process and E.P.R. situations arise. This feature is so deeply rooted in the mathematical structure of quantum mechanics that we believe one should not try to make it less stringent, e.g., by attempts like *spontaneous reduction* [63]. We prefer instead to weaken the very concept of physical system: usually the *isolation* of a physical system is taken for granted, while in our opinion the way in which isolation is achieved belongs to the very definition of the system. Any attempt inside quantum mechanics to obtain the subdynamics for a subsystem enforces the introduction of a suitable time scale in order to break up the correlations with the environment and replace physical walls by idealized boundary conditions; in a completely sharp description of the dynamics of a subsystem the physics of the whole universe would enter. The preparation procedure leading to a system, isolated during a time interval $[t_0, t_1]$ and confined in a spatial region ω, covers a time interval $[T, t_0]$, that will be called *preparation time*. Due to the confinement the basic space-time symmetries are broken and by suitable boundary conditions "peculiar" properties of the system are introduced. This obviously reduces the universal character of the dynamical description, however an important universal behavior still remains due to symmetry and locality (or short range character) of effective interactions, whose relevance becomes particularly evident in the quantum field theoretical approach. The outstanding relevance of the field aspect in the description of macroscopic systems is substantiated from the available phenomenological descriptions such as classical electrodynamics, mechanics of continua, equilibrium and non-equilibrium statistical thermodynamics [64].

We thus regard a physical system as a part of the world under control by a suitable preparation, whose local behavior is explained in terms of locally interacting quantum fields. The choice of these fields depends on the level of description of the system. A large part of physics can be explained in terms of quantum fields related to molecules with a typical time scale of the order $\approx 10^{-13}$ s; a much more refined description arises if the basic fields are related to nuclei and electrons, then the basic theory would be QED and a much smaller time scale $\approx 10^{-23}$ s could be considered: however such role of QED as basic theory of macrosystems is far from being exploited. In a sense this viewpoint [65] can appear as opposite to the most widely spread one, which we synthesize as follows: particles are the primary systems, related to non-confined quantum fields and to basic symmetries, all other systems are structure of particles; one then tries to obtain a typical macroscopic behavior in some suitable thermodynamic limit. According to us, on the contrary, macroscopic systems are to be taken as the primary systems, even if in their definition time scales and spatial confinement must be carefully taken into account; the theoretical framework for their description is quantum field theory, locality and quantization taking the place of the atomistic model. In this context particles are a derived concept. The description of non-equilibrium systems is put in the foreground and at least in principle should be performed taking boundary effects into account; procedures like *continuous limit* should be applied only at the end, if one wants to get rid of boundary effects. This standpoint is closer to thermodynamics and electromagnetism, while the former one originates from classical mechanics. The relevance of macroscopic systems for the foundations of quantum mechanics is the starting point of Ludwig's axiomatic approach to quantum mechanics, which has been surveyed in Chap. 2. The insistence on the distinction between these two attitudes is due to the fact that they lead in a natural way to two different formulations of the dynamics, already sketched in Sect. 3.2 in the simpler case of a microsystem interacting with matter. In the first approach one associates a wave function ψ to each system ($\psi(\mathbf{x}, t)$ for one particle, ..., $\psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N, t)$ for N particles); obviously if one describes situations like "unpolarized" particles it is appropriate to use a statistical operator, in order to take a lack of control of the experimental specification into account. This aspect becomes increasingly important for large N, so that statistical operators are very useful for macroscopic systems, nevertheless the basic dynamics is given by an evolution operator for the wavefunction ψ. On the other hand, starting with a macroscopic system, one is led to assume a statistical operator ϱ_t as the most appropriate mathematical representation of the preparation procedure until time t. The set $\mathcal{K}(\mathcal{H})$ of statistical operators on the Hilbert space $\mathcal{H}$ becomes most important and the space $\mathcal{T}(\mathcal{H})$ of trace-class operators, which is generated in a natural way by $\mathcal{K}(\mathcal{H})$ [$\mathcal{K}(\mathcal{H})$ is the base of the base-norm space $\mathcal{T}(\mathcal{H})$], plays a role similar to that of $\mathcal{H}$ in the previous formalism. Correspondingly unitary operators on $\mathcal{H}$ in the first approach are replaced by affine maps of $\mathcal{K}(\mathcal{H})$ in $\mathcal{K}(\mathcal{H})$, i.e., by positive, trace-preserving maps on $\mathcal{T}(\mathcal{H})$. If the system is isolated in the time interval $[t_0, t_1]$ the spontaneous repreparations ϱ_t, $t \in [t_0, t_1]$, are related together by $\varrho_t = \mathcal{M}_{tt'}\varrho_{t'}$ $(t \geq t')$, where the evolution system $\{\mathcal{M}_{t''t'}\, t'' \geq t'\}$ satisfies the composition rule $\mathcal{M}_{t'''t'} = \mathcal{M}_{t'''t''}\mathcal{M}_{t''t'}$ $(t' \leq t'' \leq t''')$. We stress the fact that there is no reason to assume that $\mathcal{M}_{t''t'}$ has an inverse. If $\mathcal{M}^{-1}_{t''t'}$ exists then $\mathcal{M}_{t''t'} = U_{t''t'} \cdot U^{\dagger}_{t''t'}$ (see the discussion in Sect. 3.2), with $U_{t''t'}$ unitary or antiunitary operator and one is brought back to the Hilbert space formalism: $\psi_{t''} = U_{t''t'}\psi_{t'}$. The dynamics in the present framework is indeed more general and has irreversibility as typical phenomenon.

To determine the maps $\mathcal{M}_{t''t'}$ a choice of relevant observables is necessary: when a time scale is introduced, only those observables should be considered, whose expectation values do not appreciably vary in a time interval of the order of the time scale. It is thus necessary to work in the Heisenberg picture, i.e., with the adjoint map $\mathcal{M}'_{tt_0}$, and consider expressions of the form $\mathcal{M}'_{tt_0}A$, A being a relevant observable. For the same system different descriptions can be given by different choices of relevant observables and corresponding time scales, as we shall exemplify in Sect. 5.2.1. Skipping questions of mathematical rigor we can assume the differential equation

$$\frac{d}{dt}\mathcal{M}'_{tt_0} = \mathcal{L}'_t\mathcal{M}'_{tt_0},$$

and represent $\mathcal{M}'_{tt_0}$ in the form $\mathcal{M}'_{tt_0} = T\left(e^{\int_{t_0}^{t} dt'\, \mathcal{L}'_{t'}}\right)$ in terms of the generator $\mathcal{L}'_t$. It is well known (rigorously for bounded $\mathcal{L}'_t$) that if $\mathcal{M}'_{t''t'}$ has the additional property of complete positivity, $\mathcal{L}'_t$ has the Lindblad structure [30, 31]:

$$\mathcal{L}'_t B = +\frac{i}{\hbar}\left(H_t B - B H_t\right) - \frac{1}{\hbar}\left(A_t B + B A_t\right) + \frac{1}{\hbar}\sum_j L^{\dagger}_{tj} B L_{tj}$$

$$H_t = H^{\dagger}_t \qquad A_t = \frac{1}{2}\sum_j L_{tj} L^{\dagger}_{tj}.$$

In our framework the assumption of complete positivity can appear too restrictive since only a suitable subset of observables is relevant and one expects that a modified concept of complete positivity of $\mathcal{M}'_{t''t'}$ relatively to these observables should be given, leading to a more general structure of $\mathcal{L}'_t$, as we shall see in Sect. 5.3.3.

The more general description of the dynamics that we are considering allows the introduction of the concept of trajectory in quantum theory. In fact in the general formalism of continuous measurement approach [32, 33, 34, 35, 36, 37, 38] (for a recent review see [24, 39]) one has that an evolution system $\{\mathcal{M}_{t''t'} \quad t'' \geq t'\}$ with $\mathcal{L}_t$ having the Lindblad structure can be decomposed on a space $Y^{t_1}_{t_0}$ of trajectories for stochastic variables. One can define σ-algebras $\mathcal{B}(Y^{t''}_{t'})$ of subsets $\Omega^{t''}_{t'}$ of $Y^{t''}_{t'}$ and construct operation valued measures $\mathcal{F}^{t''}_{t'}(\Omega^{t''}_{t'})$ on $\mathcal{B}(Y^{t''}_{t'})$ in such a way that $\mathcal{M}_{t''t'} = \mathcal{F}(Y^{t''}_{t'})$. Then for any decomposition $Y^{t''}_{t'} = \cup_\alpha(\Omega^{t''}_{t'\,\alpha})$ with disjoint subsets $\Omega^{t''}_{t'\,\alpha}$ one has

$$\mathcal{M}_{t''t'} = \sum_\alpha \mathcal{F}(\Omega^{t''}_{t'\,\alpha}). \tag{5.1.1}$$

One can therefore claim that the quantum dynamics of the system is compatible with the evolution of classical stochastic variables; typically the probability that the trajectory of these variables for $t' \leq t \leq t''$ belongs to a subset $\Omega_{t'\ \alpha}^{t''}$ is given by $p(\Omega_{t'\ \alpha}^{t''}) = \mathrm{Tr}\left(\mathcal{F}_{t'}^{t''}(\Omega_{t'\ \alpha}^{t''})\varrho(t')\right)$. The decomposition of $\mathcal{M}_{t''t'}$ by operation valued stochastic processes $\mathcal{F}_{t'}^{t''}$ on a suitable trajectory space $Y_{t'}^{t''}$ is not unique, i.e., there are many compatible objective "classical" pictures which are consistent with the quantum evolution. The very possibility of recovering some kind of classical insight into quantum mechanics is due to the non-Hamiltonian evolution; obviously (5.1.1) would be inconsistent with $\mathcal{M}_{t''t'} = U_{t''t'} \cdot U_{t''t'}^{\dagger}$, since for $\varrho_{t'} = |\psi_{t'}\rangle\langle\psi_{t'}|$ the l.h.s. of (5.1.1) is a pure state and the r.h.s. is a mixture.

In the framework we have now presented, dynamics is given by $\mathcal{L}'_t$. One can expect that near to equilibrium only the Hamiltonian part $\frac{i}{\hbar}[H, \cdot]$ is important, as it is clearly indicated by the great success of equilibrium statistical mechanics; however the non-Hamiltonian part of $\mathcal{L}'_t$ is relevant for irreversible behavior and for a full explanation of approach to equilibrium, as we shall see for example in the derivation of the quantum Boltzmann equation in Sect. 5.3.4.

5.2 Finite Isolated Macroscopic Systems

We now consider a very schematic model of macrosystem, in the non-relativistic case, built by one type of molecules with mass m confined inside a region ω, interacting by a two body potential $\Phi(|\mathbf{x} - \mathbf{y}|)$; for the sake of simplicity no internal structure of the molecules is taken into account. In the field theoretical language the system is described by a quantum Schrödinger field:

$$\psi(\mathbf{x}) = \sum_f u_f(\mathbf{x}) a_f \qquad \left[a_f, a_g^{\dagger}\right]_{\pm} = \delta_{fg}$$

$$-\frac{\hbar^2}{2m}\Delta_2 u_f(\mathbf{x}) = E_f u_f(\mathbf{x}), \qquad u_f(\mathbf{x}) = 0 \quad \mathbf{x} \notin \omega. \tag{5.2.1}$$

We shall assume the following Hamiltonian to take local interactions and confinement into account:

$$H = \int_{\omega} d^3\mathbf{x}\, e(\mathbf{x}) = H_0 + \Phi = \sum_f E_f a_f^{\dagger} a_f + \frac{1}{2} \sum_{\substack{l_1 l_2 \\ f_1 f_2}} a_{l_2}^{\dagger} a_{l_1}^{\dagger} \Phi_{l_1 l_2 f_1 f_2} a_{f_1} a_{f_2} \tag{5.2.2}$$

$$\Phi_{l_1 l_2 f_1 f_2} = \int_{\omega} d^3\mathbf{x} \int_{\omega} d^3\mathbf{y}\, u_{l_2}^*(\mathbf{x}) u_{l_1}^*(\mathbf{y}) \Phi(|\mathbf{x} - \mathbf{y}|) u_{f_1}(\mathbf{y}) u_{f_2}(\mathbf{x}).$$

Eq.(5.2.2) is linked to the basic local Hamiltonian density for the non-confined field (nc)

$$e_{\mathrm{nc}}(\mathbf{x}) \;=\; \frac{\hbar^2}{2m}\nabla\psi_{\mathrm{nc}}^{\dagger}(\mathbf{x}) \cdot \nabla\psi_{\mathrm{nc}}(\mathbf{x}) + \frac{1}{2}\int_{\omega} d^3\mathbf{y}\, \psi_{\mathrm{nc}}^{\dagger}(\mathbf{x})\, \psi_{\mathrm{nc}}^{\dagger}(\mathbf{y})\, \Phi(|\mathbf{x} - \mathbf{y}|) \psi_{\mathrm{nc}}(\mathbf{y})\, \psi_{\mathrm{nc}}(\mathbf{x})$$

$$\left[\psi_{\mathrm{nc}}(\mathbf{x}), \psi_{\mathrm{nc}}^{\dagger}(\mathbf{x}')\right]_{\pm} = \delta(\mathbf{x} - \mathbf{x}'),$$

simply selecting the part of $e_{\text{nc}}(\mathbf{x})$ related to the *normal modes* u_f typical of the confinement. Obviously it may be uncomfortable to deal with the functions $u_f(\mathbf{x})$ and to perform discrete sums, even if, but only at a final stage, one can do approximations like $\sum_f h(E_f)u_f(\mathbf{x}) = \int d\mu(\mathbf{p})\, h(\frac{\mathbf{p}^2}{2m})e^{i\frac{\mathbf{p}\cdot\mathbf{x}}{\hbar}}$. The preparation procedure should imply a kind of relaxation of $\psi_{\text{nc}}(\mathbf{x})$ to $\psi(\mathbf{x})$. Skipping this problem we shall simply take the Hamiltonian (5.2.2) containing only the normal modes of the field inside ω. Our aim is not at all a full description of the finite isolated system, but a description of it having negligible correlations with the environment; this description is related to suitable slow variables, linked to the fundamental constants of motion of the system. One has then to make a choice of relevant variables suitably slowly varying on the considered time scale; these quantities will typically be densities of conserved quantities: $A(\mathbf{x})$ with $\int_\omega d^3\mathbf{x}\, A(\mathbf{x})$ a conserved quantity. Our relevant observables, as we shall see in the examples of Sect. 5.2.1, have the general structure:

$$\sum_{hk} a_h^\dagger A_{hk}(\mathbf{x})a_k \quad , \quad \sum_{\substack{h_1h_2\\k_1k_2}} a_{h_2}^\dagger a_{h_1}^\dagger A_{h_2h_1k_1k_2}(\mathbf{x})a_{k_1}a_{k_2} \tag{5.2.3}$$

$$A_{h_2h_1k_1k_2}(\mathbf{x}) = \frac{1}{2}\int_\omega d^3\mathbf{y}\, u_{h_2}^*(\mathbf{x})u_{h_1}^*(\mathbf{y})V(\mathbf{x}-\mathbf{y})u_{k_1}(\mathbf{y})u_{k_2}(\mathbf{x}). \tag{5.2.4}$$

We thus have to study in Heisenberg picture the expressions:

$$\sum_{hk} e^{\frac{i}{\hbar}Ht}a_h^\dagger a_k e^{-\frac{i}{\hbar}Ht}A_{hk}(\mathbf{x}), \qquad \sum_{\substack{h_1h_2\\k_1k_2}} e^{\frac{i}{\hbar}Ht}a_{h_2}^\dagger a_{h_1}^\dagger a_{k_1}a_{k_2}e^{-\frac{i}{\hbar}Ht}A_{h_2h_1k_1k_2}(\mathbf{x}), \tag{5.2.5}$$

and shall take into account that by the slow variability only terms that are "diagonal enough" are really relevant, thus working near to the homogeneous case. The sums should be restricted to indexes such that:

$$\frac{1}{\hbar}|E_h - E_k| < \frac{1}{\tau_1} \qquad \frac{1}{\hbar}|E_{h_1} + E_{h_2} - E_{k_1} - E_{k_2}| < \frac{1}{\tau_1}, \tag{5.2.6}$$

where τ_1 is the characteristic variation time of the relevant quantities, the introduction of the time scale τ_1 implying that the detailed dynamics of the two-body interaction is replaced by collisions. The time scale is related to the choice of the relevant fields in terms of which $e(\mathbf{x})$ is given. The picture founded on a *mass charged* field associated to molecules holds if the physics of the system essentially depends on elastic scattering of neutral molecules, the whole underlying electromagnetic structure being hidden: the intermolecular (e.g., Lennard-Jones) potential $V(r)$ is a simple effective representation of the molecular field self-interaction. A much deeper description of dynamics is possible in terms of *electrically charged* fields (electron and nuclei) based on QED, but also in this case effective rough elements will enter in the Hamiltonian density, e.g., the electromagnetic form factors of nuclei. One can expect that the relevance of time scales in macrophysics, the increasingly deeper descriptions lowering the time scale, even if at any stage the separation procedure requires a persistence of some coarse graining of the dynamical description, indicates a link with the ultraviolet renormalization problem in field theory: such a link appears clearer if quantum field theory is seen as the basic theory of macrosystems, rather than of particles.

We would like to stress the fact that the quantum Schrödinger field is the basic tool to describe a massive continuum, just like the quantum electromagnetic field describes a massless continuum. The dynamics of the quantum Schrödinger field, $\psi(\mathbf{x},t) = e^{\frac{i}{\hbar}Ht}\psi(\mathbf{x})e^{-\frac{i}{\hbar}Ht}$, in terms of which one can rewrite (5.2.5), is given by the simple field equation

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{x},t) = -\frac{\hbar^2}{2m}\Delta_2\psi(\mathbf{x},t) + \int d^3\mathbf{y}\,\psi^\dagger(\mathbf{y},t)\Phi(|\mathbf{x}-\mathbf{y}|)\psi(\mathbf{y},t)\psi(\mathbf{x},t),$$

accounting for covariance under Galilei transformations; however no such equation holds for the expectation value of the field $\langle\psi(\mathbf{x},t)\rangle$ due to correlations in the non-linear term. Therefore a classical Schrödinger field equation for $\langle\psi(\mathbf{x},t)\rangle$ has no physical meaning in general. In this respect the case of electromagnetism, where no self-interaction of the field occurs, is deeply different and allows classical electrodynamics to play an important role.

5.2.1 Different Levels of Description

As phenomenology indicates, for the considered medium there are two meaningful descriptions: the hydrodynamic one based on energy density and mass density; the kinetic one based on energy density and phase-space density. If we are interested in a hydrodynamic description relevant observables are constructed starting with the densities of the typical constants of motion, mass and energy:

$$\begin{aligned} \rho_m(\mathbf{x}) &= m\psi^\dagger(\mathbf{x})\psi(\mathbf{x}) \\ e(\mathbf{x}) &= \frac{\hbar^2}{2m}\nabla\psi^\dagger(\mathbf{x})\cdot\nabla\psi(\mathbf{x}) + \frac{1}{2}\int_\omega d^3\mathbf{y}\,\psi^\dagger(\mathbf{x})\,\psi^\dagger(\mathbf{y})\,\Phi(|\mathbf{x}-\mathbf{y}|)\psi(\mathbf{y})\,\psi(\mathbf{x})\,. \end{aligned} \tag{5.2.7}$$

In the case of a kinetic description we replace (5.2.7) by the phase-space operator density $f(\mathbf{x},\mathbf{p}) = m\sum_{hk} a_h^\dagger\langle u_h|\mathsf{F}^{(1)}(\mathbf{x},\mathbf{p})|u_k\rangle a_k$, where $\mathsf{F}^{(1)}$ is the density of a p.o.v. measure for the joint one particle position-momentum observable [66, 18]. The first step towards a classical description is the introduction of a velocity field of the continuum, so that the former observables can be referred to a local rest frame. Denoting by an index $^{(0)}$ these observables, one has:

$$\begin{aligned} e^{(0)}(\mathbf{x}) &= \frac{1}{2m}\left(i\hbar\nabla - m\mathbf{v}(\mathbf{x},t)\right)\psi^\dagger(\mathbf{x})\cdot\left(-i\hbar\nabla - m\mathbf{v}(\mathbf{x},t)\right)\psi(\mathbf{x}) + \\ &\quad + \frac{1}{2}\int_\omega d^3\mathbf{y}\,\psi^\dagger(\mathbf{x})\,\psi^\dagger(\mathbf{y})\,\Phi(|\mathbf{x}-\mathbf{y}|)\psi(\mathbf{y})\,\psi(\mathbf{x}) \end{aligned}$$

$$\rho_m^{(0)}(\mathbf{x}) = \rho_m(\mathbf{x})$$

$$f^{(0)}(\mathbf{x},\mathbf{p}) = f(\mathbf{x},\mathbf{p}-m\mathbf{v}(\mathbf{x},t)).$$

The introduction of this external classical field allows to compensate a gauge transformation of the field $\psi(\mathbf{x}) \to \psi(\mathbf{x})e^{\frac{i}{\hbar}\Lambda(\mathbf{x})}$ with a transformation $\mathbf{v}(\mathbf{x},t) \to \mathbf{v}(\mathbf{x},t) - 1/m\nabla\Lambda(\mathbf{x},t)$ of the external parameter. The velocity field $\mathbf{v}(\mathbf{x},t)$ is linked to the expectation at time t of the momentum density $\mathbf{p}(\mathbf{x})$ through the relation $\langle \mathbf{p}^{(0)}(\mathbf{x})\rangle_t = 0$, where

$$\mathbf{p}^{(0)}(\mathbf{x}) = \frac{1}{2}\{[(i\hbar\nabla - m\mathbf{v}(\mathbf{x},t))\,\psi^\dagger(\mathbf{x})]\,\psi(\mathbf{x}) - \psi^\dagger(\mathbf{x})\,(i\hbar\nabla + m\mathbf{v}(\mathbf{x},t))\,\psi(\mathbf{x})\}$$

or equivalently $\langle \mathbf{p}(\mathbf{x})\rangle_t = \mathbf{v}(\mathbf{x},t)\langle\rho_m(\mathbf{x})\rangle_t$. The other classical state parameters are linked to the expectations $\langle e^{(0)}(\mathbf{x})\rangle_t$ and $\langle\rho_m^{(0)}(\mathbf{x})\rangle_t$ (or $\langle f^{(0)}(\mathbf{x},\mathbf{p})\rangle_t$ in the kinetic case).

5.2.2 Principle of Maximum Entropy and Thermodynamic Parameters

To the macrosystem one associates typical *thermodynamic state* parameters: the velocity field $\mathbf{v}(\mathbf{x},t)$, the temperature field $\beta(\mathbf{x},t)$, the chemical potential field $\mu(\mathbf{x},t)$ in the case of the hydrodynamic description or more generally a field $\mu(\mathbf{x},\mathbf{p},t)$ on the one-particle phase-space in the kinetic case [67]. The parameters $\beta(\mathbf{x},t)$ and $\mu(\mathbf{x},t)$ ($\mu(\mathbf{x},\mathbf{p},t)$) determine the expectation values of energy density and mass density (the phase-space distribution operator); let us briefly recall how the relation between state variables and expectation values is established according to the principle of maximum entropy [68]. At any time t one considers the whole set of statistical operators $\{w\}$ which yield the expectation values assigned at that time:

$$\langle e^{(0)}(\mathbf{x})\rangle_t = \mathrm{Tr}\left(e^{(0)}(\mathbf{x})w\right), \quad \langle\rho_m(\mathbf{x})\rangle_t = \mathrm{Tr}\left(\rho_m(\mathbf{x})w\right), \quad \langle f^{(0)}(\mathbf{x},\mathbf{p})\rangle_t = \mathrm{Tr}\left(f^{(0)}(\mathbf{x},\mathbf{p})w\right)$$

where the quantities indexed by $^{(0)}$ represent densities in the reference frame in which the continuum is locally at rest and the velocity field is assigned as above. Then one looks for a statistical operator in the set $\{w\}$ such that the von-Neumann entropy [69] $S = -k\mathrm{Tr}\,(w\log w)$ is maximal, i.e., the most unbiased choice of a statistical operator leading to the given expectation values. The unique solution of this problem is

$$w[\beta(t),\mu(t),\mathbf{v}(t)] = \frac{e^{-\int_\omega d^3\mathbf{x}\,\beta(\mathbf{x},t)\left[e^{(0)}(\mathbf{x})-\mu(\mathbf{x},t)\rho_m(\mathbf{x})\right]}}{\mathrm{Tr}\,e^{-\int_\omega d^3\mathbf{x}\,\beta(\mathbf{x},t)\left[e^{(0)}(\mathbf{x})-\mu(\mathbf{x},t)\rho_m(\mathbf{x})\right]}} \tag{5.2.8}$$

and analogously in the kinetic case.

The corresponding $S = -k\mathrm{Tr}(w[\beta(t),\mu(t),\mathbf{v}(t)]\log w[\beta(t),\mu(t),\mathbf{v}(t)])$ is the thermodynamic entropy of the macrosystem. If the time evolution of the expectation values $\langle e^{(0)}(\mathbf{x})\rangle_t$, $\langle\rho_m(\mathbf{x})\rangle_t$,

$\Big(\langle f^{(0)}(\mathbf{x},\mathbf{p})\rangle_t\Big)$ is given by the Hamiltonian evolution (5.2.5) or more generally by a map $\mathcal{M}'_{tt_0}$, having a preadjoint $\mathcal{M}_{tt_0}$ which does not decrease the von-Neumann entropy, one immediately has that the thermodynamic entropy is non-decreasing. In this way one establishes the second principle of thermodynamics on a very clear dynamical basis.

Now the problem arises to make a suitable choice for the representative of the state at some initial time t_0. According to *information thermodynamics* one takes the generalized Gibbs state determined by the given expectation values at time t_0, that is the most unbiased choice. This approach is certainly satisfying if memory effects are absent or completely negligible and if no other information about the system, apart from these expectations, is available. More general situations, for example memory effects connected to a macrophysical correlation time, demand a preparation procedure covering at least the correlation time, thus leading to memory terms in the representative of the state. The dynamical evolution law must then be fine enough to keep such effects into account. To circumvent these difficulty Zubarev, in his definition of the *non-equilibrium statistical operator* [64], takes the limit $t_0 \to -\infty$, thus removing any possible previous memory. This is obtained at the price of introducing a weighting factor $e^{\varepsilon t}$ that has to be eliminated after the thermodynamic limit has been taken, thus resorting once more to an infinite limit. Anyway a suitable memory loss mechanism must be still assumed, typically decay time of correlation functions.

In the simplest scheme of macroscopic dynamics the thermodynamic state parameters $\mathbf{v}(\mathbf{x},t)$, $\beta(\mathbf{x},t)$, $\mu(\mathbf{x},t)$ ($\mu(\mathbf{x},\mathbf{p},t)$) at time t_0 determine its evolution for $t > t_0$, e.g., by differential equations. Phenomenology shows that this is very often the case. Tackling the problem from the theoretical viewpoint one is induced, considering the operators

$$\begin{aligned} \dot{\rho}_m(\mathbf{x}) &= \tfrac{i}{\hbar}[H,\rho_m(\mathbf{x})] & \dot{\mathbf{p}}(\mathbf{x}) &= \tfrac{i}{\hbar}[H,\mathbf{p}(\mathbf{x})] \\ \dot{e}(\mathbf{x}) &= \tfrac{i}{\hbar}[H,e(\mathbf{x})] & (\dot{f}(\mathbf{x},\mathbf{p}) &= \tfrac{i}{\hbar}[H,f(\mathbf{x},\mathbf{p})]), \end{aligned}$$

to calculate their expectations with the statistical operator given by (5.2.8). This leads to wrong results as can be seen from the fact that the expectation values of the currents which can be associated, through a conservation equation, to these operators would vanish [64], due to time reversal invariance of microphysics, thus failing to describe any dissipative flow (e.g., heat conduction, viscosity, etc.). The idea of a time scale for the thermodynamic evolution and of a related subdynamics for the basic densities leads to a refinement of the aforementioned procedure: assume that $\frac{i}{\hbar}[H,\cdot]$ can be replaced by a mapping $\mathcal{L}'$, defined on the linearly independent elements $a^\dagger_h a_k$, $a^\dagger_{h_2} a^\dagger_{h_1} a_{k_1} a_{k_2}$, giving the slow time evolution of the relevant variables. In this way not only the statistical operator $w[\beta(t),\mu(t),\mathbf{v}(t)]$, but also the evolution operator is tuned to the relevant observables. Then one has the following set of closed evolution equations for the thermodynamic fields $\mathbf{v}(\mathbf{x},t)$, $\beta(\mathbf{x},t)$,

$\mu(\mathbf{x},t)$, $(\mu(\mathbf{x},\mathbf{p},t))$ related to the basic observables $A=\rho_m(\mathbf{x})$, $\mathbf{p}(\mathbf{x})$, $e(\mathbf{x})$, $(f(\mathbf{x},\mathbf{p}))$:

$$\frac{d}{dt}\mathrm{Tr}\left(Aw[\beta(t),\mu(t),\mathbf{v}(t)]\right)=\mathrm{Tr}\left((\mathcal{L}'A)w[\beta(t),\mu(t),\mathbf{v}(t)]\right).$$

The non-Hamiltonian form of the map $\mathcal{L}'$ should eliminate the aforementioned difficulties with vanishing dissipative flows. The classical fields $\mathbf{v}$, β, μ entering in the construction of w provide an objective description of the isolated macrosystem, compatible with quantum field dynamics, once the time-scale of the relevant variables has been taken into account. These classical state variables control the expectations of the relevant variables, that can be attributed to collections of prepared systems independently of an actual measuring process. If a concrete measuring process is performed the system is no longer isolated and the dynamics of the open system can be assumed to be still Markovian with $\mathcal{U}'(t)$ replaced by an evolution generated by a superoperator $\mathcal{L}'$ which takes the interaction with the measuring apparatus into account. Then one can attribute trajectories to the relevant quantum field variables in the context of continuous measurement theory: one can see that the part of $\mathcal{L}'$ related to the interaction with the measuring apparatus strongly affects the probability measures in this trajectory space, e.g., providing dispersions for the relevant observables that diverge in the limit of an isolated system. In this way expectation values of the relevant observables can be linked to actual probability distributions for open systems and retain a physical meaning in the limit in which the perturbation due to measurement vanishes. Examples of this situation arise in quantum optics when atomic systems are considered, pumped by an external laser field and behaving as open systems due to the interaction with the quantum radiation field. In [65] a model is given for a continuous observation of the Schrödinger field, in which a trajectory space for the relevant variables that we are considering in this chapter has been introduced, in this thesis this point is not further examined. However it appears that a first step has been made in the direction of an objective of a macrosystem inside quantum mechanics, which was indeed the starting point described in Chap. 2. The problem of decomposing the dynamics of an isolated macrosystem first into independent components, then into components independent "but for a microsystem" appears as the most natural strategy to study interaction between macrosystems; this should lead to to microsystems as carrier of interaction.

5.3 Time Scale and Scattering Map

After the presentation of the formal and conceptual scheme for the description of the dynamics of macroscopic systems put forward in the previous sections, exploiting the notion of time scale and relevant, slowly varying variables, we now devote our attention to the detailed evaluation of the time evolution of these variables. As seen in Sect. 5.2 our relevant variables, in the case of a kinetic or hydrodynamic description, have the general form (5.2.3), so that we actually have to study expressions of the form $\mathcal{U}'(a^\dagger_h a_k)$, $\mathcal{U}'(a^\dagger_{h_1} a^\dagger_{h_2} a_{k_2} a_{k_1})$, $\mathcal{U}'$ being the time evolution mapping in Heisenberg picture (the prime denotes in fact, here and in the sequel, the adjoint mapping with respect to the Schrödinger picture), acting on the algebra of creation and annihilation operators in Fock-space

$$\mathcal{U}' \cdot = e^{+\frac{i}{\hbar}Ht} \cdot e^{-\frac{i}{\hbar}Ht},$$

looking for an asymptotic representation for $t \geq \tau_1 \gg \tau_0$, where τ_1 is the typical variation time of our relevant variables, as given by (5.2.6), while τ_0 can be interpreted as the typical duration of a collision between two particles interacting through the potential $\Phi(|\mathbf{x}-\mathbf{y}|)$. The time scale given by τ_0 is therefore supposed to be much smaller than the time scale τ_1 associated to the selected variables. Our approach, related to relevant field variables in Heisenberg picture, differs strongly from master equation theory or investigations (e.g., Prigogine's approach) aiming at a subdynamics for the statistical operator and the procedure essentially consists in transferring to the space of observables $\mathcal{B}(\mathcal{H})$ standard methods of scattering theory related to $\mathcal{H}$, analogously to what we have done in Sect. 3.2.1. The mapping $\mathcal{T}(z)$, reminiscent of the T-matrix, plays a central role in this treatment and will be called *scattering map*, the existence of τ_0 being connected to suitable smoothness properties of $\mathcal{T}(z)$, so that essentially only the poles of $(z-\mathcal{H}'_0)^{-1}$ contribute to the calculations in (5.3.1). The final result will have the simple structure

$$\mathcal{U}'(t)\,(a^\dagger_h a_k) = a^\dagger_h a_k + t\mathcal{L}'\,(a^\dagger_h a_k) \qquad \tau_0 \ll t \ll \frac{\hbar}{|E_h - E_k|},$$

and similarly for higher order polynomials of the field operators. The linear mapping $\mathcal{L}'$ acting in $\mathcal{B}(\mathcal{H})$ and defined on the linearly independent elements $a^\dagger_h a_k$, $a^\dagger_{h_2} a^\dagger_{h_1} a_{k_1} a_{k_2}$ is given by (5.3.25), formally the same as in (3.2.24).

5.3.1 Derivation of the Scattering Map

We want to study the expression

$$\mathcal{U}'(a^\dagger_h a_k) = e^{+\frac{i}{\hbar}Ht} a^\dagger_h a_k e^{-\frac{i}{\hbar}Ht},$$

where H is the Hamiltonian given by (5.2.2) and the time t is such that $t \geq \tau_1 \gg \tau_0$. As in Sect. 3.2.1 we introduce the superoperators

$$\mathcal{H}' = \frac{i}{\hbar}[H,\cdot], \quad \mathcal{H}'_0 = \frac{i}{\hbar}[H_0,\cdot], \quad \mathcal{V}' = \frac{i}{\hbar}[\Phi,\cdot]$$

recalling that $a^\dagger_h, a_k$ are "eigenstates" of the superoperator $\mathcal{H}'_0$

$$\mathcal{H}'_0 a^\dagger_h = +\frac{i}{\hbar}E_h a^\dagger_h \qquad \mathcal{H}'_0 a_k = -\frac{i}{\hbar}E_k a_k.$$

We make use again of the integral representation

$$\mathcal{U}'(t)\,(a_h^\dagger a_k) = e^{\mathcal{H}'t}\left[a_h^\dagger a_k\right] = \int_{-i\infty+\eta}^{+i\infty+\eta} \frac{dz}{2\pi i}\, e^{zt}(z-\mathcal{H}')^{-1}\left[a_h^\dagger a_k\right], \tag{5.3.1}$$

where

$$(z-\mathcal{H}')^{-1} = (z-\mathcal{H}_0')^{-1} + (z-\mathcal{H}_0')^{-1}\mathcal{T}(z)(z-\mathcal{H}_0')^{-1} \tag{5.3.2}$$

and thanks to (3.2.14) one has the analog of the usual resolvent series

$$(z-\mathcal{H}')^{-1} = (z-\mathcal{H}_0')^{-1} + (z-\mathcal{H}_0')^{-1}\mathcal{V}'(z-\mathcal{H}_0')^{-1} + (z-\mathcal{H}_0')^{-1}\mathcal{V}'(z-\mathcal{H}_0')^{-1}\mathcal{V}'(z-\mathcal{H}_0')^{-1} + \ldots \tag{5.3.3}$$

We may therefore write

$$\mathcal{U}'(t)\,(a_h^\dagger a_k) = e^{(e_h-e_k)t}a_h^\dagger a_k + \int_{-i\infty+\eta}^{+i\infty+\eta} \frac{dz}{2\pi i}\, e^{zt}\frac{1}{z-e_h+e_k}\sum_{n=1}^{\infty}\mathcal{A}_{hk}^n \tag{5.3.4}$$

where we have set for simplicity $e_h = \frac{i}{\hbar}E_h$ and

$$\mathcal{A}_{hk}^n \equiv \left\{(z-\mathcal{H}_0')^{-1}\mathcal{V}'\right\}^n\left[a_h^\dagger a_k\right], \qquad \mathcal{A}_{hk}^{n+1} = (z-\mathcal{H}_0')^{-1}\mathcal{V}'\left[\mathcal{A}_{hk}^n\right].$$

Our aim is therefore to obtain a suitable expression for $\sum_{n=1}^{\infty}\mathcal{A}_{hk}^n$. In order to make the first step let us observe that the matrix elements of the potential

$$\Phi = \frac{1}{2}\sum_{\substack{l_1 l_2\\ f_1 f_2}} a_{l_2}^\dagger a_{l_1}^\dagger \Phi_{l_1 l_2 f_1 f_2} a_{f_1} a_{f_2}$$

have the following symmetry properties ($\pm$ denoting Bose or Fermi statistics respectively)

$$\Phi_{l_1 l_2 f_1 f_2} = \pm\Phi_{l_2 l_1 f_1 f_2} = \pm\Phi_{l_1 l_2 f_2 f_1} = \Phi_{l_2 l_1 f_2 f_1} = \left(\Phi_{f_1 f_2 l_1 l_2}\right)^*, \tag{5.3.5}$$

so that

$$\mathcal{V}(a_h^\dagger) = \frac{i}{\hbar}\sum_{\substack{l_1 l_2\\ f}} a_{l_2}^\dagger a_{l_1}^\dagger \Phi_{l_1 l_2 f h} a_f, \qquad \mathcal{V}(a_k) = -\frac{i}{\hbar}\sum_{\substack{f_1 f_2\\ l}} a_l^\dagger \Phi_{l k f_1 f_2} a_{f_1} a_{f_2}. \tag{5.3.6}$$

At first order we have therefore simply

$$\begin{aligned}\mathcal{A}_{hk}^1 &= (z-\mathcal{H}_0')^{-1}\mathcal{V}'\left[a_h^\dagger a_k\right] = (z-\mathcal{H}_0')^{-1}\left\{\mathcal{V}'\left[a_h^\dagger\right]a_k + a_h^\dagger\mathcal{V}'\left[a_k\right]\right\} \\ &= +\sum_{\substack{l_1 l_2\\ \lambda}}\left(\frac{i}{\hbar}\right)\frac{1}{z-e_{l_1}-e_{l_2}+e_\lambda+e_k}a_{l_2}^\dagger a_{l_1}^\dagger\Phi_{l_1 l_2 \lambda h}a_\lambda a_k \qquad \mathtt{l} \\ &\quad+\sum_{\substack{f_1 f_2\\ \lambda}}\left(-\frac{i}{\hbar}\right)\frac{1}{z-e_h-e_\lambda+e_{f_1}+e_{f_2}}a_h^\dagger a_\lambda^\dagger\Phi_{\lambda k f_1 f_2}a_{f_1}a_{f_2}, \qquad \mathtt{r}\end{aligned} \tag{5.3.7}$$

where the letters `l` and `r`, here and in the sequel, denote the contributions obtained by acting with the mapping $\mathcal{V}'$ on the left or right block of field operators respectively; `llr` will denote for example the term obtained acting at first order on $a^{\dagger}_{h}$, at second order on $a^{\dagger}_{l_2}a^{\dagger}_{l_1}$ and at third order on $a_{f_1}a_{f_2}$. This notation, that will become clearer in the sequel, is helpful in keeping track of the logical structure of the expressions obtained at the higher perturbative orders. By conservation of total mass the scattering map applied to a couple of creation and annihilation operators should have the general structure

$$\begin{aligned}\mathcal{T}(z)[a^{\dagger}_{h}a_k] &= \sum_{l_1 f_1} a^{\dagger}_{l_1} C_{l_1 hk f_1} a_{f_1}(z,n) + \sum_{\substack{l_1 l_2 \\ f_1 f_2}} a^{\dagger}_{l_2}a^{\dagger}_{l_1} C_{l_1 l_2 hk f_1 f_2}(z,n) a_{f_1}a_{f_2} \\ &+ \sum_{\substack{l_1 l_2 l_3 \\ f_1 f_2 f_3}} a^{\dagger}_{l_3}a^{\dagger}_{l_2}a^{\dagger}_{l_1} C_{l_1 l_2 l_3 hk f_1 f_2 f_3}(z,n) a_{f_1}a_{f_2}a_{f_3} + \ldots\end{aligned} \tag{5.3.8}$$

where the coefficients $C_{l_1 hk f_1} a_{l_1}(z,n)$, $C_{l_1 l_2 hk f_1 f_2}(z,n)$, ... are operator functions of the set of number operators $\{n_g = a^{\dagger}_{g}a_g\}$, diagonal with respect to the basis in Fock-space generated by the creation operators. A very natural approximation in usual kinetic theory is the evolution by two-particle collisions, reliable if the system is not too dense. In our field description the corresponding approximation seems to be the following: a *one-mode* approximation in which we consider the part of the evolution involving only one other field mode, so that in (5.3.8) we consider only the first two terms in the expansion; however all the *spectator modes* are also relevant through the n dependence of the coefficients and provide the Pauli principle corrections. We now calculate $\mathcal{A}^2_{hk}$ within this *one-mode* approximation. The relevant part of the calculation is the evaluation of expressions of the form

$$\mathcal{V}'\left[a^{\dagger}_{l_2}a^{\dagger}_{l_1}a_{f_1}a_{f_2}\right]\Phi_{l_1 l_2 f_1 f_2} = \mathcal{V}'\left[a^{\dagger}_{l_2}a^{\dagger}_{l_1}\right]\Phi_{l_1 l_2 f_1 f_2}a_{f_1}a_{f_2} + a^{\dagger}_{l_2}a^{\dagger}_{l_1}\Phi_{l_1 l_2 f_1 f_2}\mathcal{V}'\left[a_{f_1}a_{f_2}\right],$$

discarding contributions containing more modes but keeping statistical corrections expressed by the number operators $n_g = a^{\dagger}_{g}a_g$. We have

$$\mathcal{V}'\left[a^{\dagger}_{l_2}a^{\dagger}_{l_1}\right]\Phi_{l_1 l_2 f_1 f_2}a_{f_1}a_{f_2} = \frac{i}{\hbar}\frac{1}{2}\sum_{\substack{r_1 r_2 \\ g_1 g_2}} a^{\dagger}_{r_2}a^{\dagger}_{r_1}\Phi_{r_1 r_2 g_1 g_2}\left[a_{g_1}a_{g_2}, a^{\dagger}_{l_2}a^{\dagger}_{l_1}\right]\Phi_{l_1 l_2 f_1 f_2}a_{f_1}a_{f_2}$$

$$= \frac{i}{\hbar}\sum_{\substack{r_1 r_2 \\ g}} a^{\dagger}_{r_2}a^{\dagger}_{r_1}\frac{1}{2}\left\{\Phi_{r_1 r_2 g l_2}a_g a^{\dagger}_{l_1} \pm \Phi_{r_1 r_2 g l_1}a_g a^{\dagger}_{l_2} + \Phi_{r_1 r_2 l_2 g}a^{\dagger}_{l_1}a_g \pm \Phi_{r_1 r_2 l_1 g}a^{\dagger}_{l_2}a_g\right\}\Phi_{l_1 l_2 f_1 f_2}a_{f_1}a_{f_2}$$

and putting the operators in normal order, exploiting also the symmetry property of the potential given by (5.3.5)

$$\mathcal{V}'\left[a^{\dagger}_{l_2}a^{\dagger}_{l_1}\right]\Phi_{l_1 l_2 f_1 f_2}a_{f_1}a_{f_2} =$$

$$\frac{i}{\hbar}\sum_{r_1r_2} a^\dagger_{r_2}a^\dagger_{r_1}\left\{\Phi_{r_1r_2l_1l_2} \pm \sum_g \Phi_{r_1r_2gl_2}a^\dagger_{l_1}a_g \pm \sum_g \Phi_{r_1r_2l_1g}a^\dagger_{l_2}a_g\right\}\Phi_{l_1l_2f_1f_2}a_{f_1}a_{f_2}.$$

At this point, exploiting the *one-mode* approximation as explained above, we keep only the summands in which either $g = l_1$ or $g = l_2$, which do not introduce further modes, but contribute, through the n_{l_1}, n_{l_2} operators, to the statistical corrections. The final expression is

$$\mathcal{V}'\left[a^\dagger_{l_2}a^\dagger_{l_1}\right]\Phi_{l_1l_2f_1f_2}a_{f_1}a_{f_2} \approx \frac{i}{\hbar}\sum_{r_1r_2} a^\dagger_{r_2}a^\dagger_{r_1}\Phi_{r_1r_2l_1l_2}\left(1 \pm n_{l_1} \pm n_{l_2}\right)\Phi_{l_1l_2f_1f_2}a_{f_1}a_{f_2}, \tag{5.3.9}$$

and in the same way we obtain

$$a^\dagger_{l_2}a^\dagger_{l_1}\Phi_{l_1l_2f_1f_2}\mathcal{V}'\left[a_{f_1}a_{f_2}\right] \approx -\frac{i}{\hbar}\sum_{r_1r_2} a^\dagger_{l_2}a^\dagger_{l_1}\Phi_{l_1l_2f_1f_2}\left(1 \pm n_{f_1} \pm n_{f_2}\right)\Phi_{f_1f_2r_1r_2}a_{r_1}a_{r_2}. \tag{5.3.10}$$

Exploiting (5.3.9) and (5.3.10) our second order contribution becomes

$$\begin{aligned}
\mathcal{A}^2_{hk} \quad = \quad & \sum_{\substack{l_1l_2\\ l'_1l'_2}}\sum_{\lambda}\left(\frac{i}{\hbar}\right)\frac{1}{z - e_{l_1} - e_{l_2} + e_\lambda + e_k}a^\dagger_{l_2}a^\dagger_{l_1}\Phi_{l_1l_2l'_1l'_2} \\
& \times\left(\frac{i}{\hbar}\right)\frac{\left(1 \pm n_{l'_1} \pm n_{l'_2}\right)}{z - e_{l'_1} - e_{l'_2} + e_\lambda + e_k}\Phi_{l'_1l'_2\lambda h}a_\lambda a_k \qquad \texttt{ll} \\
& + \sum_{\substack{l_1l_2\\ f_1f_2}}\sum_{\lambda}\left(\frac{i}{\hbar}\right)\frac{1}{z - e_{l_1} - e_{l_2} + e_{f_1} + e_{f_2}}a^\dagger_{l_2}a^\dagger_{l_1}\Phi_{l_1l_2\lambda h} \\
& \times\left(-\frac{i}{\hbar}\right)\frac{\left(1 \pm n_\lambda \pm n_k\right)}{z - e_{l_1} - e_{l_2} + e_\lambda + e_k}\Phi_{\lambda kf_1f_2}a_{f_1}a_{f_2} \qquad \texttt{lr} \\
& + \sum_{\substack{f_1f_2\\ f'_1f'_2}}\sum_{\lambda}\left(-\frac{i}{\hbar}\right)\frac{1}{z - e_h - e_\lambda + e_{f_1} + e_{f_2}}a^\dagger_h a^\dagger_\lambda\Phi_{\lambda kf'_1f'_2} \\
& \times\left(-\frac{i}{\hbar}\right)\frac{\left(1 \pm n_{f'_1} \pm n_{f'_2}\right)}{z - e_h - e_\lambda + e_{f'_1} + e_{f'_2}}\Phi_{f'_1f'_2f_1f_2}a_{f_1}a_{f_2} \qquad \texttt{rr} \\
& + \sum_{\substack{l_1l_2\\ f_1f_2}}\sum_{\lambda}\left(-\frac{i}{\hbar}\right)\frac{1}{z - e_{l_1} - e_{l_2} + e_{f_1} + e_{f_2}}a^\dagger_{l_2}a^\dagger_{l_1}\Phi_{l_1l_2\lambda h} \\
& \times\left(\frac{i}{\hbar}\right)\frac{\left(1 \pm n_\lambda \pm n_h\right)}{z - e_h - e_\lambda + e_{f_1} + e_{f_2}}\Phi_{\lambda kf_1f_2}a_{f_1}a_{f_2}. \qquad \texttt{rl}
\end{aligned}$$

Let us note that in front of each contribution we have a term with a pole for the z variable corresponding to the difference in energy between the in and out states. We now go over to the third order contribution $\mathcal{A}^3_{hk}$, always in the *one-mode* approximation, so that the action of $\mathcal{V}'$ on the statistical corrections, bringing in new modes, has been neglected; after some tedious bookkeeping we have

$$\mathcal{A}^3_{hk} =$$

$$\sum_{\substack{l_1 l_2\\ l'_1 l'_2\\ l''_1 l''_2}} \sum_{\lambda} \left(\frac{i}{\hbar}\right) \frac{1}{z - e_{l_1} - e_{l_2} + e_\lambda + e_k} a^\dagger_{l_2} a^\dagger_{l_1} \Phi_{l_1 l_2 l''_1 l''_2} \left(\frac{i}{\hbar}\right) \frac{\left(1 \pm n_{l''_1} \pm n_{l''_2}\right)}{z - e_{l''_1} - e_{l''_2} + e_\lambda + e_k} \Phi_{l''_1 l''_2 l'_1 l'_2}$$

$$\times \left(\frac{i}{\hbar}\right) \frac{\left(1 \pm n_{l'_1} \pm n_{l'_2}\right)}{z - e_{l'_1} - e_{l'_2} + e_\lambda + e_k} \Phi_{l'_1 l'_2 \lambda h} a_\lambda a_k \qquad \texttt{lll}$$

$$+ \sum_{\substack{l_1 l_2\\ l'_1 l'_2}} \sum_{f_1 f_2} \sum_{\lambda} \left(\frac{i}{\hbar}\right) \frac{1}{z - e_{l_1} - e_{l_2} + e_{f_1} + e_{f_2}} a^\dagger_{l_2} a^\dagger_{l_1} \Phi_{l_1 l_2 l'_1 l'_2} \left(\frac{i}{\hbar}\right) \frac{\left(1 \pm n_{l'_1} \pm n_{l'_2}\right)}{z - e_{l'_1} - e_{l'_2} + e_\lambda + e_k} \Phi_{l'_1 l'_2 \lambda h}$$

$$\times \left(-\frac{i}{\hbar}\right) \frac{(1 \pm n_\lambda \pm n_k)}{z - e_{l_1} - e_{l_2} + e_\lambda + e_k} \Phi_{\lambda k f_1 f_2} a_{f_1} a_{f_2} \qquad \texttt{llr}$$

$$+ \sum_{\substack{l_1 l_2\\ l'_1 l'_2}} \sum_{f_1 f_2} \sum_{\lambda} \left(\frac{i}{\hbar}\right) \frac{1}{z - e_{l_1} - e_{l_2} + e_{f_1} + e_{f_2}} a^\dagger_{l_2} a^\dagger_{l_1} \Phi_{l_1 l_2 l'_1 l'_2} \left(\frac{i}{\hbar}\right) \frac{\left(1 \pm n_{l'_1} \pm n_{l'_2}\right)}{z - e_{l'_1} - e_{l'_2} + e_{f_1} + e_{f_2}} \Phi_{l'_1 l'_2 \lambda h}$$

$$\times \left(-\frac{i}{\hbar}\right) \frac{(1 \pm n_\lambda \pm n_k)}{z - e_{l'_1} - e_{l'_2} + e_\lambda + e_k} \Phi_{\lambda k f_1 f_2} a_{f_1} a_{f_2} \qquad \texttt{lrl}$$

$$+ \sum_{l_1 l_2} \sum_{\substack{f_1 f_2\\ f'_1 f'_2}} \sum_{\lambda} \left(\frac{i}{\hbar}\right) \frac{1}{z - e_{l_1} - e_{l_2} + e_{f_1} + e_{f_2}} a^\dagger_{l_2} a^\dagger_{l_1} \Phi_{l_1 l_2 \lambda h} \left(-\frac{i}{\hbar}\right) \frac{(1 \pm n_\lambda \pm n_k)}{z - e_{l_1} - e_{l_2} + e_\lambda + e_k} \Phi_{\lambda k f'_1 f'_2}$$

$$\times \left(-\frac{i}{\hbar}\right) \frac{\left(1 \pm n_{f'_1} \pm n_{f'_2}\right)}{z - e_{l_1} - e_{l_2} + e_{f'_1} + e_{f'_2}} \Phi_{f'_1 f'_2 f_1 f_2} a_{f_1} a_{f_2} \qquad \texttt{lrr}$$

$$+ \sum_{l_1 l_2} \sum_{\substack{f_1 f_2\\ f'_1 f'_2}} \sum_{\lambda} \left(-\frac{i}{\hbar}\right) \frac{1}{z - e_{l_1} - e_{l_2} + e_{f_1} + e_{f_2}} a^\dagger_{l_2} a^\dagger_{l_1} \Phi_{l_1 l_2 \lambda h} \left(\frac{i}{\hbar}\right) \frac{(1 \pm n_\lambda \pm n_h)}{z - e_h - e_\lambda + e_{f_1} + e_{f_2}} \Phi_{\lambda k f'_1 f'_2}$$

$$\times \left(-\frac{i}{\hbar}\right) \frac{\left(1 \pm n_{f'_1} \pm n_{f'_2}\right)}{z - e_h - e_\lambda + e_{f'_1} + e_{f'_2}} \Phi_{f'_1 f'_2 f_1 f_2} a_{f_1} a_{f_2} \qquad \texttt{rrl}$$

$$+\sum_{\substack{f_1f_2\\f_1'f_2'\\f_1''f_2''}}\sum_{\lambda}\left(-\frac{i}{\hbar}\right)\frac{1}{z-e_h-e_\lambda+e_{f_1}+e_{f_2}}a_h^\dagger a_\lambda^\dagger\Phi_{\lambda k f_1'f_2'}\left(-\frac{i}{\hbar}\right)\frac{\left(1\pm n_{f_1'}\pm n_{f_2'}\right)}{z-e_h-e_\lambda+e_{f_1'}+e_{f_2'}}\Phi_{f_1'f_2'f_1''f_2''}$$

$$\times\left(-\frac{i}{\hbar}\right)\frac{\left(1\pm n_{f_1''}\pm n_{f_2''}\right)}{z-e_h-e_\lambda+e_{f_1''}+e_{f_2''}}\Phi_{f_1''f_2''f_1f_2}a_{f_1}a_{f_2}\qquad \texttt{rrr}$$

$$+\sum_{\substack{l_1l_2\\l_1'l_2'}}\sum_{f_1f_2}\sum_{\lambda}\left(-\frac{i}{\hbar}\right)\frac{1}{z-e_{l_1}-e_{l_2}+e_{f_1}+e_{f_2}}a_{l_2}^\dagger a_{l_1}^\dagger\Phi_{l_1l_2l_1'l_2'}\left(\frac{i}{\hbar}\right)\frac{\left(1\pm n_{l_1'}\pm n_{l_2'}\right)}{z-e_{l_1'}-e_{l_2'}+e_{f_1}+e_{f_2}}\Phi_{l_1'l_2'\lambda h}$$

$$\times\left(\frac{i}{\hbar}\right)\frac{(1\pm n_\lambda\pm n_h)}{z-e_h-e_\lambda+e_{f_1}+e_{f_2}}\Phi_{\lambda k f_1f_2}a_{f_1}a_{f_2}\qquad \texttt{rll}$$

$$+\sum_{l_1l_2}\sum_{\substack{f_1f_2\\f_1'f_2'}}\sum_{\lambda}\left(-\frac{i}{\hbar}\right)\frac{1}{z-e_{l_1}-e_{l_2}+e_{f_1}+e_{f_2}}a_{l_2}^\dagger a_{l_1}^\dagger\Phi_{l_1l_2\lambda h}\left(\frac{i}{\hbar}\right)\frac{(1\pm n_\lambda\pm n_h)}{z-e_h-e_\lambda+e_{f_1'}+e_{f_2'}}\Phi_{\lambda k f_1'f_2'}$$

$$\times\left(-\frac{i}{\hbar}\right)\frac{\left(1\pm n_{f_1'}\pm n_{f_2'}\right)}{z-e_{l_1}-e_{l_2}+e_{f_1'}+e_{f_2'}}\Phi_{f_1'f_2'f_1f_2}a_{f_1}a_{f_2}.\qquad \texttt{rlr}$$

We now sort the different summands, collecting the terms with the same operator structure and putting into evidence the contributions having a pole in the z variable corresponding to the difference in energy between the in and out states. We have

$$\texttt{llr}+\texttt{lrl}=$$

$$\sum_{\substack{l_1l_2\\l_1'l_2'}}\sum_{f_1f_2}\sum_{\lambda}\left(\frac{i}{\hbar}\right)\frac{1}{z-e_{l_1}-e_{l_2}+e_{f_1}+e_{f_2}}a_{l_2}^\dagger a_{l_1}^\dagger\Phi_{l_1l_2l_1'l_2'}$$

$$\times\left(\frac{i}{\hbar}\right)\left(1\pm n_{l_1'}\pm n_{l_2'}\right)\Phi_{l_1'l_2'\lambda h}\left(-\frac{i}{\hbar}\right)\frac{(1\pm n_\lambda\pm n_k)}{z-e_{l_1'}-e_{l_2'}+e_\lambda+e_k}\Phi_{\lambda k f_1f_2}a_{f_1}a_{f_2}$$

$$\times\frac{[z-e_{l_1}-e_{l_2}+e_{f_1}+e_{f_2}]+[z-e_{l_1'}-e_{l_2'}+e_\lambda+e_k]}{(z-e_{l_1}-e_{l_2}+e_\lambda+e_k)\,(z-e_{l_1'}-e_{l_2'}+e_{f_1}+e_{f_2})}$$

and therefore

$$\texttt{llr}+\texttt{lrl}+\texttt{rll}=$$

$$+\sum_{\substack{l_1l_2\\l_1'l_2'}}\sum_{f_1f_2}\sum_{\lambda}\left(\frac{i}{\hbar}\right)\frac{1}{z-e_{l_1}-e_{l_2}+e_{f_1}+e_{f_2}}a_{l_2}^\dagger a_{l_1}^\dagger\Phi_{l_1l_2l_1'l_2'}\left(\frac{i}{\hbar}\right)\frac{\left(1\pm n_{l_1'}\pm n_{l_2'}\right)}{z-e_{l_1'}-e_{l_2'}+e_{f_1}+e_{f_2}}$$

$$\times \Phi_{l_1' l_2' \lambda h} \left[\left(-\frac{i}{\hbar}\right) \frac{(1 \pm n_\lambda \pm n_k)}{z - e_{l_1} - e_{l_2} + e_\lambda + e_k} - \left(\frac{i}{\hbar}\right) \frac{(1 \pm n_\lambda \pm n_h)}{z - e_h - e_\lambda + e_{f_1} + e_{f_2}} \right] \Phi_{\lambda k f_1 f_2} a_{f_1} a_{f_2}$$

$$+ \sum_{\substack{l_1 l_2 \\ l_1' l_2'}} \sum_{f_1 f_2} \sum_\lambda \left(\frac{i}{\hbar}\right) \frac{1}{z - e_{l_1} - e_{l_2} + e_\lambda + e_k} a_{l_2}^\dagger a_{l_1}^\dagger \Phi_{l_1 l_2 l_1' l_2'}$$

$$\times \left(\frac{i}{\hbar}\right) \frac{\left(1 \pm n_{l_1'} \pm n_{l_2'}\right)}{z - e_{l_1'} - e_{l_2'} + e_{f_1} + e_{f_2}} \Phi_{l_1' l_2' \lambda h} \left(-\frac{i}{\hbar}\right) \frac{(1 \pm n_\lambda \pm n_k)}{z - e_{l_1'} - e_{l_2'} + e_\lambda + e_k} \Phi_{\lambda k f_1 f_2} a_{f_1} a_{f_2}.$$

Similarly

$$\texttt{rrl} + \texttt{rlr} =$$

$$\sum_{l_1 l_2} \sum_{\substack{f_1 f_2 \\ f_1' f_2'}} \sum_\lambda \left(-\frac{i}{\hbar}\right) \frac{1}{z - e_{l_1} - e_{l_2} + e_{f_1} + e_{f_2}} a_{l_2}^\dagger a_{l_1}^\dagger \Phi_{l_1 l_2 \lambda h}$$

$$\times \left(\frac{i}{\hbar}\right) \frac{(1 \pm n_\lambda \pm n_h)}{z - e_h - e_\lambda + e_{f_1'} + e_{f_2'}} \Phi_{\lambda k f_1' f_2'} \left(-\frac{i}{\hbar}\right) \left(1 \pm n_{f_1'} \pm n_{f_2'}\right) \Phi_{f_1' f_2' f_1 f_2} a_{f_1} a_{f_2}$$

$$\times \frac{[z - e_{l_1} - e_{l_2} + e_{f_1} + e_{f_2}] + [z - e_h - e_\lambda + e_{f_1'} + e_{f_2'}]}{\left(z - e_{l_1} - e_{l_2} + e_{f_1'} + e_{f_2'}\right)\left(z - e_h - e_\lambda + e_{f_1} + e_{f_2}\right)}$$

and therefore

$$\texttt{rrl} + \texttt{rlr} + \texttt{lrr} =$$

$$\sum_{l_1 l_2} \sum_{\substack{f_1 f_2 \\ f_1' f_2'}} \sum_\lambda \left(\frac{i}{\hbar}\right) \frac{1}{z - e_{l_1} - e_{l_2} + e_{f_1} + e_{f_2}} a_{l_2}^\dagger a_{l_1}^\dagger$$

$$\times \Phi_{l_1 l_2 \lambda h} \left[\left(-\frac{i}{\hbar}\right) \frac{(1 \pm n_\lambda \pm n_k)}{z - e_{l_1} - e_{l_2} + e_\lambda + e_k} - \left(\frac{i}{\hbar}\right) \frac{(1 \pm n_\lambda \pm n_h)}{z - e_h - e_\lambda + e_{f_1} + e_{f_2}} \right] \Phi_{\lambda k f_1' f_2'}$$

$$\times \left(-\frac{i}{\hbar}\right) \frac{\left(1 \pm n_{f_1'} \pm n_{f_2'}\right)}{z - e_{l_1} - e_{l_2} + e_{f_1'} + e_{f_2'}} \Phi_{f_1' f_2' f_1 f_2} a_{f_1} a_{f_2}$$

$$+ \sum_{l_1 l_2} \sum_{\substack{f_1 f_2 \\ f_1' f_2'}} \sum_\lambda \left(\frac{i}{\hbar}\right) \frac{1}{z - e_h - e_\lambda + e_{f_1} + e_{f_2}} a_{l_2}^\dagger a_{l_1}^\dagger \Phi_{l_1 l_2 \lambda h}$$

$$\times \left(\frac{i}{\hbar}\right) \frac{(1 \pm n_\lambda \pm n_h)}{z - e_h - e_\lambda + e_{f_1'} + e_{f_2'}} \Phi_{\lambda k f_1' f_2'} \left(-\frac{i}{\hbar}\right) \frac{\left(1 \pm n_{f_1'} \pm n_{f_2'}\right)}{z - e_{l_1} - e_{l_2} + e_{f_1'} + e_{f_2'}} \Phi_{f_1' f_2' f_1 f_2} a_{f_1} a_{f_2}.$$

Up to third order we thus obtain the result

$$
\begin{aligned}
&\mathcal{A}^1_{hk}+\mathcal{A}^2_{hk}+\mathcal{A}^3_{hk}= \\
&\quad \sum_{l_1 l_2}\sum_{\lambda}\left(\frac{i}{\hbar}\right)\frac{1}{z-e_{l_1}-e_{l_2}+e_\lambda+e_k}a^\dagger_{l_2}a^\dagger_{l_1} \\
&\quad \times\Bigg[\Phi_{l_1 l_2 \lambda h}+\left(\frac{i}{\hbar}\right)\sum_{l'_1 l'_2}\Phi_{l_1 l_2 l'_1 l'_2}\frac{\left(1\pm n_{l'_1}\pm n_{l'_2}\right)}{z-e_{l'_1}-e_{l'_2}+e_\lambda+e_k}\Phi_{l'_1 l'_2 \lambda h} \\
&\qquad +\left(\frac{i}{\hbar}\right)^2\sum_{\substack{l'_1 l'_2\\ l''_1 l''_2}}\Phi_{l_1 l_2 l''_1 l''_2}\frac{\left(1\pm n_{l''_1}\pm n_{l''_2}\right)}{z-e_{l''_1}-e_{l''_2}+e_\lambda+e_k}\Phi_{l''_1 l''_2 c l'_1 l'_2}\frac{\left(1\pm n_{l'_1}\pm n_{l'_2}\right)}{z-e_{l'_1}-e_{l'_2}+e_\lambda+e_k}\Phi_{l'_1 l'_2 \lambda h}\Bigg]a_\lambda a_k \\
&+\sum_{f_1 f_2}\sum_{\lambda}\left(-\frac{i}{\hbar}\right)\frac{1}{z-e_h-e_\lambda+e_{f_1}+e_{f_2}}a^\dagger_h a^\dagger_\lambda \\
&\quad \times\Bigg[\Phi_{\lambda k f_1 f_2}+\left(-\frac{i}{\hbar}\right)\sum_{f'_1 f'_2}\Phi_{\lambda k f'_1 f'_2}\frac{\left(1\pm n_{f'_1}\pm n_{f'_2}\right)}{z-e_h-e_\lambda+e_{f'_1}+e_{f'_2}}\Phi_{f'_1 f'_2 f_1 f_2} \\
&\qquad +\left(-\frac{i}{\hbar}\right)^2\sum_{\substack{f'_1 f'_2\\ f''_1 f''_2}}\Phi_{\lambda k f'_1 f'_2}\frac{\left(1\pm n_{f'_1}\pm n_{f'_2}\right)}{z-e_h-e_\lambda+e_{f'_1}+e_{f'_2}}\Phi_{f'_1 f'_2 f''_1 f''_2}\frac{\left(1\pm n_{f''_1}\pm n_{f''_2}\right)}{z-e_h-e_\lambda+e_{f''_1}+e_{f''_2}}\Phi_{f''_1 f''_2 \lambda h}\Bigg]a_{f_1}a_{f_2} \\
&+\sum_{l_1 l_2}\sum_{f_1 f_2}\sum_{\lambda}\left(\frac{i}{\hbar}\right)\frac{1}{z-e_{l_1}-e_{l_2}+e_{f_1}+e_{f_2}}a^\dagger_{l_2}a^\dagger_{l_1} \\
&\quad \times\Phi_{l_1 l_2 \lambda h}\left[\left(-\frac{i}{\hbar}\right)\frac{(1\pm n_\lambda\pm n_k)}{z-e_{l_1}-e_{l_2}+e_\lambda+e_k}-\left(\frac{i}{\hbar}\right)\frac{(1\pm n_\lambda\pm n_h)}{z-e_h-e_\lambda+e_{f_1}+e_{f_2}}\right]\Phi_{\lambda k f_1 f_2}a_{f_1}a_{f_2} \\
&+\sum_{\substack{l_1 l_2\\ l'_1 l'_2}}\sum_{f_1 f_2}\sum_{\lambda}\left(\frac{i}{\hbar}\right)\frac{1}{z-e_{l_1}-e_{l_2}+e_{f_1}+e_{f_2}}a^\dagger_{l_2}a^\dagger_{l_1}\Phi_{l_1 l_2 l'_1 l'_2}\left(\frac{i}{\hbar}\right)\frac{\left(1\pm n_{l'_1}\pm n_{l'_2}\right)}{z-e_{l'_1}-e_{l'_2}+e_{f_1}+e_{f_2}} \\
&\quad \times\Phi_{l'_1 l'_2 \lambda h}\left[\left(-\frac{i}{\hbar}\right)\frac{(1\pm n_\lambda\pm n_k)}{z-e_{l_1}-e_{l_2}+e_\lambda+e_k}-\left(\frac{i}{\hbar}\right)\frac{(1\pm n_\lambda\pm n_h)}{z-e_h-e_\lambda+e_{f_1}+e_{f_2}}\right]\Phi_{\lambda k f_1 f_2}a_{f_1}a_{f_2} \\
&+\sum_{l_1 l_2}\sum_{\substack{f_1 f_2\\ f'_1 f'_2}}\sum_{\lambda}\left(\frac{i}{\hbar}\right)\frac{1}{z-e_{l_1}-e_{l_2}+e_{f_1}+e_{f_2}}a^\dagger_{l_2}a^\dagger_{l_1}
\end{aligned}
$$

$$\times\, \Phi_{l_1 l_2 \lambda h} \left[\left(-\frac{i}{\hbar}\right) \frac{(1 \pm n_\lambda \pm n_k)}{z - e_{l_1} - e_{l_2} + e_\lambda + e_k} - \left(\frac{i}{\hbar}\right) \frac{(1 \pm n_\lambda \pm n_h)}{z - e_h - e_\lambda + e_{f_1} + e_{f_2}} \right] \Phi_{\lambda k f_1' f_2'}$$

$$\times \left(-\frac{i}{\hbar}\right) \frac{\left(1 \pm n_{f_1'} \pm n_{f_2'}\right)}{z - e_{l_1} - e_{l_2} + e_{f_1'} + e_{f_2'}} \Phi_{f_1' f_2' f_1 f_2} a_{f_1} a_{f_2}$$

$$+ \frac{i}{\hbar} \sum_{l_1 l_2} \sum_{f_1 f_2} a^\dagger_{l_2} a^\dagger_{l_1} F^{hk}_{l_1 l_2 f_1 f_2}(z) a_{f_1} a_{f_2},$$

where $F^{hk}_{l_1 l_2 f_1 f_2}(z)$ is an expression which is not singular in $(e_{l_1} + e_{l_2} - e_{f_1} - e_{f_2})$. One can check that the same mechanism holds also at higher perturbation orders, even though a precise formal proof of this fact is still under study, so that the following relevant operator expressions come into evidence

$$\langle \lambda k \left| t(E_h + E_\lambda + i\hbar z) \right| f_1 f_2 \rangle \tag{5.3.11}$$

$$= \langle \lambda k |\Phi| f_1 f_2 \rangle + \sum_{f_1' f_2'} \langle \lambda k |\Phi| f_1' f_2' \rangle \frac{\left(1 \pm n_{f_1'} \pm n_{f_2'}\right)}{E_h + E_\lambda - E_{f_1'} - E_{f_2'} + i\hbar z} \langle f_1' f_2' |\Phi| f_1 f_2 \rangle$$

$$+ \sum_{\substack{f_1' f_2' \\ f_1'' f_2''}} \langle \lambda k |\Phi| f_1' f_2' \rangle \frac{\left(1 \pm n_{f_1'} \pm n_{f_2'}\right)}{E_h + E_\lambda - E_{f_1'} - E_{f_2'} + i\hbar z} \langle f_1' f_2' |\Phi| f_1'' f_2'' \rangle$$

$$\times \frac{\left(1 \pm n_{f_1''} \pm n_{f_2''}\right)}{E_h + E_\lambda - E_{f_1''} - E_{f_2''} + i\hbar z} \langle f_1'' f_2'' |\Phi| f_1 f_2 \rangle + \ldots$$

$$= \Phi_{\lambda k f_1 f_2} + \sum_{f_1' f_2'} \Phi_{\lambda k f_1' f_2'} \left(-\frac{i}{\hbar}\right) \frac{\left(1 \pm n_{f_1'} \pm n_{f_2'}\right)}{z - e_h - e_\lambda + e_{f_1'} + e_{f_2'}} \Phi_{f_1' f_2' f_1 f_2}$$

$$+ \sum_{\substack{f_1' f_2' \\ f_1'' f_2''}} \Phi_{\lambda k f_1' f_2'} \left(-\frac{i}{\hbar}\right) \frac{\left(1 \pm n_{f_1'} \pm n_{f_2'}\right)}{z - e_h - e_\lambda + e_{f_1'} + e_{f_2'}} \Phi_{f_1' f_2' f_1'' f_2''}$$

$$\times \left(-\frac{i}{\hbar}\right) \frac{\left(1 \pm n_{f_1''} \pm n_{f_2''}\right)}{z - e_h - e_\lambda + e_{f_1''} + e_{f_2''}} \Phi_{f_1'' f_2'' f_1 f_2} + \ldots$$

and setting $t^\dagger(z) \equiv [t(z)]^\dagger$ we have

$$\langle l_1 l_2 \left| t^\dagger(E_k + E_\lambda + i\hbar z^*) \right| \lambda h \rangle \tag{5.3.12}$$

$$
\begin{aligned}
&= \langle l_1 l_2 |\Phi| \lambda h\rangle + \sum_{l_1' l_2'} \langle l_1 l_2 |\Phi| l_1' l_2'\rangle \frac{\left(1 \pm n_{l_1'} \pm n_{l_2'}\right)}{E_k + E_\lambda - E_{l_1'} - E_{l_2'} - i\hbar z} \langle l_1' l_2' |\Phi| \lambda h\rangle \\
&\quad + \sum_{\substack{l_1' l_2' \\ l_1'' l_2''}} \langle l_1 l_2 |\Phi| l_1'' l_2''\rangle \frac{\left(1 \pm n_{l_1''} \pm n_{l_2''}\right)}{E_k + E_\lambda - E_{l_1''} - E_{l_2''} - i\hbar z} \\
&\qquad \times \langle l_1'' l_2'' |\Phi| l_1' l_2'\rangle \frac{\left(1 \pm n_{l_1'} \pm n_{l_2'}\right)}{E_k + E_\lambda - E_{l_1'} - E_{l_2'} - i\hbar z} \langle l_1' l_2' |\Phi| \lambda h\rangle + \dots \\
&= \Phi_{l_1 l_2 \lambda h} + \sum_{l_1' l_2'} \Phi_{l_1 l_2 l_1' l_2'} \left(\frac{i}{\hbar}\right) \frac{\left(1 \pm n_{l_1'} \pm n_{l_2'}\right)}{z - e_{l_1'} - e_{l_2'} + e_\lambda + e_k} \Phi_{l_1' l_2' \lambda h} \\
&\quad + \sum_{\substack{l_1' l_2' \\ l_1'' l_2''}} \Phi_{l_1 l_2 l_1'' l_2''} \frac{\left(1 \pm n_{l_1''} \pm n_{l_2''}\right)}{z - e_{l_1''} - e_{l_2''} + e_\lambda + e_k} \Phi_{l_1'' l_2'' l_1' l_2'} \\
&\qquad \times \left(\frac{i}{\hbar}\right) \frac{\left(1 \pm n_{l_1'} \pm n_{l_2'}\right)}{z - e_{l_1'} - e_{l_2'} + e_\lambda + e_k} \Phi_{l_1' l_2' \lambda h} + \dots
\end{aligned}
$$

corresponding to the matrix elements of a two-particle scattering operator, bearing Pauli-principle corrections of the form $(1 \pm n_{l_1} \pm n_{l_2})$ and therefore operator valued, even though this makes no problem for the definition of $t(z)$, since for all l_1, l_2 these statistical corrections commute. The final result obtained resumming the whole perturbation series is then

$$
\begin{aligned}
\sum_{n=1}^{\infty} \mathcal{A}_{hk}^n \quad = \quad & + \sum_{l_1 l_2} \sum_{\lambda} \left(\frac{i}{\hbar}\right) \frac{1}{z - e_{l_1} - e_{l_2} + e_\lambda + e_k} a_{l_2}^\dagger a_{l_1}^\dagger \langle l_1 l_2 |t^\dagger(E_k + E_\lambda + i\hbar z^*)| \lambda h\rangle a_\lambda a_k \\
& + \sum_{f_1 f_2} \sum_{\lambda} \left(-\frac{i}{\hbar}\right) \frac{1}{z - e_h - e_\lambda + e_{f_1} + e_{f_2}} a_h^\dagger a_\lambda^\dagger \langle \lambda k |t(E_h + E_\lambda + i\hbar z)| f_1 f_2\rangle a_{f_1} a_{f_2} \\
& + \sum_{l_1 l_2} \sum_{f_1 f_2} \sum_{\lambda} \left(\frac{i}{\hbar}\right) \frac{1}{z - e_{l_1} - e_{l_2} + e_{f_1} + e_{f_2}} a_{l_2}^\dagger a_{l_1}^\dagger \langle l_1 l_2 |t^\dagger(E_{f_1} + E_{f_2} + i\hbar z^*)| \lambda h\rangle \\
& \qquad \times \left[\frac{(1 \pm n_\lambda \pm n_k)}{E_{l_1} + E_{l_2} - E_\lambda - E_k + i\hbar z} + \frac{(1 \pm n_\lambda \pm n_h)}{E_h + E_\lambda - E_{f_1} - E_{f_2} + i\hbar z}\right] \\
& \qquad \times \langle \lambda k |t(E_{l_1} + E_{l_2} + i\hbar z)| f_1 f_2\rangle a_{f_1} a_{f_2} \\
& + \frac{i}{\hbar} \sum_{l_1 l_2} \sum_{f_1 f_2} a_{l_2}^\dagger a_{l_1}^\dagger F_{l_1 l_2 f_1 f_2}^{hk}(z) a_{f_1} a_{f_2},
\end{aligned}
\tag{5.3.13}
$$

where $F^{hk}_{l_1 l_2 f_1 f_2}(z)$ is again an expression which is not singular for $z = e_{l_1} + e_{l_2} - e_{f_1} - e_{f_2}$. In order to make our expressions somehow more compact we introduce the notation

$$S^{hk}_{l_1 l_2 f_1 f_2}(z) = \sum_\lambda \langle l_1 l_2 | t^\dagger (E_{f_1} + E_{f_2} + i\hbar z^*) | \lambda h \rangle$$

$$\left[\frac{(1 \pm n_\lambda \pm n_k)}{E_{l_1} + E_{l_2} - E_\lambda - E_k + i\hbar z} + \frac{(1 \pm n_\lambda \pm n_h)}{E_h + E_\lambda - E_{f_1} - E_{f_2} + i\hbar z} \right] \langle \lambda k | t(E_{l_1} + E_{l_2} + i\hbar z) | f_1 f_2 \rangle .$$

We are now in the position to evaluate $\mathcal{U}'(t)\,(a^\dagger_h a_k)$ making use of (5.3.4) and (5.3.13)

$$\mathcal{U}'(t)\,(a^\dagger_h a_k) = e^{(e_h - e_k)t} a^\dagger_h a_k + \int_{-i\infty+\eta}^{+i\infty+\eta} \frac{dz}{2\pi i}\, e^{zt} \tag{5.3.14}$$

$$\Bigg\{ + \frac{i}{\hbar} \sum_{l_1 l_2} \sum_\lambda \frac{1}{z - e_h + e_k} \frac{1}{z - e_{l_1} - e_{l_2} + e_\lambda + e_k} a^\dagger_{l_2} a^\dagger_{l_1} \langle l_1 l_2 | t^\dagger (E_k + E_\lambda + i\hbar z^*) | \lambda h \rangle a_\lambda a_k$$

$$- \frac{i}{\hbar} \sum_{f_1 f_2} \sum_\lambda \frac{1}{z - e_h + e_k} \frac{1}{z - e_h - e_\lambda + e_{f_1} + e_{f_2}} a^\dagger_h a^\dagger_\lambda \langle \lambda k | t(E_h + E_\lambda + i\hbar z) | f_1 f_2 \rangle a_{f_1} a_{f_2}$$

$$+ \frac{i}{\hbar} \sum_{l_1 l_2} \sum_{f_1 f_2} \frac{1}{z - e_h + e_k} \frac{1}{z - e_{l_1} - e_{l_2} + e_{f_1} + e_{f_2}} a^\dagger_{l_2} a^\dagger_{l_1} S^{hk}_{l_1 l_2 f_1 f_2}(z) a_{f_1} a_{f_2}$$

$$+ \frac{i}{\hbar} \sum_{l_1 l_2} \sum_{f_1 f_2} \frac{1}{z - e_h + e_k} a^\dagger_{l_2} a^\dagger_{l_1} F^{hk}_{l_1 l_2 f_1 f_2}(z) a_{f_1} a_{f_2} \Bigg\} .$$

Let us note that the contributions apart from the last one, which will prove to be not relevant, in (5.3.14) may be obtained simply setting for the scattering map in (5.3.2)

$$\begin{aligned} \mathcal{T}(z)\,[a^\dagger_h a_k] \quad = \quad & + \frac{i}{\hbar} \sum_{l_1 l_2} \sum_\lambda a^\dagger_{l_2} a^\dagger_{l_1} \langle l_1 l_2 | t^\dagger (E_k + E_\lambda + i\hbar z^*) | \lambda h \rangle a_\lambda a_k \\ & - \frac{i}{\hbar} \sum_{f_1 f_2} \sum_\lambda a^\dagger_h a^\dagger_\lambda \langle \lambda k | t(E_h + E_\lambda + i\hbar z) | f_1 f_2 \rangle a_{f_1} a_{f_2} \\ & + \frac{i}{\hbar} \sum_{l_1 l_2} \sum_{f_1 f_2} a^\dagger_{l_2} a^\dagger_{l_1} S^{hk}_{l_1 l_2 f_1 f_2}(z) a_{f_1} a_{f_2}, \end{aligned}$$

so that

$$(z - \mathcal{H}'_0)^{-1} \mathcal{T}(z) (z - \mathcal{H}'_0)^{-1}\, [a^\dagger_h a_k] =$$

$$+ \frac{i}{\hbar} \sum_{l_1 l_2} \sum_\lambda \frac{1}{z - e_h + e_k} \frac{1}{z - e_{l_1} - e_{l_2} + e_\lambda + e_k} a^\dagger_{l_2} a^\dagger_{l_1} \langle l_1 l_2 | t^\dagger (E_k + E_\lambda + i\hbar z^*) | \lambda h \rangle a_\lambda a_k$$

$$- \frac{i}{\hbar} \sum_{f_1 f_2} \sum_{\lambda} \frac{1}{z - e_h + e_k} \frac{1}{z - e_h - e_\lambda + e_{f_1} + e_{f_2}} a_h^\dagger a_\lambda^\dagger \left\langle \lambda k \left| t(E_h + E_\lambda + i\hbar z) \right| f_1 f_2 \right\rangle a_{f_1} a_{f_2}$$

$$+ \frac{i}{\hbar} \sum_{l_1 l_2} \sum_{f_1 f_2} \frac{1}{z - e_h + e_k} \frac{1}{z - e_{l_1} - e_{l_2} + e_{f_1} + e_{f_2}} a_{l_2}^\dagger a_{l_1}^\dagger S_{l_1 l_2 f_1 f_2}^{hk}(z) a_{f_1} a_{f_2}.$$

We now have to evaluate the contribution of the different poles to (5.3.14), assuming for simplicity that no bound states between the molecules can be formed. Then the time scale is introduced by the following modifications. The scattering map $\mathcal{T}(z)$ is replaced by $\mathcal{T}\left(z + \frac{\varepsilon}{\hbar}\right)$, with $\varepsilon \approx \frac{\hbar}{\tau_0}$, τ_0 being of the order of the collision time. So that (5.3.14) becomes

$$\mathcal{U}'(t)\left(a_h^\dagger a_k\right) = e^{(e_h - e_k)t} a_h^\dagger a_k + \int_{-i\infty+\eta}^{+i\infty+\eta} \frac{dz}{2\pi i} e^{zt}$$

$$\left\{ + \frac{i}{\hbar} \sum_{l_1 l_2} \sum_{\lambda} \frac{1}{z - e_h + e_k} \frac{1}{z - e_{l_1} - e_{l_2} + e_\lambda + e_k} a_{l_2}^\dagger a_{l_1}^\dagger \left\langle l_1 l_2 \left| t^\dagger(E_k + E_\lambda + i\hbar z^* + i\varepsilon) \right| \lambda h \right\rangle a_\lambda a_k \right.$$

$$- \frac{i}{\hbar} \sum_{f_1 f_2} \sum_{\lambda} \frac{1}{z - e_h + e_k} \frac{1}{z - e_h - e_\lambda + e_{f_1} + e_{f_2}} a_h^\dagger a_\lambda^\dagger \left\langle \lambda k \left| t(E_h + E_\lambda + i\hbar z + i\varepsilon) \right| f_1 f_2 \right\rangle a_{f_1} a_{f_2}$$

$$+ \frac{i}{\hbar} \sum_{l_1 l_2} \sum_{f_1 f_2} \frac{1}{z - e_h + e_k} \frac{1}{z - e_{l_1} - e_{l_2} + e_{f_1} + e_{f_2}} a_{l_2}^\dagger a_{l_1}^\dagger S_{l_1 l_2 f_1 f_2}^{hk}\left(z + \frac{\varepsilon}{\hbar}\right) a_{f_1} a_{f_2}$$

$$\left. + \frac{i}{\hbar} \sum_{l_1 l_2} \sum_{f_1 f_2} \frac{1}{z - e_h + e_k} a_{l_2}^\dagger a_{l_1}^\dagger F_{l_1 l_2 f_1 f_2}^{hk}\left(z + \frac{\varepsilon}{\hbar}\right) a_{f_1} a_{f_2} \right\}.$$

Final results for expectations of the relevant variables, having a typical variation time $\tau_1 \gg \tau_0$ are practically independent on ε; ε dependence would mean dependence on the distribution of the huge set of poles that $\mathcal{T}(z)$ has on the imaginary axis, which in turn is related to the confinement of the system, only roughly represented by the boundary conditions we assumed in (5.2.1). So ε dependence is more an artifact of the idealized confinement, rather than a physical feature. For a finite confined system this treatment unavoidably relies on an approximation. The situation can be improved considering the limit of no confinement: then the set of poles of $\mathcal{T}\left(z + \frac{\varepsilon}{\hbar}\right)$ becomes a continuum and its matrix elements become analytic functions for $\operatorname{Re} z > -\varepsilon$, having a cut on the imaginary axis, and the existence of the limit $\delta \to 0$ (δ being the typical spacing between the poles) can be reasonably assumed. The analytic continuation across the cut can be considered and one can assume that the singularities of this continuation are located in the left half-plane far enough from the imaginary axis to give contributions that rapidly decay for $\tau \gg \tau_0$, thus providing the precise reason that makes the previously considered terms indeed negligible. We therefore consider only the poles relative to $(z - \mathcal{H}_0')^{-1}$. Due to (5.3.16) the term with $F_{l_1 l_2 f_1 f_2}^{hk}(z)$ gives no contribution to the dynamics on this time scale, and will be therefore neglected. It could be relevant if, due to the existence of bound states, poles of $\mathcal{T}(z)$ should also be taken into account. Of course this analysis might be refined, allowing to treat more general physical situations. We have an expression of the form

$$I(\alpha,\beta)=\oint \frac{dz}{2\pi i}e^{zt}\frac{1}{z-\beta}\frac{1}{z-\alpha}f(z)$$

where β equals (e_h-e_k), while α equals either $(e_{l_1}+e_{l_2}-e_k-e_\lambda)$ or $(e_h+e_\lambda-e_{f_1}-e_{f_2})$ or $(e_{l_1}+e_{l_2}-e_{f_1}-e_{f_2})$, and the poles of $f(z)$ are suppose to give no contribution. The expression is symmetric in α and β and may be written

$$I(\alpha,\beta)=\frac{e^{\alpha t}f(\alpha)-e^{\beta t}f(\beta)}{\alpha-\beta}, \tag{5.3.15}$$

but since we are considering variables with suitably slowly varying expectations, on the considered time scale t, which is much longer than typical microphysical interaction times, but still much shorter than the macrophysical variation time of the relevant observables, we have

$$|e_h-e_k|t\ll 1, \qquad |e_{l_1}+e_{l_2}-e_{f_1}-e_{f_2}|t\ll 1. \tag{5.3.16}$$

Exploiting (5.3.16) and analogous relations, we can expand the exponentials in (5.3.15), thus obtaining, up to the linear term in t

$$I(\alpha,\beta)=\frac{f(\alpha)-f(\beta)}{\alpha-\beta}+t\frac{\alpha f(\alpha)-\beta f(\beta)}{\alpha-\beta},$$

that is to say

$$\mathcal{U}'(t)\,(a^\dagger_h a_k)=a^\dagger_h a_k+\frac{i}{\hbar}t(e_h-e_k)a^\dagger_h a_k$$

$$+\frac{i}{\hbar}t\sum_{l_1l_2}\sum_{\lambda}\frac{1}{e_{l_1}+e_{l_2}-e_h-e_\lambda}a^\dagger_{l_2}a^\dagger_{l_1}\left[(e_{l_1}+e_{l_2}-e_k-e_\lambda)\left\langle l_1l_2\left|t^\dagger(E_{l_1}+E_{l_2}+i\varepsilon)\right|\lambda h\right\rangle\right.$$

$$\left.-(e_h-e_k)\left\langle l_1l_2\left|t^\dagger(E_h+E_\lambda+i\varepsilon)\right|\lambda h\right\rangle\right]a_\lambda a_k$$

$$-\frac{i}{\hbar}t\sum_{f_1f_2}\sum_{\lambda}\frac{1}{e_k+e_\lambda-e_{f_1}-e_{f_2}}a^\dagger_h a^\dagger_\lambda\left[(e_h+e_\lambda-e_{f_1}-e_{f_2})\left\langle\lambda k\left|t(E_{f_1}+E_{f_2}+i\varepsilon)\right|f_1f_2\right\rangle\right.$$

$$\left.-(e_h-e_k)\left\langle\lambda k\left|t(E_k+E_\lambda+i\varepsilon)\right|f_1f_2\right\rangle\right]a_{f_1}a_{f_2}$$

$$+\frac{i}{\hbar}t\sum_{l_1l_2}\sum_{f_1f_2}\frac{1}{e_{l_1}+e_{l_2}+e_k-e_{f_1}-e_{f_2}-e_h}a^\dagger_{l_2}a^\dagger_{l_1}$$

$$\left[(e_{l_1}+e_{l_2}-e_{f_1}-e_{f_2})S^{hk}_{l_1l_2f_1f_2}\left(e_{l_1}+e_{l_2}-e_{f_1}-e_{f_2}+\frac{\varepsilon}{\hbar}\right)\right.$$

$$- (e_h - e_k) S^{hk}_{l_1 l_2 f_1 f_2} \left(e_h - e_k + \frac{\varepsilon}{\hbar} \right) \Bigg] a_{f_1} a_{f_2}$$

$$+ \frac{i}{\hbar} \sum_{l_1 l_2} \sum_{\lambda} a^\dagger_{l_2} a^\dagger_{l_1} \frac{\langle l_1 l_2 \,| [t^\dagger (E_{l_1} + E_{l_2} + i\varepsilon) - t^\dagger (E_h + E_\lambda + i\varepsilon)] |\, \lambda h \rangle}{\frac{i}{\hbar} [(E_{l_1} + E_{l_2} + i\varepsilon) - (E_h + E_\lambda + i\varepsilon)]} a_\lambda a_k$$

$$- \frac{i}{\hbar} \sum_{f_1 f_2} \sum_{\lambda} a^\dagger_h a^\dagger_\lambda \frac{\langle \lambda k \,| [t (E_{f_1} + E_{f_2} + i\varepsilon) - t (E_k + E_\lambda + i\varepsilon)] |\, f_1 f_2 \rangle}{-\frac{i}{\hbar} [(E_{f_1} + E_{f_2} + i\varepsilon) - (E_k + E_\lambda + i\varepsilon)]} a_{f_1} a_{f_2}$$

$$+ \frac{i}{\hbar} \sum_{l_1 l_2} \sum_{f_1 f_2} e^{(e_h - e_k)t} a^\dagger_{l_2} a^\dagger_{l_1} \frac{S^{hk}_{l_1 l_2 f_1 f_2} \left(e_{l_1} + e_{l_2} - e_{f_1} - e_{f_2} + \frac{\varepsilon}{\hbar} \right) - S^{hk}_{l_1 l_2 f_1 f_2} \left(e_h - e_k + \frac{\varepsilon}{\hbar} \right)}{\left(e_{l_1} + e_{l_2} - e_{f_1} - e_{f_2} - \frac{\varepsilon}{\hbar} \right) - \left(e_h - e_k + \frac{\varepsilon}{\hbar} \right)} a_{f_1} a_{f_2}.$$

Keeping the slow energy dependence of $\mathcal{T}(z)$ into account we also have

$$\left| \frac{\langle g f \,| t (E_g + E_f + i\varepsilon) |\, r s \rangle - \langle g f \,| t (E_r + E_s + i\varepsilon) |\, r s \rangle}{(E_g + E_f) - (E_r + E_s)} \right| \approx \tau_0 |\langle g f | t (E_g + E_f + i\varepsilon) | r s \rangle|,$$

so that we may leave out the constant terms, not contributing to the time evolution. It may also be checked that these terms do not spoil particle number conservation (see Sect. 5.3.2). We are thus left with

$$\mathcal{U}'(t)\, (a^\dagger_h a_k) = a^\dagger_h a_k + \frac{i}{\hbar} t (e_h - e_k) a^\dagger_h a_k \tag{5.3.17}$$

$$+ \frac{i}{\hbar} t \sum_{l_1 l_2} \sum_{\lambda} \frac{1}{e_{l_1} + e_{l_2} - e_h - e_\lambda} a^\dagger_{l_2} a^\dagger_{l_1} \left[(e_{l_1} + e_{l_2} - e_k - e_\lambda) \langle l_1 l_2 \,| t^\dagger (E_{l_1} + E_{l_2} + i\varepsilon) |\, \lambda h \rangle \right.$$

$$\left. - (e_h - e_k) \langle l_1 l_2 \,| t^\dagger (E_h + E_\lambda + i\varepsilon) |\, \lambda h \rangle \right] a_\lambda a_k$$

$$- \frac{i}{\hbar} t \sum_{f_1 f_2} \sum_{\lambda} \frac{1}{e_k + e_\lambda - e_{f_1} - e_{f_2}} a^\dagger_h a^\dagger_\lambda \left[(e_h + e_\lambda - e_{f_1} - e_{f_2}) \langle \lambda k \,| t (E_{f_1} + E_{f_2} + i\varepsilon) |\, f_1 f_2 \rangle \right.$$

$$\left. - (e_h - e_k) \langle \lambda k \,| t (E_k + E_\lambda + i\varepsilon) |\, f_1 f_2 \rangle \right] a_{f_1} a_{f_2}$$

$$+ \frac{i}{\hbar} t \sum_{l_1 l_2} \sum_{f_1 f_2} \frac{1}{e_{l_1} + e_{l_2} + e_k - e_{f_1} - e_{f_2} - e_h} a^\dagger_{l_2} a^\dagger_{l_1}$$

$$\left[(e_{l_1} + e_{l_2} - e_{f_1} - e_{f_2}) S^{hk}_{l_1 l_2 f_1 f_2} \left(e_{l_1} + e_{l_2} - e_{f_1} - e_{f_2} + \frac{\varepsilon}{\hbar} \right) \right.$$

$$\left. - (e_h - e_k) S^{hk}_{l_1 l_2 f_1 f_2} \left(e_h - e_k + \frac{\varepsilon}{\hbar} \right) \right] a_{f_1} a_{f_2}.$$

The asymptotic form of $\mathcal{U}'(t)\, (a^\dagger_h a_k)$ thus obtained, however, does not have the typical structure of a completely positive mapping, as the one we obtained in Chap. 3 for the microsystem. The relevance of the completely positive property in the case of one-particle quantum mechanics, which accounts for the generality of the Lindblad structure, seems to suggest that a similar property could be important also in more general physical situations. In fact the terms spoiling a generalized completely positive structure in (5.3.17) are exactly those expressions which become null in the homogeneous case. Considering slowly varying, that is to say quasi-diagonal, quantities, it seems quite natural to keep, instead of the symmetric choice (5.3.17), the contribution relevant in the quasi-diagonal case, that is to say $tf(\alpha)$

$$
\begin{aligned}
\mathcal{U}'(t)\left(a_h^\dagger a_k\right) = {} & + a_h^\dagger a_k + \frac{i}{\hbar} t (E_h - E_k) a_h^\dagger a_k \\
& + \frac{i}{\hbar} t \sum_{l_1 l_2} \sum_{\lambda} a_{l_2}^\dagger a_{l_1}^\dagger \left\langle l_1 l_2 \left| t^\dagger (E_{l_1} + E_{l_2} + i\varepsilon) \right| \lambda h \right\rangle a_\lambda a_k \\
& - \frac{i}{\hbar} t \sum_{f_1 f_2} \sum_{\lambda} a_h^\dagger a_\lambda^\dagger \left\langle \lambda k \left| t (E_{f_1} + E_{f_2} + i\varepsilon) \right| f_1 f_2 \right\rangle a_{f_1} a_{f_2} \\
& + \frac{i}{\hbar} t \sum_{l_1 l_2} \sum_{f_1 f_2} \sum_{\lambda} a_{l_2}^\dagger a_{l_1}^\dagger \left\langle l_1 l_2 \left| t^\dagger (E_{l_1} + E_{l_2} + i\varepsilon) \right| \lambda h \right\rangle \\
& \times \left[\frac{(1 \pm n_\lambda \pm n_k)}{E_{f_1} + E_{f_2} - E_\lambda - E_k + i\varepsilon} - \frac{(1 \pm n_\lambda \pm n_h)}{E_{l_1} + E_{l_2} - E_h - E_\lambda - i\varepsilon} \right] \\
& \times \left\langle \lambda k \left| t (E_{f_1} + E_{f_2} + i\varepsilon) \right| f_1 f_2 \right\rangle a_{f_1} a_{f_2} .
\end{aligned}
\tag{5.3.18}
$$

5.3.2 Particle Number Conservation

Now that we have obtained the desired expression for the time evolution of the field operators $a_h^\dagger a_k$ we want to check the fact that the mapping thus obtained warrants particle number conservation, or equivalently mass conservation. This fact will provide us with a confirmation of the meaningfulness of the approximations used in order to introduce the time scale. Setting $N = \sum_g a_g^\dagger a_g$ we have

$$
\begin{aligned}
& \mathcal{U}'(t)(N) = N \\
& + \frac{i}{\hbar} t \sum_{l_1 l_2} \sum_{f_1 f_2} a_{l_2}^\dagger a_{l_1}^\dagger \left[\left\langle l_1 l_2 \left| t^\dagger (E_{l_1} + E_{l_2} + i\varepsilon) \right| f_1 f_2 \right\rangle - \left\langle l_1 l_2 \left| t (E_{f_1} + E_{f_2} + i\varepsilon) \right| f_1 f_2 \right\rangle \right] a_{f_1} a_{f_2} \\
& + \frac{i}{\hbar} t \sum_{l_1 l_2} \sum_{f_1 f_2} \sum_{\lambda_1 \lambda_2} a_{l_2}^\dagger a_{l_1}^\dagger \left\langle l_1 l_2 \left| t^\dagger (E_{l_1} + E_{l_2} + i\varepsilon) \right| \lambda_1 \lambda_2 \right\rangle \\
& \qquad \times \left[\frac{(1 \pm n_{\lambda_1} \pm n_{\lambda_2})}{E_{f_1} + E_{f_2} - E_{\lambda_1} - E_{\lambda_2} + i\varepsilon} - \frac{(1 \pm n_{\lambda_1} \pm n_{\lambda_2})}{E_{l_1} + E_{l_2} - E_{\lambda_1} - E_{\lambda_2} - i\varepsilon} \right] \\
& \qquad \times \left\langle \lambda_1 \lambda_2 \left| t (E_{f_1} + E_{f_2} + i\varepsilon) \right| f_1 f_2 \right\rangle a_{f_1} a_{f_2} .
\end{aligned}
\tag{5.3.19}
$$

We now come back to the definition of the $t(z)$ operator in (5.3.11). Setting $z_2 = (E_{f_1} + E_{f_2} + i\varepsilon)$ and defining the following operator potential

$$\langle l_1 l_2 |\Phi_{\rm R}| f_1 f_2\rangle \equiv \langle l_1 l_2 |\Phi| f_1 f_2\rangle (1 \pm n_{f_1} \pm n_{f_2}),$$

the subscript R recalling the fact that the statistical corrections are on the right, with reference to (5.3.11) we may write

$$\begin{aligned}\langle l_1 l_2 | t(z_2) | f_1 f_2\rangle &= \langle l_1 l_2 | \Phi + \Phi_{\rm R} \frac{1}{z_2 - H_0} \Phi + \Phi_{\rm R} \frac{1}{z_2 - H_0} \Phi_{\rm R} \frac{1}{z_2 - H_0} \Phi + \ldots | f_1 f_2\rangle \\ &\equiv \langle l_1 l_2 | \Phi + \Phi_{\rm R} \frac{1}{z_2 - H_0 - \Phi_{\rm R}} \Phi | f_1 f_2\rangle,\end{aligned}$$

where the operator $(z_2 - H_0 - \Phi_{\rm R})^{-1}$ is actually defined by the series given in this expression. On the same footing, setting $z_1 = (E_{l_1} + E_{l_2} - i\varepsilon)$ and recalling (5.3.12) we have

$$\begin{aligned}\langle l_1 l_2 | t^\dagger(z_1^*) | f_1 f_2\rangle &= \langle l_1 l_2 | \Phi + \Phi_{\rm R} \frac{1}{z_1 - H_0} \Phi + \Phi_{\rm R} \frac{1}{z_1 - H_0} \Phi_{\rm R} \frac{1}{z_1 - H_0} \Phi + \ldots | f_1 f_2\rangle \\ &\equiv \langle l_1 l_2 | \Phi + \Phi_{\rm R} \frac{1}{z_1 - H_0 - \Phi_{\rm R}} \Phi | f_1 f_2\rangle.\end{aligned}$$

Let us note that a fully equivalent analysis may be put forward in terms of the operator potential $\Phi_{\rm L}$ given by

$$\langle l_1 l_2 |\Phi_{\rm L}| f_1 f_2\rangle \equiv (1 \pm n_{l_1} \pm n_{l_2}) \langle l_1 l_2 |\Phi| f_1 f_2\rangle ,$$

that is to say formally the adjoint of $\Phi_{\rm R}$. We stress the fact that $\langle l_1 l_2 |\Phi_{\rm R}| f_1 f_2\rangle$ is not a c-number, but is operator valued in the Fock-space of the quantum Schrödinger field, diagonal in the basis created by the operators $\{a_g^\dagger\}$. Eq. (5.3.19) thus becomes

$$\begin{aligned}\mathcal{U}'(t)(N) &= N + \frac{i}{\hbar} t \sum_{l_1 l_2} \sum_{f_1 f_2} a_{l_2}^\dagger a_{l_1}^\dagger \langle l_1 l_2 | t^\dagger(z_1^*) - t(z_2) | f_1 f_2\rangle a_{f_1} a_{f_2} \\ &\quad + \frac{i}{\hbar} t \sum_{l_1 l_2} \sum_{f_1 f_2} \sum_{\lambda_1 \lambda_2} a_{l_2}^\dagger a_{l_1}^\dagger \langle l_1 l_2 | t^\dagger(z_1^*) | \lambda_1 \lambda_2\rangle (1 \pm n_{\lambda_1} \pm n_{\lambda_2}) \\ &\qquad \times \left(\frac{1}{z_2 - E_{\lambda_1} - E_{\lambda_2}} - \frac{1}{z_1 - E_{\lambda_1} - E_{\lambda_2}} \right) \langle \lambda_1 \lambda_2 | t(z_2) | f_1 f_2\rangle a_{f_1} a_{f_2} \\ &= N + \frac{i}{\hbar} t \sum_{l_1 l_2} \sum_{f_1 f_2} a_{l_2}^\dagger a_{l_1}^\dagger \langle l_1 l_2 | \left\{ \Phi_{\rm R} \frac{1}{z_1 - H_0 - \Phi_{\rm R}} \Phi - \Phi_{\rm R} \frac{1}{z_2 - H_0 - \Phi_{\rm R}} \Phi \right. \\ &\qquad + \left(\Phi_{\rm R} + \Phi_{\rm R} \frac{1}{z_1 - H_0 - \Phi_{\rm R}} \Phi_{\rm R} \right)\end{aligned}$$

$$\times \left(\frac{1}{z_2 - H_0} - \frac{1}{z_1 - H_0} \right)$$

$$\times \left(\Phi + \Phi_{\mathrm{R}} \frac{1}{z_2 - H_0 - \Phi_{\mathrm{R}}} \Phi \right) \Big\} |f_1 f_2\rangle a_{f_1} a_{f_2},$$

but exploiting the relations analogous to (5.3.3) for the resolvent series which defines $(z_2 - H_0 - \Phi_{\mathrm{R}})^{-1}$ we have

$$- \left[\Phi_{\mathrm{R}} \frac{1}{z_1 - H_0 - \Phi_{\mathrm{R}}} \Phi - \Phi_{\mathrm{R}} \frac{1}{z_2 - H_0 - \Phi_{\mathrm{R}}} \Phi \right] =$$

$$= \Phi_{\mathrm{R}} \frac{z_2 - z_1}{(z_1 - H_0 - \Phi_{\mathrm{R}})(z_2 - H_0 - \Phi_{\mathrm{R}})} \Phi$$

$$= (z_2 - z_1) \Phi_{\mathrm{R}} \left(\frac{1}{z_1 - H_0} + \frac{1}{z_1 - H_0 - \Phi_{\mathrm{R}}} \Phi_{\mathrm{R}} \frac{1}{z_1 - H_0} \right) \left(\frac{1}{z_2 - H_0} + \frac{1}{z_2 - H_0} \Phi_{\mathrm{R}} \frac{1}{z_2 - H_0 - \Phi_{\mathrm{R}}} \right) \Phi$$

$$= \left(\Phi_{\mathrm{R}} + \Phi_{\mathrm{R}} \frac{1}{z_1 - H_0 - \Phi_{\mathrm{R}}} \Phi_{\mathrm{R}} \right) \left(\frac{1}{z_2 - H_0} - \frac{1}{z_1 - H_0} \right) \left(\Phi + \Phi_{\mathrm{R}} \frac{1}{z_2 - H_0 - \Phi_{\mathrm{R}}} \Phi \right),$$

and therefore $\mathcal{U}'(N) = N$, that is particle number conservation.

5.3.3 Structure of the Generator

We can now read off from (5.3.18) the expression of the generator of the time evolution in Heisenberg picture $\mathcal{L}'$

$$\begin{aligned}
\mathcal{L}' \left(a_h^\dagger a_k \right) &= \frac{i}{\hbar} (E_h - E_k) a_h^\dagger a_k \\
&+ \frac{i}{\hbar} \sum_{l_1 l_2} \sum_{\lambda} a_{l_2}^\dagger a_{l_1}^\dagger \left\langle l_1 l_2 \left| t^\dagger (E_{l_1} + E_{l_2} + i\varepsilon) \right| \lambda h \right\rangle a_\lambda a_k \\
&- \frac{i}{\hbar} \sum_{f_1 f_2} \sum_{\lambda} a_h^\dagger a_\lambda^\dagger \left\langle \lambda k \left| t (E_{f_1} + E_{f_2} + i\varepsilon) \right| f_1 f_2 \right\rangle a_{f_1} a_{f_2} \\
&+ \frac{i}{\hbar} \sum_{l_1 l_2} \sum_{f_1 f_2} \sum_{\lambda} a_{l_2}^\dagger a_{l_1}^\dagger \left\langle l_1 l_2 \left| t^\dagger (E_{l_1} + E_{l_2} + i\varepsilon) \right| \lambda h \right\rangle \\
&\qquad \times \left[\frac{(1 \pm n_\lambda \pm n_k)}{E_{f_1} + E_{f_2} - E_\lambda - E_k + i\varepsilon} - \frac{(1 \pm n_\lambda \pm n_h)}{E_{l_1} + E_{l_2} - E_h - E_\lambda - i\varepsilon} \right] \\
&\qquad \times \left\langle \lambda k \left| t (E_{f_1} + E_{f_2} + i\varepsilon) \right| f_1 f_2 \right\rangle a_{f_1} a_{f_2}.
\end{aligned} \tag{5.3.20}$$

Considering in particular the contribution containing both $t(z)$ and $t^\dagger(z)$ we see that the expression between square brackets may be written in the form

$$\frac{2\varepsilon}{\hbar} \frac{1 \pm n_\lambda \pm \frac{1}{2}(n_h + n_k)}{(E_{f_1} + E_{f_2} - E_\lambda - E_k + i\varepsilon)(E_{l_1} + E_{l_2} - E_h - E_\lambda - i\varepsilon)}$$

$$+ \quad \frac{(1 \pm n_\lambda \pm n_k)(E_{l_1} + E_{l_2} - E_h - E_\lambda) - (1 \pm n_\lambda \pm n_h)(E_{f_1} + E_{f_2} - E_\lambda - E_k)}{(E_{f_1} + E_{f_2} - E_\lambda - E_k + i\varepsilon)(E_{l_1} + E_{l_2} - E_h - E_\lambda - i\varepsilon)}$$

and provided $|n_h - n_k| \ll 1$, $\varepsilon \gg |E_k - E_{f_1} - E_{f_2} - E_h + E_{l_1} + E_{l_2}|$ we can keep only the first contribution. Assuming small statistical corrections, so that

$$1 \pm n_\lambda \pm \frac{1}{2}(n_h + n_k) \approx \sqrt{(1 \pm n_\lambda \pm n_h)}\sqrt{(1 \pm n_\lambda \pm n_k)}$$

the last term of (5.3.20) assumes the following factorized form

$$\frac{2\varepsilon}{\hbar} \sum_{l_1 l_2} \sum_{f_1 f_2} a^\dagger_{l_2} a^\dagger_{l_1} \frac{\langle l_1 l_2 | t^\dagger (E_{l_1} + E_{l_2} + i\varepsilon) | \lambda h \rangle}{E_{l_1} + E_{l_2} - E_h - E_\lambda - i\varepsilon} \sqrt{(1 \pm n_\lambda \pm n_h)}$$

$$\sqrt{(1 \pm n_\lambda \pm n_k)} \frac{\langle \lambda k | t(E_{f_1} + E_{f_2} + i\varepsilon) | f_1 f_2 \rangle}{E_{f_1} + E_{f_2} - E_\lambda - E_k + i\varepsilon} a_{f_1} a_{f_2}.$$

In strict analogy with (3.2.22) we introduce the operators

$$T^{[2]} = \frac{1}{2} \sum_{l_1 l_2} \sum_{f_1 f_2} a^\dagger_{l_2} a^\dagger_{l_1} \langle l_1 l_2 | t(E_{f_1} + E_{f_2} + i\varepsilon) | f_1 f_2 \rangle a_{f_1} a_{f_2} \tag{5.3.21}$$

$$T^{[2]\dagger} = \frac{1}{2} \sum_{l_1 l_2} \sum_{f_1 f_2} a^\dagger_{l_2} a^\dagger_{l_1} \langle l_1 l_2 | t^\dagger (E_{l_1} + E_{l_2} + i\varepsilon) | f_1 f_2 \rangle a_{f_1} a_{f_2}$$

$$R^{[2]}_{k\lambda} = \sum_{f_1 f_2} \sqrt{2\varepsilon (1 \pm n_\lambda \pm n_k)} \frac{\langle \lambda k | t(E_{f_1} + E_{f_2} + i\varepsilon) | f_1 f_2 \rangle}{E_{f_1} + E_{f_2} - E_\lambda - E_k + i\varepsilon} a_{f_1} a_{f_2}$$

$$R^{[2]\dagger}_{h\lambda} = \sum_{l_1 l_2} a^\dagger_{l_2} a^\dagger_{l_1} \frac{\langle l_1 l_2 | t^\dagger (E_{l_1} + E_{l_2} + i\varepsilon) | \lambda h \rangle}{E_{l_1} + E_{l_2} - E_h - E_\lambda - i\varepsilon} \sqrt{2\varepsilon (1 \pm n_\lambda \pm n_h)}$$

and we can write

$$\mathcal{L}' (a^\dagger_h a_k) = \frac{i}{\hbar} [H_0, a^\dagger_h a_k] + \frac{i}{\hbar} \left[T^{[2]\dagger}, a^\dagger_h \right] a_k + \frac{i}{\hbar} a^\dagger_h \left[T^{[2]}, a_k \right] + \frac{1}{\hbar} \sum_\lambda R^{[2]\dagger}_{h\lambda} R^{[2]}_{k\lambda}. \tag{5.3.22}$$

Following (3.2.23) we have

$$\begin{aligned} V^{[2]} &= \frac{1}{2} \left[T^{[2]} + T^{[2]\dagger} \right] \\ &= \frac{1}{2} \sum_{l_1 l_2} \sum_{f_1 f_2} a^\dagger_{l_2} a^\dagger_{l_1} \langle l_1 l_2 | [t(E_{f_1} + E_{f_2} + i\varepsilon) + t^\dagger (E_{l_1} + E_{l_2} + i\varepsilon)] | f_1 f_2 \rangle a_{f_1} a_{f_2} \\ \Gamma^{[2]} &= \frac{i}{2} \left[T^{[2]} - T^{[2]\dagger} \right] \\ &= \frac{i}{2} \sum_{l_1 l_2} \sum_{f_1 f_2} a^\dagger_{l_2} a^\dagger_{l_1} \langle l_1 l_2 | [t(E_{f_1} + E_{f_2} + i\varepsilon) - t^\dagger (E_{l_1} + E_{l_2} + i\varepsilon)] | f_1 f_2 \rangle a_{f_1} a_{f_2} \end{aligned} \tag{5.3.23}$$

and therefore

$$T^{[2]} = V^{[2]} - i\Gamma^{[2]}, \qquad V^{[2]} = V^{[2]\dagger}, \qquad \Gamma^{[2]} = \Gamma^{[2]\dagger}, \tag{5.3.24}$$

so that $\Gamma^{[2]}$ is different from zero only if one goes beyond the Born approximation. The final expression is

$$\mathcal{L}'\left(a_h^\dagger a_k\right) = \frac{i}{\hbar}\left[H_0 + V^{[2]}, a_h^\dagger a_k\right] - \frac{1}{\hbar}\left\{\left[\Gamma^{[2]}, a_h^\dagger\right] a_k - a_h^\dagger\left[\Gamma^{[2]}, a_k\right]\right\} + \frac{1}{\hbar}\sum_\lambda R_{h\lambda}^{[2]\dagger} R_{k\lambda}^{[2]}, \tag{5.3.25}$$

formally exactly the same as eq. (3.2.24) obtained for the particle interacting with a system having many degrees of freedom, so that an analogous demonstration of the complete positivity property holds. The difference lies in the structure of the operators appearing in it, one-particle operators in the first case (as stressed by the superscript $^{[1]}$), two-particle operators including statistical corrections in the second one (denoted by $^{[2]}$). Neglecting the operator structure due to statistical corrections we have

$$\sum_h \left[\Gamma^{[2]}, a_h^\dagger\right] a_h = 2\Gamma^{[2]}, \qquad \sum_h a_h^\dagger\left[\Gamma^{[2]}, a_h\right] = -2\Gamma^{[2]}$$

and therefore

$$\mathcal{L}'(N) = -\frac{4}{\hbar}\Gamma^{[2]} + \frac{1}{\hbar}\sum_{h\lambda} R_{h\lambda}^{[2]\dagger} R_{h\lambda}^{[2]},$$

so that within our approximations particle number conservation amounts to

$$\Gamma^{[2]} \approx \frac{1}{4}\sum_{gf} R_{gf}^{[2]\dagger} R_{gf}^{[2]}. \tag{5.3.26}$$

The expression thus obtained, ensuring mass conservation, is

$$\begin{aligned}\mathcal{L}'\left(a_h^\dagger a_k\right) &= \frac{i}{\hbar}\left[H_0 + V^{[2]}, a_h^\dagger a_k\right] - \frac{1}{\hbar}\left\{\left[\frac{1}{4}\sum_{gf} R_{gf}^{[2]\dagger} R_{gf}^{[2]}, a_h^\dagger\right] a_k - a_h^\dagger\left[\frac{1}{4}\sum_{gf} R_{gf}^{[2]\dagger} R_{gf}^{[2]}, a_k\right]\right\} \\ &\quad + \frac{1}{\hbar}\sum_\lambda R_{h\lambda}^{[2]\dagger} R_{k\lambda}^{[2]}. \end{aligned} \tag{5.3.27}$$

5.3.4 Homogeneous Boltzmann Equation with Statistical Corrections

As a first application of the results obtained so far we will now show how (5.3.27) goes simply over to a Boltzmann equation with statistical corrections, the so called Uehling – Uhlenbeck equation. For simplicity we will consider the homogeneous case; setting $h = k$ and exploiting the following simple relations

$$\left[R_{gf}^{[2]}, a_h\right] = 0, \qquad \left[R_{gf}^{[2]\dagger}, a_h^\dagger\right] = 0$$

eq. (5.3.27) becomes

$$\frac{d}{dt}n_h = \frac{i}{\hbar}\left[V^{[2]}, n_h\right] - \frac{1}{4\hbar}\sum_{gf}\left\{R^{[2]\dagger}_{gf}\left[R^{[2]}_{gf}, a^\dagger_h\right]a_h - a^\dagger_h\left[R^{[2]\dagger}_{gf}, a_h\right]R^{[2]}_{gf}\right\} + \frac{1}{\hbar}\sum_\lambda R^{[2]\dagger}_{h\lambda}R^{[2]}_{h\lambda},$$

and using further

$$\begin{aligned}\left[R^{[2]}_{gf}, a^\dagger_h\right] &= 2\sum_\lambda \sqrt{2\varepsilon\left(1\pm n_f \pm n_g\right)}\frac{\langle fg\left|t(E_\lambda+E_h+i\varepsilon)\right|\lambda h\rangle}{E_\lambda+E_h-E_f-E_g+i\varepsilon}a_\lambda \\ \left[R^{[2]\dagger}_{gf}, a_h\right] &= -2\sum_\lambda a^\dagger_\lambda\frac{\langle \lambda h\left|t^\dagger(E_h+E_\lambda+i\varepsilon)\right|fg\rangle}{E_h+E_\lambda-E_f-E_g-i\varepsilon}\sqrt{2\varepsilon\left(1\pm n_f\pm n_g\right)}\end{aligned}$$

we come to

$$\begin{aligned}\frac{d}{dt}n_h &= \frac{i}{\hbar}\left[V^{[2]}, n_h\right] \\ &- \frac{1}{2\hbar}\sum_{\substack{gf\\ l_1l_2\\ \lambda}} a^\dagger_{l_2}a^\dagger_{l_1}\frac{\langle l_1l_2\left|t^\dagger(E_{l_1}+E_{l_2}+i\varepsilon)\right|fg\rangle}{E_{l_1}+E_{l_2}-E_f-E_g-i\varepsilon}2\varepsilon\left(1\pm n_f\pm n_g\right)\frac{\langle fg\left|t(E_h+E_\lambda+i\varepsilon)\right|\lambda h\rangle}{E_\lambda+E_h-E_f-E_g+i\varepsilon}a_\lambda a_k \\ &- \frac{1}{2\hbar}\sum_{\substack{gf\\ f_1f_2\\ \lambda}} a^\dagger_h a^\dagger_\lambda\frac{\langle \lambda h\left|t^\dagger(E_h+E_\lambda+i\varepsilon)\right|fg\rangle}{E_\lambda+E_h-E_f-E_g-i\varepsilon}2\varepsilon\left(1\pm n_f\pm n_g\right)\frac{\langle fg\left|t(E_{f_1}+E_{f_2}+i\varepsilon)\right|f_1f_2\rangle}{E_{f_1}+E_{f_2}-E_f-E_g+i\varepsilon}a_{f_1}a_{f_2} \\ &+ \frac{1}{\hbar}\sum_{\substack{l_1l_2\\ f_1f_2\\ \lambda}} a^\dagger_{l_2}a^\dagger_{l_1}\frac{\langle l_1l_2\left|t^\dagger(E_{l_1}+E_{l_2}+i\varepsilon)\right|\lambda h\rangle}{E_{l_1}+E_{l_2}-E_h-E_\lambda-i\varepsilon}2\varepsilon\left(1\pm n_f\pm n_g\right)\frac{\langle \lambda h\left|t(E_{f_1}+E_{f_2}+i\varepsilon)\right|l_1f_2\rangle}{E_{f_1}+E_{f_2}-E_\lambda-E_h+i\varepsilon}a_{f_1}a_{f_2}.\end{aligned}$$

We now consider the expectation value of this expression with a statistical operator ϱ_{m} having the canonical form, diagonal with respect to the basis generated by the operators $\{n_g\}$, so that we are left with

$$\begin{aligned}\frac{d}{dt}\langle n_h\rangle &= \frac{2}{\hbar}\sum_{gf}\sum_\lambda\frac{\varepsilon}{(E_\lambda+E_h-E_f-E_g)^2+\varepsilon^2} \\ &\times\left\{\left|\langle\lambda h\left|t(E_f+E_g+i\varepsilon)\right|fg\rangle\right|^2\langle 1\pm n_\lambda\pm n_h\rangle\langle n_f\rangle\langle n_g\rangle\right. \\ &\left.-\left|\langle fg\left|t(E_h+E_\lambda+i\varepsilon)\right|\lambda h\rangle\right|^2\langle n_\lambda\rangle\langle n_h\rangle\langle 1\pm n_f\pm n_g\rangle\right\},\end{aligned}$$

and we have used the same notation for the t operators, even though the expectation value has brought to the replacement $n_g \to \langle n_g\rangle$, and the factorization property is linked to the structure of ϱ_{m}. Using the time reversal invariance of the T-matrix we have

$$\begin{aligned}\frac{d}{dt}\langle n_h\rangle &= \frac{2}{\hbar}\sum_{gf}\sum_\lambda\frac{\varepsilon}{(E_\lambda+E_h-E_f-E_g)^2+\varepsilon^2}\left|\langle\lambda h\left|t(E_f+E_g+i\varepsilon)\right|fg\rangle\right|^2 \\ &\times\left\{\langle 1\pm n_\lambda\pm n_h\rangle\langle n_f\rangle\langle n_g\rangle-\langle n_\lambda\rangle\langle n_h\rangle\langle 1\pm n_f\pm n_g\rangle\right\},\end{aligned}$$

or equivalently

$$\frac{d}{dt}\langle n_h \rangle = \frac{2}{\hbar}\sum_{gf}\sum_{\lambda}\frac{\varepsilon}{(E_\lambda + E_h - E_f - E_g)^2 + \varepsilon^2}\left|\langle \lambda h \left| t(E_f + E_g + i\varepsilon) \right| fg \rangle\right|^2$$

$$\times \left\{ \langle 1 \pm n_\lambda \rangle \langle 1 \pm n_h \rangle \langle n_f \rangle \langle n_g \rangle - \langle n_\lambda \rangle \langle n_h \rangle \langle 1 \pm n_f \rangle \langle 1 \pm n_g \rangle \right\}.$$

Recalling the fact that the indexes f, g now denote momenta, we extract the delta of momentum conservation from the matrix element of the t operator, changing the notation from f, g to $\mathbf{p}_f, \mathbf{p}_g$, thus obtaining

$$\langle \mathbf{p}_\lambda \mathbf{p}_h \left| t(E_f + E_g + i\varepsilon) \right| \mathbf{p}_f \mathbf{p}_g \rangle = \delta_{p_\lambda + p_h, p_f + p_g} \mathsf{T}\left(\mathbf{q}_{\lambda h} \leftarrow \mathbf{q}_{fg}\right)$$

where

$$\mathbf{q}_{fg} = \frac{1}{2}\left(\mathbf{p}_f - \mathbf{p}_g\right), \qquad \mathbf{q}_{\lambda h} = \frac{1}{2}\left(\mathbf{p}_\lambda - \mathbf{p}_h\right)$$

denote initial and final relative momenta, and the expression T is such that

$$\left|\mathsf{T}\left(\mathbf{q}_{\lambda h} \leftarrow \mathbf{q}_{fg}\right)\right|^2 = \frac{1}{(2\pi)^4 \hbar^2 (m/2)^2}\left|f(\theta)\right|^2,$$

with θ the angle of rotation of the relative momentum between the colliding particles. In the continuum limit we have

$$\frac{d}{dt} f(\mathbf{p}_h) = \frac{2\pi}{\hbar}(2\pi\hbar)^3 \int d^3\mathbf{p}_\lambda \int d^3\mathbf{p}_f \int d^3\mathbf{p}_g \, \delta\left(E_\lambda + E_h - E_f - E_g\right) \delta^3\left(\mathbf{p}_\lambda + \mathbf{p}_h - \mathbf{p}_f - \mathbf{p}_g\right)$$

$$\times \left|\mathsf{T}\left(\mathbf{q}_{\lambda h} \leftarrow \mathbf{q}_{fg}\right)\right|^2 \left\{ \left[1 \pm (2\pi\hbar)^3 f(\mathbf{p}_\lambda)\right]\left[1 \pm (2\pi\hbar)^3 f(\mathbf{p}_h)\right] f(\mathbf{p}_f) f(\mathbf{p}_g)\right.$$

$$\left. - \, f(\mathbf{p}_\lambda) f(\mathbf{p}_h)\left[1 \pm (2\pi\hbar)^3 f(\mathbf{p}_f)\right]\left[1 \pm (2\pi\hbar)^3 f(\mathbf{p}_g)\right]\right\} \quad (5.3.28)$$

where $f(\mathbf{p})$ is the distribution function for the homogeneous case

$$f(\mathbf{p}) = \frac{1}{\mathsf{V}}\langle n(\mathbf{p}) \rangle, \qquad \int_\omega d^3\mathbf{x} \int_\omega d^3\mathbf{p}\, f(\mathbf{p}) = N.$$

As we have seen there is a strict connection between (5.3.27) and the Boltzmann equation with statistical corrections given by (5.3.28), in particular the expression

$$+\frac{1}{\hbar}\sum_{\lambda} R^{[2]\dagger}_{h\lambda} R^{[2]}_{h\lambda}$$

goes over to the gain term, while

$$-\frac{1}{\hbar}\left\{ \left[\frac{1}{4}\sum_{gf} R^{[2]\dagger}_{gf} R^{[2]}_{gf}, a^\dagger_h\right] a_h - a^\dagger_h \left[\frac{1}{4}\sum_{gf} R^{[2]\dagger}_{gf} R^{[2]}_{gf}, a_h\right]\right\}$$

goes over to the loss term.

5.3.5 Extension of the Formalism to Higher Polynomials of Field Operators

We will now show how the formalism of Sect. 5.3.1 for the evaluation of the time evolution of the couple of field operators $a^\dagger_h a_k$ can be suitably generalized to the case of higher polynomials of field operators. As we have seen in Sect. 5.2, the typical structure of the relevant observables one should consider for the description of the macroscopic system on a given time scale is given by (5.2.3) and (5.2.4), together with generalizations of these expressions to the case of $2n$ field operators. We therefore intend to give an asymptotic evaluation of the expression $\mathcal{U}'(a^\dagger_{h_n} \dots a^\dagger_{h_1} a_{k_1} \dots a_{k_n})$ for $t \geq \tau_1 \gg \tau_0$. Dealing with suitably slowly varying quantities, so that, at least with respect to the considered observables, the system is not too far from equilibrium, one has that the indexes h_i, k_i referring to the normal modes are not completely independent. In the case of two operators $a^\dagger_h a_k$ considering slow variables implied a neighborhood of the two modes h and k, which played an important role in the calculation, especially in obtaining the completely positive structure given by (5.3.25). This condition of almost homogeneity becomes clear if one supposes that the system is described by an equilibrium statistical operator diagonal with respect to the normal modes, so that the equilibrium value of quantities of the form $\sum_{hk} a^\dagger_h A_{hk}(\mathbf{x}) a_k$ actually implies $h = k$. The natural generalization of this physical approximation to the case of observables having a more complex operator structure is therefore the following: in expressions of the form $a^\dagger_{h_n} \dots a^\dagger_{h_1} a_{k_1} \dots a_{k_n}$ we suppose that the indexes are linked in couples, so that between the modes h_j and k_j a relation exists, similar to the one between h and k exploited in the calculation of Sect. 5.3.1. In the following we will therefore develop the calculations paying attention to the couples $a^\dagger_{h_j} a_{k_j}$ as a whole, rather than to the single field operators, keeping the relation between the indexes into account. To understand the meaning of this approximation more clearly, let us consider in more detail the typical observable given by (5.2.3) and (5.2.4)

$$\frac{1}{2} \int_\omega d^3\mathbf{y}\, \psi^\dagger(\mathbf{x})\, \psi^\dagger(\mathbf{y})\, V(\mathbf{x}-\mathbf{y}) \psi(\mathbf{y})\, \psi(\mathbf{x}) = \sum_{\substack{h_1 h_2 \\ k_1 k_2}} a^\dagger_{h_2} a^\dagger_{h_1} A_{h_2 h_1 k_1 k_2}(\mathbf{x}) a_{k_1} a_{k_2} \quad (5.3.29)$$

$$= \frac{1}{2} \sum_{\substack{h_1 h_2 \\ k_1 k_2}} \int_\omega d^3\mathbf{y}\, a^\dagger_{h_2} a^\dagger_{h_1} u^*_{h_2}(\mathbf{x}) u^*_{h_1}(\mathbf{y}) V(\mathbf{x}-\mathbf{y}) u_{k_1}(\mathbf{y}) u_{k_2}(\mathbf{x}) a_{k_1} a_{k_2}.$$

If we consider the expectation value of (5.3.29) with a statistical operator, diagonal with respect to the normal modes of the system supposed to be at equilibrium, we obtain

$$\sum_{fg} \int_\omega d^3\mathbf{y}\, |u_f(\mathbf{x})|^2\, V(\mathbf{x}-\mathbf{y})\, |u_g(\mathbf{y})|^2 \left\langle a^\dagger_g a^\dagger_f a_f a_g \right\rangle,$$

so that the interaction kernel actually describes an interaction between the local densities of the different modes of the field, weighted according to the population of the modes. A similar approximation, however more restrictive, due to its statistical consequences, would consist in setting

$$\langle \psi^\dagger(\mathbf{x})\, \psi^\dagger(\mathbf{y})\, \psi(\mathbf{y})\, \psi(\mathbf{x}) \rangle \approx \langle \psi^\dagger(\mathbf{x})\, \psi(\mathbf{x}) \rangle \langle \psi^\dagger(\mathbf{y})\, \psi(\mathbf{y}) \rangle ,$$

thus reconducting the expectation value of $2n$ operators to suitable multiples of expectation value of couples of creation and annihilation operators. For the relevant variables we consider a generalization of this situation, so that the different indexes h_j, k_j are related, though not necessarily identical. Keeping this feature into account we will now develop the calculations in strict analogy with Sect. 5.3.1.

To start with let us introduce the following operator structures

$$\mathcal{A}^\dagger_{hn} = a^\dagger_{h_n} \dots a^\dagger_{h_1}, \qquad \mathcal{A}_{kn} = a_{k_1} \dots a_{k_n},$$

which will be helpful both in having a more compact notation and in keeping track of the structure of the different expressions. We intend to evaluate $\mathcal{U}'(t)\,(\mathcal{A}^\dagger_{hn}\mathcal{A}_{kn})$ and analogously to (5.3.4) we exploit the following integral representation

$$\mathcal{U}'(t)\,(\mathcal{A}^\dagger_{hn}\mathcal{A}_{kn}) = \exp\left(\sum_{i=1}^{n}(e_{h_i} - e_{k_i})t\right) \mathcal{A}^\dagger_{hn}\mathcal{A}_{kn} + \int_{-i\infty+\eta}^{+i\infty+\eta} \frac{dz}{2\pi i}\, e^{zt} \frac{1}{z - \sum_{i=1}^{n}(e_{h_i} - e_{k_i})} \sum_{m=1}^{\infty} \mathcal{N}^m_{hk},$$

where again

$$\mathcal{N}^m_{hk} \equiv \left\{ (z - \mathcal{H}'_0)^{-1} \mathcal{V}' \right\}^m [\mathcal{A}^\dagger_{hn}\mathcal{A}_{kn}] .$$

Exploiting (5.3.6) and the simple property

$$[A, B_1 \dots B_N] = [A, B_1]\, B_2 \dots B_N + B_1\, [A, B_2]\, B_3 \dots B_N + \dots + B_1 \dots B_{N-1}\, [A, B_N] \tag{5.3.30}$$

we come to

$$\begin{aligned}\mathcal{N}^1_{hk} \;=\;& (z - \mathcal{H}'_0)^{-1} \frac{i}{\hbar} \sum_{j=1}^{n} \sum_{\lambda} \Bigg[\sum_{l_1 l_2} a^\dagger_{h_n} \dots a^\dagger_{h_{j+1}} \left(a^\dagger_{l_2} a^\dagger_{l_1} \Phi_{l_1 l_2 \lambda h_j} a_\lambda \right) a^\dagger_{h_{j-1}} \dots a^\dagger_{h_1} \mathcal{A}_{kn} \\ & - \sum_{f_1 f_2} \mathcal{A}^\dagger_{hn} a_{k_1} \dots a_{k_{j-1}} \left(a^\dagger_\lambda \Phi_{\lambda k_j f_1 f_2} a_{f_1} a_{f_2} \right) a_{k_{j+1}} \dots a_{k_n} \Bigg] .\end{aligned}$$

For both Bose and Fermi statistics one has

$$\left[a^\dagger_{l_2} a^\dagger_{l_1}, a^\dagger_{g_1} \dots a^\dagger_{g_r} \right] = 0, \qquad \left[a_{f_1} a_{f_2}, a_{g_1} \dots a_{g_r} \right] = 0 \tag{5.3.31}$$

so that the couples $a^\dagger_{l_2} a^\dagger_{l_1}$ and $a_{f_1} a_{f_2}$ can be moved to the left and to the right respectively:

$$\begin{aligned}\mathcal{N}^1_{hk} \;=\;& (z - \mathcal{H}'_0)^{-1} \frac{i}{\hbar} \sum_{j=1}^{n} \sum_{\lambda} \Bigg[\sum_{l_1 l_2} a^\dagger_{l_1} a^\dagger_{l_2} \Phi_{l_1 l_2 \lambda h_j} a^\dagger_{h_n} \dots a^\dagger_{h_{j+1}} a_\lambda a^\dagger_{h_{j-1}} \dots a^\dagger_{h_1} \mathcal{A}_{kn} \\ & - \sum_{f_1 f_2} \mathcal{A}^\dagger_{hn} a_{k_1} \dots a_{k_{j-1}} a^\dagger_\lambda a_{k_{j+1}} \dots a_{k_n} \Phi_{\lambda k_j f_1 f_2} a_{f_1} a_{f_2} \Bigg] .\end{aligned}$$

We now proceed to normal order; considering the identity

$$a_\lambda a_h^\dagger = \pm a_h^\dagger a_\lambda + [a_\lambda, a_h^\dagger]_\pm = \pm a_h^\dagger a_\lambda + \delta_{\lambda h}$$

(the $\pm$ sign denoting as usual Bose or Fermi statistics respectively) we see that moving the operator a_λ to the right, apart from an overall sign further contributions arise, having the typical structure

$$\sum_{l_1 l_2} a_{l_1}^\dagger a_{l_2}^\dagger \Phi_{l_1 l_2 h_{j-1} h_j} a_{h_n}^\dagger \dots a_{h_{j+1}}^\dagger a_{h_{j-2}}^\dagger \dots a_{h_1}^\dagger \mathcal{A}_{kn},$$

these terms however, because of the missing sum over λ, have a different volume dependence in the continuum limit and will therefore be neglected with respect to the other ones. Noting that the operator a_λ comes from the action of the potential $\mathcal{V}'$ on the operator $a_{h_j}^\dagger$ and recalling that we are considering a situation in which the two indexes are linked, we move the operator a_{k_j} to the left, in order to put into evidence the pair $a_\lambda a_{k_j}$, thus generating an overall sign that exactly compensates the sign obtained in bringing the operator a_λ to normal order. A similar reasoning applies to the term with $a_\lambda^\dagger$, so that setting for simplicity

$$\begin{aligned} (\mathcal{A}_{hn}^\dagger)_j &= a_{h_n}^\dagger \dots a_{h_{j+1}}^\dagger a_{h_{j-1}}^\dagger \dots a_{h_1}^\dagger \quad 1 \le j \le n \\ (\mathcal{A}_{kn})_i &= a_{k_1} \dots a_{k_{i-1}} a_{k_{i+1}} \dots a_{k_n} \quad 1 \le i \le n \end{aligned} \tag{5.3.32}$$

$\mathcal{N}_{hk}^1$ becomes

$$(z - \mathcal{H}_0')^{-1} \frac{i}{\hbar} \sum_{j=1}^n \sum_\lambda \left[\sum_{l_1 l_2} a_{l_1}^\dagger a_{l_2}^\dagger \Phi_{l_1 l_2 \lambda h_j} (\mathcal{A}_{hn}^\dagger)_j a_\lambda a_{k_j} (\mathcal{A}_{kn})_j \right.$$
$$\left. - \sum_{f_1 f_2} (\mathcal{A}_{hn}^\dagger)_j a_{h_j}^\dagger a_\lambda^\dagger (\mathcal{A}_{kn})_j \Phi_{\lambda k_j f_1 f_2} a_{f_1} a_{f_2} \right]$$

and using further (5.3.31), so that

$$[\mathcal{A}_{hn}^\dagger, a_h^\dagger a_\lambda^\dagger] = 0, \qquad [\mathcal{A}_{kn}, a_\lambda a_k] = 0$$

and similarly for $(\mathcal{A}_{hn}^\dagger)_j$, $(\mathcal{A}_{kn})_i$, we finally obtain

$$\begin{aligned} \mathcal{N}_{hk}^1 &= (z - \mathcal{H}_0')^{-1} \mathcal{V}' [\mathcal{A}_{hn}^\dagger \mathcal{A}_{kn}] \\ &= + \sum_{j=1}^n \sum_{\substack{l_1 l_2 \\ \lambda}} \left(\frac{i}{\hbar}\right) \frac{1}{z - e_{l_1} - e_{l_2} - \sum_{i \neq j}(e_{h_i} - e_{k_i}) + e_\lambda + e_{k_j}} \\ &\qquad \times a_{l_2}^\dagger a_{l_1}^\dagger \Phi_{l_1 l_2 \lambda h_j} (\mathcal{A}_{hn}^\dagger)_j (\mathcal{A}_{kn})_j a_\lambda a_{k_j} \qquad \mathtt{L} \\ &\quad + \sum_{j=1}^n \sum_{\substack{f_1 f_2 \\ \lambda}} \left(-\frac{i}{\hbar}\right) \frac{1}{z - e_{h_j} - e_\lambda - \sum_{i \neq j}(e_{h_i} - e_{k_i}) + e_{f_1} + e_{f_2}} \\ &\qquad \times a_{h_j}^\dagger a_\lambda^\dagger (\mathcal{A}_{hn}^\dagger)_j (\mathcal{A}_{kn})_j \Phi_{\lambda k_j f_1 f_2} a_{f_1} a_{f_2}, \qquad \mathtt{R} \end{aligned} \tag{5.3.33}$$

where the letters L, R have a similar meaning to the letters l, r used in (5.3.7). The structure of (5.3.33) is in fact strongly similar to that of (5.3.7). The same procedure has been applied to the n couples $h_j k_j$, so that one has n terms analogous to the l and r terms of (5.3.7), having a slightly more complicated operator structure, due to the presence of the block of operators $(\mathcal{A}^\dagger_{hn})_j\,(\mathcal{A}_{kn})_j$. We now go over to second order, always within the *one-mode* approximation introduced in Sect. 5.3.1. The further mode has already been added, so that only statistical corrections are to be taken into account, exploiting the usual relations (5.3.9) and (5.3.10) on the couples $a^\dagger_{l_2}a^\dagger_{l_1}$, $a_\lambda a_{k_j}$, $a^\dagger_{h_j}a^\dagger_\lambda$, $a_{f_1}a_{f_2}$, the grouping between the terms being determined by the fact that the modes h_j and k_j are supposed to be close to each other. Moreover terms coming from the action of $\mathcal{V}'$ on couples such as $a^\dagger_{h_{j+1}}a^\dagger_{h_j}$, $a_{k_j}a_{k_{j+1}}$ or $a^\dagger_{h_j}a_{k_j}$ would be negligible with respect to the others in the continuum limit. Similarly to $\mathcal{A}^2_{hk}$ we therefore obtain

$$
\begin{aligned}
\mathcal{N}^2_{hk} = & \\
& \sum_{j=1}^{n}\sum_{\substack{l_1 l_2\\ l'_1 l'_2}}\sum_{\lambda}\left(\frac{i}{\hbar}\right)\frac{1}{z-e_{l_1}-e_{l_2}-\sum_{i\neq j}(e_{h_i}-e_{k_i})+e_\lambda+e_{k_j}}a^\dagger_{l_2}a^\dagger_{l_1}\Phi_{l_1 l_2 l'_1 l'_2}\\
& \times\left(\frac{i}{\hbar}\right)\frac{\left(1\pm n_{l'_1}\pm n_{l'_2}\right)}{z-e_{l'_1}-e_{l'_2}-\sum_{i\neq j}(e_{h_i}-e_{k_i})+e_\lambda+e_{k_j}}\Phi_{l'_1 l'_2 \lambda h_j}\,(\mathcal{A}^\dagger_{hn})_j\,(\mathcal{A}_{kn})_j\,a_\lambda a_{k_j} \qquad \texttt{LL}\\
& +\sum_{j=1}^{n}\sum_{\substack{l_1 l_2\\ f_1 f_2}}\sum_{\lambda}\left(\frac{i}{\hbar}\right)\frac{1}{z-e_{l_1}-e_{l_2}-\sum_{i\neq j}(e_{h_i}-e_{k_i})+e_{f_1}+e_{f_2}}a^\dagger_{l_2}a^\dagger_{l_1}\Phi_{l_1 l_2 \lambda h_j}\,(\mathcal{A}^\dagger_{hn})_j\,(\mathcal{A}_{kn})_j\\
& \times\left(-\frac{i}{\hbar}\right)\frac{\left(1\pm n_\lambda\pm n_{k_j}\right)}{z-e_{l_1}-e_{l_2}-\sum_{i\neq j}(e_{h_i}-e_{k_i})+e_\lambda+e_{k_j}}\Phi_{\lambda k_j f_1 f_2}a_{f_1}a_{f_2} \qquad \texttt{LR}\\
& +\sum_{j=1}^{n}\sum_{\substack{f_1 f_2\\ f'_1 f'_2}}\sum_{\lambda}\left(-\frac{i}{\hbar}\right)\frac{1}{z-e_{h_j}-e_\lambda-\sum_{i\neq j}(e_{h_i}-e_{k_i})+e_{f_1}+e_{f_2}}a^\dagger_{h_j}a^\dagger_\lambda\,(\mathcal{A}^\dagger_{hn})_j\,(\mathcal{A}_{kn})_j\,\Phi_{\lambda k_j f'_1 f'_2}\\
& \times\left(-\frac{i}{\hbar}\right)\frac{\left(1\pm n_{f'_1}\pm n_{f'_2}\right)}{z-e_{h_j}-e_\lambda-\sum_{i\neq j}(e_{h_i}-e_{k_i})+e_{f'_1}+e_{f'_2}}\Phi_{f'_1 f'_2 f_1 f_2}a_{f_1}a_{f_2} \qquad \texttt{RR}\\
& +\sum_{j=1}^{n}\sum_{\substack{l_1 l_2\\ f_1 f_2}}\sum_{\lambda}\left(-\frac{i}{\hbar}\right)\frac{1}{z-e_{l_1}-e_{l_2}-\sum_{i\neq j}(e_{h_i}-e_{k_i})+e_{f_1}+e_{f_2}}a^\dagger_{l_2}a^\dagger_{l_1}\Phi_{l_1 l_2 \lambda h_j}\\
& \times\left(\frac{i}{\hbar}\right)\frac{\left(1\pm n_\lambda\pm n_{h_j}\right)}{z-e_{h_j}-e_\lambda-\sum_{i\neq j}(e_{h_i}-e_{k_i})+e_{f_1}+e_{f_2}}\,(\mathcal{A}^\dagger_{hn})_j\,(\mathcal{A}_{kn})_j\,\Phi_{\lambda k_j f_1 f_2}a_{f_1}a_{f_2}. \qquad \texttt{RL}
\end{aligned}
$$

Let us note that, within the adopted approximations, statistical corrections and operators of the form $\mathcal{A}^\dagger_{hn}$,$\mathcal{A}_{kn}$ commute, in fact

$$\begin{aligned} n_l a^\dagger_h &= a^\dagger_h n_l + [n_l, a^\dagger_h] &= a^\dagger_h (n_l + \delta_{lh}) \\ n_f a_k &= a_k n_f + [n_f, a_k] &= a_k (n_f - \delta_{fk}) \end{aligned}$$

and the terms with the Kronecker's delta would have once more a different volume dependence. On the other hand n_{h_j} and $\left(\mathcal{A}^\dagger_{hn}\right)_j$ commute having different indexes, and similarly for n_{k_j} and $\left(\mathcal{A}_{kn}\right)_j$ or the other possible combinations. We refrain from giving the result for the expressions that one obtains at higher perturbative orders, because they can be simply obtained from the results for the couple of operators $a^\dagger_h a_k$, as can be seen comparing $\mathcal{A}^1_{hk}$ with $\mathcal{N}^1_{hk}$ and $\mathcal{A}^2_{hk}$ with $\mathcal{N}^2_{hk}$. Also the recombination of the denominators, in order to put into evidence the contribution having a pole depending on the difference in energy between the in and out states, takes place in the very same way. We therefore go over directly to the expression for $\sum_{m=1}^\infty \mathcal{N}^m_{hk}$. Instead of (5.3.11) and (5.3.12) we now have the following matrix elements, being operators in the Fock-space due to the presence of statistical corrections:

$$\langle \lambda k_j | t(E_{h_j} + E_\lambda + \textstyle\sum_{i\neq j}(E_{h_i} - E_{k_i}) + i\hbar z) | f_1 f_2 \rangle, \quad \langle l_1 l_2 | t^\dagger (E_\lambda + E_{k_j} - \textstyle\sum_{i\neq j}(E_{h_i} - E_{k_i}) + i\hbar z^*) | \lambda h_j \rangle$$

and therefore

$$\begin{aligned}
&\sum_{m=1}^{\infty} \mathcal{N}^m_{hk} = \\
&\quad + \sum_{j=1}^{n} \sum_{l_1 l_2} \sum_{\lambda} \left(\frac{i}{\hbar}\right) \frac{1}{z - e_{l_1} - e_{l_2} - \sum_{i\neq j}(e_{h_i} - e_{k_i}) + e_\lambda + e_{k_j}} \\
&\qquad \times a^\dagger_{l_2} a^\dagger_{l_1} \langle l_1 l_2 | t^\dagger (E_\lambda + E_{k_j} - \textstyle\sum_{i\neq j}(E_{h_i} - E_{k_i}) + i\hbar z^*) | \lambda h_j \rangle \left(\mathcal{A}^\dagger_{hn}\right)_j \left(\mathcal{A}_{kn}\right)_j a_\lambda a_{k_j} \\
&\quad + \sum_{j=1}^{n} \sum_{f_1 f_2} \sum_{\lambda} \left(-\frac{i}{\hbar}\right) \frac{1}{z - e_{h_j} - e_\lambda - \sum_{i\neq j}(e_{h_i} - e_{k_i}) + e_{f_1} + e_{f_2}} \\
&\qquad \times a^\dagger_{h_j} a^\dagger_\lambda \left(\mathcal{A}^\dagger_{hn}\right)_j \left(\mathcal{A}_{kn}\right)_j \langle \lambda k_j | t(E_{h_j} + E_\lambda + \textstyle\sum_{i\neq j}(E_{h_i} - E_{k_i}) + i\hbar z) | f_1 f_2 \rangle a_{f_1} a_{f_2} \\
&\quad + \sum_{j=1}^{n} \sum_{l_1 l_2} \sum_{f_1 f_2} \sum_{\lambda} \left(\frac{i}{\hbar}\right) \frac{1}{z - e_{l_1} - e_{l_2} - \sum_{i\neq j}(e_{h_i} - e_{k_i}) + e_{f_1} + e_{f_2}} \\
&\qquad \times a^\dagger_{l_2} a^\dagger_{l_1} \langle l_1 l_2 | t^\dagger (E_\lambda + E_{k_j} - \textstyle\sum_{i\neq j}(E_{h_i} - E_{k_i}) + i\hbar z^*) | \lambda h_j \rangle \\
&\qquad \times \left(\mathcal{A}^\dagger_{hn}\right)_j \left[\frac{\left(1 \pm n_\lambda \pm n_{k_j}\right)}{E_{l_1} + E_{l_2} + \sum_{i\neq j}(E_{h_i} - E_{k_i}) - E_\lambda - E_{k_j} + i\hbar z} \right.
\end{aligned}$$

$$+ \frac{\left(1 \pm n_\lambda \pm n_{h_j}\right)}{E_{h_j} + E_\lambda + \sum_{i \neq j}(E_{h_i} - E_{k_i}) - E_{f_1} - E_{f_2} + i\hbar z}\Bigg] \left(\mathcal{A}_{kn}\right)_j$$

$$\times \langle \lambda k_j | t(E_{h_j} + E_\lambda + \textstyle\sum_{i \neq j}(E_{h_i} - E_{k_i}) + i\hbar z) | f_1 f_2 \rangle a_{f_1} a_{f_2}$$

$$+ \frac{i}{\hbar} \sum_{j=1}^{n} \sum_{l_1 l_2} \sum_{f_1 f_2} a^\dagger_{l_2} a^\dagger_{l_1} \left(\mathcal{A}^\dagger_{hn}\right)_j F^{h_n \ldots h_1 k_1 \ldots k_n}_{l_1 l_2 f_1 f_2}(z) \left(\mathcal{A}_{kn}\right)_j a_{f_1} a_{f_2},$$

$F^{h_n \ldots h_1 k_1 \ldots k_n}_{l_1 l_2 f_1 f_2}(z)$ being once more a term not exhibiting the pole relative to the difference in energy between the in and out states. Corresponding to (5.3.14) we have

$$\mathcal{U}'(t) \left(\mathcal{A}^\dagger_{hn} \mathcal{A}_{kn}\right) = \exp\left(\sum_{i=1}^{n} (e_{h_i} - e_{k_i}) t\right) \mathcal{A}^\dagger_{hn} \mathcal{A}_{kn} + \int_{-i\infty+\eta}^{+i\infty+\eta} \frac{dz}{2\pi i}\, e^{zt} \frac{1}{z - \sum_{i=1}^{n}(e_{h_i} - e_{k_i})} \sum_{j=1}^{n}$$

$$\Bigg\{ + \frac{i}{\hbar} \sum_{l_1 l_2} \sum_{\lambda} \frac{1}{z - e_{l_1} - e_{l_2} - \sum_{i \neq j}(e_{h_i} - e_{k_i}) + e_\lambda + e_{k_j}}$$

$$\times a^\dagger_{l_2} a^\dagger_{l_1} \langle l_1 l_2 | t^\dagger(E_\lambda + E_{k_j} - \textstyle\sum_{i \neq j}(E_{h_i} - E_{k_i}) + i\hbar z^*) | \lambda h_j \rangle \left(\mathcal{A}^\dagger_{hn}\right)_j \left(\mathcal{A}_{kn}\right)_j a_\lambda a_{k_j}$$

$$- \frac{i}{\hbar} \sum_{f_1 f_2} \sum_{\lambda} \frac{1}{z - e_{h_j} - e_\lambda - \sum_{i \neq j}(e_{h_i} - e_{k_i}) + e_{f_1} + e_{f_2}}$$

$$\times a^\dagger_{h_j} a^\dagger_\lambda \left(\mathcal{A}^\dagger_{hn}\right)_j \left(\mathcal{A}_{kn}\right)_j \langle \lambda k_j | t(E_{h_j} + E_\lambda + \textstyle\sum_{i \neq j}(E_{h_i} - E_{k_i}) + i\hbar z) | f_1 f_2 \rangle a_{f_1} a_{f_2}$$

$$+ \frac{i}{\hbar} \sum_{l_1 l_2} \sum_{f_1 f_2} \sum_{\lambda} \frac{1}{z - e_{l_1} - e_{l_2} - \sum_{i \neq j}(e_{h_i} - e_{k_i}) + e_{f_1} + e_{f_2}}$$

$$\times a^\dagger_{l_2} a^\dagger_{l_1} \langle l_1 l_2 | t^\dagger(E_\lambda + E_{k_j} - \textstyle\sum_{i \neq j}(E_{h_i} - E_{k_i}) + i\hbar z^*) | \lambda h_j \rangle$$

$$\times \left(\mathcal{A}^\dagger_{hn}\right)_j \Bigg[\frac{\left(1 \pm n_\lambda \pm n_{k_j}\right)}{E_{l_1} + E_{l_2} + \sum_{i \neq j}(E_{h_i} - E_{k_i}) - E_\lambda - E_{k_j} + i\hbar z}$$

$$+ \frac{\left(1 \pm n_\lambda \pm n_{h_j}\right)}{E_{h_j} + E_\lambda + \sum_{i \neq j}(E_{h_i} - E_{k_i}) - E_{f_1} - E_{f_2} + i\hbar z}\Bigg] \left(\mathcal{A}_{kn}\right)_j$$

$$\times \langle \lambda k_j | t(E_{h_j} + E_\lambda + \textstyle\sum_{i \neq j}(E_{h_i} - E_{k_i}) + i\hbar z) | f_1 f_2 \rangle a_{f_1} a_{f_2}$$

$$+ \frac{i}{\hbar} \sum_{l_1 l_2} \sum_{f_1 f_2} a^\dagger_{l_2} a^\dagger_{l_1} \left(\mathcal{A}^\dagger_{hn}\right)_j F^{h_n \ldots h_1 k_1 \ldots k_n}_{l_1 l_2 f_1 f_2}(z) \left(\mathcal{A}_{kn}\right)_j a_{f_1} a_{f_2} \Bigg\}.$$

The evaluation of the integral is exactly the same as in Sect. 5.3.1, where the substitution $z \to z + \frac{\varepsilon}{\hbar}$

in the T-matrix contribution is considered, so that we have

$$\mathcal{U}'(t)\left(\mathcal{A}^{\dagger}_{hn}\mathcal{A}_{kn}\right) = +\mathcal{A}^{\dagger}_{hn}\mathcal{A}_{kn} + \frac{i}{\hbar}t\sum_{i=1}^{n}(e_{h_i}-e_{k_i})\mathcal{A}^{\dagger}_{hn}\mathcal{A}_{kn}$$

$$+\frac{i}{\hbar}t\sum_{j=1}^{n}\sum_{l_1l_2}\sum_{\lambda}a^{\dagger}_{l_2}a^{\dagger}_{l_1}\left\langle l_1l_2\left|t^{\dagger}(E_{l_1}+E_{l_2}+i\varepsilon)\right|\lambda h_j\right\rangle\left(\mathcal{A}^{\dagger}_{hn}\right)_j\left(\mathcal{A}_{kn}\right)_j a_{\lambda}a_{k_j}$$

$$-\frac{i}{\hbar}t\sum_{j=1}^{n}\sum_{f_1f_2}\sum_{\lambda}a^{\dagger}_{h_j}a^{\dagger}_{\lambda}\left(\mathcal{A}^{\dagger}_{hn}\right)_j\left(\mathcal{A}_{kn}\right)_j\left\langle\lambda k_j\left|t(E_{f_1}+E_{f_2}+i\varepsilon)\right|f_1f_2\right\rangle a_{f_1}a_{f_2}$$

$$+\frac{i}{\hbar}t\sum_{j=1}^{n}\sum_{l_1l_2}\sum_{f_1f_2}\sum_{\lambda}a^{\dagger}_{l_2}a^{\dagger}_{l_1}\left\langle l_1l_2\left|t^{\dagger}(E_{l_1}+E_{l_2}+i\varepsilon)\right|\lambda h_j\right\rangle$$

$$\times\left(\mathcal{A}^{\dagger}_{hn}\right)_j\left[\frac{\left(1\pm n_{\lambda}\pm n_{k_j}\right)}{E_{f_1}+E_{f_2}-E_{\lambda}-E_k+i\varepsilon}-\frac{\left(1\pm n_{\lambda}\pm n_{h_j}\right)}{E_{l_1}+E_{l_2}-E_h-E_{\lambda}-i\varepsilon}\right]\left(\mathcal{A}_{kn}\right)_j$$

$$\times\left\langle\lambda k_j\left|t(E_{f_1}+E_{f_2}+i\varepsilon)\right|f_1f_2\right\rangle a_{f_1}a_{f_2}.$$

5.3.6 Conservation Laws and Structure of the Generator in the General Case

We now want to consider the consequences of the property of particle number conservation proved in Sect. 5.3.2 for the generator obtained in Sect. 5.3.5. As one might naturally expect, the conserved quantities are obtained simply setting exactly equal all couples of related modes, that is to say $h_j = k_j\ \forall j = 1,\ldots,n$. They have therefore the general form

$$\sum_{f_1}a^{\dagger}_{f_1}a_{f_1}=N,\quad \sum_{f_1f_2}a^{\dagger}_{f_2}a^{\dagger}_{f_1}a_{f_1}a_{f_2}=N(N-1),\quad \sum_{f_1f_2f_3}a^{\dagger}_{f_3}a^{\dagger}_{f_2}a^{\dagger}_{f_1}a_{f_1}a_{f_2}a_{f_3}=N(N-1)(N-2),\ldots$$

and in the general case of $2n$ operators

$$\sum_{f_1\cdots f_n}\mathcal{A}^{\dagger}_{fn}\mathcal{A}_{fn}=N(N-1)\ldots(N-n+1).$$

These conservation laws may be written

$$\mathcal{L}'\left(\sum_{f_1\cdots f_n}\mathcal{A}^{\dagger}_{fn}\mathcal{A}_{fn}\right)=\mathcal{L}'\left(N(N-1)\ldots(N-n+1)\right)=0, \tag{5.3.34}$$

and express the fact that the generator $\mathcal{L}'$ gives no contribution to the time evolution of quantities already diagonal with respect to the normal modes. In order to prove this property let us consider

$$\mathcal{L}'\left(\mathcal{A}^{\dagger}_{hn}\mathcal{A}_{kn}\right) = \frac{i}{\hbar}\left[H_0,\mathcal{A}^{\dagger}_{hn}\mathcal{A}_{kn}\right] \tag{5.3.35}$$

$$+\frac{i}{\hbar}\sum_{j=1}^{n}\sum_{l_1l_2}\sum_{\lambda} a^\dagger_{l_2}a^\dagger_{l_1}\left\langle l_1l_2\left|t^\dagger(E_{l_1}+E_{l_2}+i\varepsilon)\right|\lambda h_j\right\rangle \left(\mathcal{A}^\dagger_{hn}\right)_j \left(\mathcal{A}_{kn}\right)_j a_\lambda a_{k_j}$$

$$-\frac{i}{\hbar}\sum_{j=1}^{n}\sum_{f_1f_2}\sum_{\lambda} a^\dagger_{h_j}a^\dagger_{\lambda}\left(\mathcal{A}^\dagger_{hn}\right)_j \left(\mathcal{A}_{kn}\right)_j \left\langle \lambda k_j\left|t(E_{f_1}+E_{f_2}+i\varepsilon)\right|f_1f_2\right\rangle a_{f_1}a_{f_2}$$

$$+\frac{i}{\hbar}\sum_{j=1}^{n}\sum_{l_1l_2}\sum_{f_1f_2}\sum_{\lambda} a^\dagger_{l_2}a^\dagger_{l_1}\left\langle l_1l_2\left|t^\dagger(E_{l_1}+E_{l_2}+i\varepsilon)\right|\lambda h_j\right\rangle$$

$$\times\left(\mathcal{A}^\dagger_{hn}\right)_j\left[\frac{\left(1\pm n_\lambda\pm n_{k_j}\right)}{E_{f_1}+E_{f_2}-E_\lambda-E_k+i\varepsilon}-\frac{\left(1\pm n_\lambda\pm n_{h_j}\right)}{E_{l_1}+E_{l_2}-E_h-E_\lambda-i\varepsilon}\right]\left(\mathcal{A}_{kn}\right)_j$$

$$\times\left\langle \lambda k_j\left|t(E_{f_1}+E_{f_2}+i\varepsilon)\right|f_1f_2\right\rangle a_{f_1}a_{f_2}$$

setting equal a couple of related indexes; we will set $h_{\bar r}=k_{\bar r}=\lambda$, being $1\le\bar r\le n$. Before doing this let us note that for $\bar r\neq j$, and supposing without loss of generality $\bar r<j$, we have the obvious relation

$$\begin{aligned}&\sum_\lambda \left(\mathcal{A}^\dagger_{hn}\right)_j\left(\mathcal{A}_{kn}\right)_{j|_{h_{\bar r}=k_{\bar r}=\lambda}} =\\ &= \sum_\lambda a^\dagger_{h_n}\dots a^\dagger_{h_{j+1}}a^\dagger_{h_{j-1}}\dots a^\dagger_{h_{\bar r+1}}a^\dagger_\lambda a^\dagger_{h_{\bar r-1}}\dots a^\dagger_{h_1}a_{k_1}\dots a_{k_{\bar r-1}}a_\lambda a_{k_{\bar r+1}}\dots a_{k_{j-1}}a_{k_{j+1}}\dots a_{k_n}\\ &= (N-n+2)\left(\mathcal{A}^\dagger_{hn}\right)_{j\bar r}\left(\mathcal{A}_{kn}\right)_{j\bar r}\end{aligned}$$

where analogously to (5.3.32) we have set

$$\left(\mathcal{A}^\dagger_{hn}\right)_{ji}=a^\dagger_{h_n}\dots a^\dagger_{h_{j+1}}a^\dagger_{h_{j-1}}\dots a^\dagger_{h_{i+1}}a^\dagger_{h_{i-1}}\dots a^\dagger_{h_1}$$

supposing as an example $1<i<j<n$ and similarly for $\mathcal{A}_{kn}$. No overall sign factor appears, because the sign generated by moving the operator $a^\dagger_\lambda$ to the right is exactly compensated by the sign obtained moving the operator a_λ to the left. The factor $(N-n+2)$ arises bringing the operator $N=\sum_\lambda a^\dagger_\lambda a_\lambda$ to the outermost left. For $1\le\bar r\le n$ we may therefore write

$$\mathcal{L}'\left(\sum_{h_{\bar r}}\mathcal{A}^\dagger_{hn}\mathcal{A}_{kn|_{h_{\bar r}=k_{\bar r}}}\right)=(N-n+1)\frac{i}{\hbar}\left[H_0,\left(\mathcal{A}^\dagger_{hn}\right)_{\bar r}\left(\mathcal{A}_{kn}\right)_{\bar r}\right]$$

$$+\sum_{j\neq\bar r}(N-n)$$

$$\times\left\{+\frac{i}{\hbar}\sum_{l_1l_2}\sum_\lambda a^\dagger_{l_2}a^\dagger_{l_1}\left\langle l_1l_2\left|t^\dagger(E_{l_1}+E_{l_2}+i\varepsilon)\right|\lambda h_j\right\rangle\left(\mathcal{A}^\dagger_{hn}\right)_{j\bar r}\left(\mathcal{A}_{kn}\right)_{j\bar r}a_\lambda a_{k_j}\right.$$

$$-\frac{i}{\hbar}\sum_{f_1f_2}\sum_{\lambda} a^\dagger_{h_j} a^\dagger_\lambda \left(\mathcal{A}^\dagger_{hn}\right)_{j\bar{r}} \left(\mathcal{A}_{kn}\right)_{j\bar{r}} \langle \lambda k_j \left| t(E_{f_1}+E_{f_2}+i\varepsilon) \right| f_1 f_2\rangle\, a_{f_1} a_{f_2}$$

$$+\frac{i}{\hbar}\sum_{l_1l_2}\sum_{f_1f_2}\sum_{\lambda} a^\dagger_{l_2} a^\dagger_{l_1} \langle l_1 l_2 \left| t^\dagger(E_{l_1}+E_{l_2}+i\varepsilon) \right| \lambda h_j\rangle$$

$$\times \left(\mathcal{A}^\dagger_{hn}\right)_{j\bar{r}} \left[\frac{\left(1\pm n_\lambda \pm n_{k_j}\right)}{E_{f_1}+E_{f_2}-E_\lambda-E_k+i\varepsilon} - \frac{\left(1\pm n_\lambda \pm n_{h_j}\right)}{E_{l_1}+E_{l_2}-E_h-E_\lambda-i\varepsilon}\right] \left(\mathcal{A}_{kn}\right)_{j\bar{r}}$$

$$\left.\times \langle \lambda k_j \left| t(E_{f_1}+E_{f_2}+i\varepsilon) \right| f_1 f_2\rangle\, a_{f_1} a_{f_2}\right\}$$

$$+ \left(\mathcal{A}^\dagger_{hn}\right)_{\bar{r}} \mathcal{L}'(N) \left(\mathcal{A}_{kn}\right)_{\bar{r}}$$

where the term $(N-n)$ instead of $(N-n+2)$ appears because of the presence of two creation operators to the left of $\left(\mathcal{A}^\dagger_{hn}\right)_j$ in (5.3.35). According to Sect. 5.3.2 however $\mathcal{L}'(N)=0$, so that apart from the factor $(N-n)$ one obtains for the *collision* part $\mathcal{L}'_{\rm coll}$ (that is, leaving out the free contribution) the same structure restricted to $(n-1)$ couples of creation and annihilation operators:

$$\mathcal{L}'_{\rm coll}\left(\sum_{h_{\bar{r}}} \mathcal{A}^\dagger_{hn}\mathcal{A}_{kn|_{h_{\bar{r}}=k_{\bar{r}}}}\right) = (N-n)\mathcal{L}'_{\rm coll}\left(\left(\mathcal{A}^\dagger_{hn}\right)_{\bar{r}}\left(\mathcal{A}_{kn}\right)_{\bar{r}}\right).$$

The same mechanism can be easily reiterated, so that we have

$$\mathcal{L}'_{\rm coll}\left(\sum_{h_1\ldots h_n} \mathcal{A}^\dagger_{hn}\mathcal{A}_{kn|_{h_1=k_1,\ldots,h_n=k_n}}\right) = (N-n)\ldots(N-2)\mathcal{L}'_{\rm coll}(N)=0,$$

that is to say the above mentioned result.

We will now show that a structure, which is the natural generalization of (5.3.25) and sharing the same generalized complete positivity property, can be obtained also in this more general case. We proceed exactly in the same way as in Sect. 5.3.3, exploiting the fact that thanks to the relation between the couples of indexes h_j and k_j the condition $|n_{h_j}-n_{k_j}|\ll 1$ is satisfied, so that introducing the operators

$$R^{[2]}_{k_j\lambda} = \sum_{f_1f_2}\sqrt{2\varepsilon\left(1\pm n_\lambda\pm n_{k_j}\right)}\frac{\langle \lambda k_j \left| t(E_{f_1}+E_{f_2}+i\varepsilon) \right| f_1 f_2\rangle}{E_{f_1}+E_{f_2}-E_\lambda-E_{k_j}+i\varepsilon} a_{f_1}a_{f_2}$$

$$R^{[2]}_{h_j\lambda}{}^\dagger = \sum_{l_1l_2} a^\dagger_{l_2}a^\dagger_{l_1}\frac{\langle l_1 l_2 \left| t^\dagger(E_{l_1}+E_{l_2}+i\varepsilon) \right| \lambda h_j\rangle}{E_{l_1}+E_{l_2}-E_{h_j}-E_\lambda-i\varepsilon}\sqrt{2\varepsilon\left(1\pm n_\lambda\pm n_{h_j}\right)}$$

we may write the last contribution of (5.3.35) in the factorized form

$$+\frac{1}{\hbar}\sum_{j=1}^{n}\sum_{\lambda} R^{[2]}_{h_j\lambda}{}^\dagger \left(\mathcal{A}^\dagger_{hn}\right)_j \left(\mathcal{A}_{kn}\right)_j R^{[2]}_{k_j\lambda}.$$

Considering the operator $T^{[2]}$ defined in (5.3.21) let us evaluate

$$\begin{aligned}
\frac{i}{\hbar}\left[T^{[2]\dagger},\mathcal{A}_{hn}^{\dagger}\right]\mathcal{A}_{kn} &= \frac{i}{\hbar}\frac{1}{2}\sum_{l_1l_2}\sum_{f_1f_2} a_{l_2}^{\dagger}a_{l_1}^{\dagger}\left\langle l_1l_2\left|t^{\dagger}(E_{l_1}+E_{l_2}+i\varepsilon)\right|f_1f_2\right\rangle\left[a_{f_1}a_{f_2},\mathcal{A}_{hn}^{\dagger}\right]\mathcal{A}_{kn} \\
&= \frac{i}{\hbar}\frac{1}{2}\sum_{l_1l_2}\sum_{f_1f_2} a_{l_2}^{\dagger}a_{l_1}^{\dagger}\left\langle l_1l_2\left|t^{\dagger}(E_{l_1}+E_{l_2}+i\varepsilon)\right|f_1f_2\right\rangle \qquad (5.3.36)\\
&\quad\times\left\{\left[a_{f_1}a_{f_2},a_{h_n}^{\dagger}\right]a_{h_{n-1}}^{\dagger}\dots a_{h_1}^{\dagger}+\dots+a_{h_n}^{\dagger}\dots a_{h_2}^{\dagger}\left[a_{f_1}a_{f_2},a_{h_1}^{\dagger}\right]\right\}\mathcal{A}_{kn},
\end{aligned}$$

where we have used (5.3.30). Since

$$\frac{1}{2}\sum_{f_1f_2}\left\langle l_1l_2\left|t^{\dagger}(E_{l_1}+E_{l_2}+i\varepsilon)\right|f_1f_2\right\rangle\left[a_{f_1}a_{f_2},a_h^{\dagger}\right]=\sum_{\lambda}\left\langle l_1l_2\left|t^{\dagger}(E_{l_1}+E_{l_2}+i\varepsilon)\right|\lambda h\right\rangle a_{\lambda}$$

eq. (5.3.36) becomes

$$\begin{aligned}
&\frac{i}{\hbar}\sum_{l_1l_2}\sum_{\lambda}a_{l_2}^{\dagger}a_{l_1}^{\dagger}\left\{\left\langle l_1l_2\left|t^{\dagger}(E_{l_1}+E_{l_2}+i\varepsilon)\right|\lambda h_n\right\rangle a_{\lambda}a_{h_{n-1}}^{\dagger}\dots a_{h_1}^{\dagger}+\dots\right.\\
&\qquad\left.+\left\langle l_1l_2\left|t^{\dagger}(E_{l_1}+E_{l_2}+i\varepsilon)\right|\lambda h_1\right\rangle a_{h_n}^{\dagger}\dots a_{h_2}^{\dagger}a_{\lambda}\right\}\mathcal{A}_{kn}
\end{aligned}$$

and we put the operators in normal order, leaving out the commutators which bring contributions negligible in the continuum limit, so that

$$\frac{i}{\hbar}\left[T^{[2]\dagger},\mathcal{A}_{hn}^{\dagger}\right]\mathcal{A}_{kn}=\frac{i}{\hbar}\sum_{j=1}^{n}\sum_{l_1l_2}\sum_{\lambda}a_{l_2}^{\dagger}a_{l_1}^{\dagger}\left\langle l_1l_2\left|t^{\dagger}(E_{l_1}+E_{l_2}+i\varepsilon)\right|\lambda h_j\right\rangle\left(\mathcal{A}_{hn}^{\dagger}\right)_j\left(\mathcal{A}_{kn}\right)_j a_{\lambda}a_{k_j}.$$

Making a similar calculation for $T^{[2]}$ we finally find that (5.3.35) may be written in the compact form

$$\begin{aligned}
\mathcal{L}'\left(\mathcal{A}_{hn}^{\dagger}\mathcal{A}_{kn}\right)&=\frac{i}{\hbar}\left[H_0,\mathcal{A}_{hn}^{\dagger}\mathcal{A}_{kn}\right]\\
&+\frac{i}{\hbar}\left[T^{[2]\dagger},\mathcal{A}_{hn}^{\dagger}\right]\mathcal{A}_{kn}+\frac{i}{\hbar}\mathcal{A}_{hn}^{\dagger}\left[T^{[2]},\mathcal{A}_{kn}\right]+\frac{1}{\hbar}\sum_{j=1}^{n}\sum_{\lambda}R_{h_j\lambda}^{[2]\dagger}\left(\mathcal{A}_{hn}^{\dagger}\right)_j\left(\mathcal{A}_{kn}\right)_j R_{k_j\lambda}^{[2]},
\end{aligned}$$

and therefore, exploiting (5.3.23) and (5.3.24) also

$$\begin{aligned}
\mathcal{L}'\left(\mathcal{A}_{hn}^{\dagger}\mathcal{A}_{kn}\right)&=\frac{i}{\hbar}\left[H_0,\mathcal{A}_{hn}^{\dagger}\mathcal{A}_{kn}\right]+\frac{i}{\hbar}\left[V^{[2]},\mathcal{A}_{hn}^{\dagger}\mathcal{A}_{kn}\right] \qquad (5.3.37)\\
&-\frac{1}{\hbar}\left\{\left[\Gamma^{[2]},\mathcal{A}_{hn}^{\dagger}\right]\mathcal{A}_{kn}-\mathcal{A}_{hn}^{\dagger}\left[\Gamma^{[2]},\mathcal{A}_{kn}\right]\right\}+\frac{1}{\hbar}\sum_{j=1}^{n}\sum_{\lambda}R_{h_j\lambda}^{[2]\dagger}\left(\mathcal{A}_{hn}^{\dagger}\right)_j\left(\mathcal{A}_{kn}\right)_j R_{k_j\lambda}^{[2]},
\end{aligned}$$

in strict analogy with (5.3.22) and (5.3.25) respectively. As in Sect. 5.3.3 the conservation laws (5.3.34) are verified provided (5.3.26) is satisfied, that is to say

$$\Gamma^{[2]}\approx\frac{1}{4}\sum_{gf}R_{gf}^{[2]\dagger}R_{gf}^{[2]}.$$

The mapping $\mathcal{L}'$ defined on linear combinations of operator structures of the form

$$a_h^\dagger a_k, \quad a_{h_2}^\dagger a_{h_1}^\dagger a_{k_1} a_{k_2}, \quad \ldots \quad , a_{h_n}^\dagger \ldots a_{h_1}^\dagger a_{k_1} \ldots a_{k_n},$$

which are sufficiently diagonal in the operator indexes ensures complete positivity of the mapping of time evolution $\mathcal{U}'$ restricted to these typical structures, and the proof of this property is the same as in Sect. 3.2.2.

5.4 Summary and outlook

The present chapter has been devoted to the study of the simplest example of macroscopic system: a self-interacting Schrödinger field describing a collection of structureless particles interacting via a two body short range potential. As explained in Sect. 5.1 according to Ludwig's view, briefly surveyed in Chap. 2, the fundamental objects in quantum mechanics, in order to avoid paradoxes and inconsistencies, should be phenomenologically, objectively described macroscopic systems. Following this point of view we try to start from finite, confined macroscopic systems to be described in terms of quantum fields. The Schrödinger field is decomposed in terms of its normal modes

$$\psi(\mathbf{x}) = \sum_f u_f(\mathbf{x}) a_f$$

which keep boundary conditions into account. According to Sect. 5.2 in order to neglect correlations with the environment a time scale has to be introduced and only quantities slowly varying within this time scale are considered. Typical possible examples of reduced dynamics are given in Sect. 5.2.1, while Sect. 5.2.2 shows how the statistical operator has to be chosen depending on the relevant observables, according to the principle of maximum entropy. The calculations are developed in Sect. 5.3, where we study the time evolution in Heisenberg picture of operator structures of the form $a_h^\dagger a_k$, in terms of which the observables are constructed and where due to the slow variability the indexes referring to the normal modes should be sufficiently diagonal. The calculations have been put forward in a superoperator formalism, using techniques of scattering theory and restricting to a *one-mode* approximation in which three particle collisions are neglected, though statistical corrections are accounted for. The generator of the time evolution (5.3.25)

$$\mathcal{L}'\left(a_h^\dagger a_k\right) = \frac{i}{\hbar}\left[H_0 + V^{[2]}, a_h^\dagger a_k\right] - \frac{1}{\hbar}\left\{\left[\Gamma^{[2]}, a_h^\dagger\right] a_k - a_h^\dagger \left[\Gamma^{[2]}, a_k\right]\right\} + \frac{1}{\hbar}\sum_\lambda R_{h\lambda}^{[2]\dagger} R_{k\lambda}^{[2]}$$

is structurally the same as the one obtained in Chap. 3 for the particle interacting with matter, only the form of the operators appearing in it and given in Sect. 5.3.3 are different, since they are here connected to a two particle T-operator keeping statistical corrections into account. The property of particle number conservation $\mathcal{L}'(N) = 0$ is shown in Sect. 5.3.2, while complete positivity of the obtained time evolution for these couples of field operators can be proved formally in the same way as in Sect. 3.2.2. As a first result a homogeneous Boltzmann equation with statistical corrections for the normal modes is obtained in Sect. 5.3.4, while in Sect. 5.3.5 the formalism is extended to higher polynomials of field operators having the typical structures

$$\mathcal{A}^\dagger_{hn} = a^\dagger_{h_n} \dots a^\dagger_{h_1}, \qquad \mathcal{A}_{kn} = a_{k_1} \dots a_{k_n}$$

and being sufficiently diagonal in the couples of related indexes h_j, k_j. The final result is (5.3.37)

$$\mathcal{L}'\left(\mathcal{A}^\dagger_{hn}\mathcal{A}_{kn}\right) = \frac{i}{\hbar}\left[H_0, \mathcal{A}^\dagger_{hn}\mathcal{A}_{kn}\right] + \frac{i}{\hbar}\left[V^{[2]}, \mathcal{A}^\dagger_{hn}\mathcal{A}_{kn}\right]$$

$$-\frac{1}{\hbar}\left\{\left[\Gamma^{[2]}, \mathcal{A}^\dagger_{hn}\right]\mathcal{A}_{kn} - \mathcal{A}^\dagger_{hn}\left[\Gamma^{[2]}, \mathcal{A}_{kn}\right]\right\} + \frac{1}{\hbar}\sum_{j=1}^{n}\sum_{\lambda} R^{[2]}_{h_j\lambda}{}^\dagger \left(\mathcal{A}^\dagger_{hn}\right)_j \left(\mathcal{A}_{kn}\right)_j R^{[2]}_{k_j\lambda},$$

where $\left(\mathcal{A}^\dagger_{hn}\right)_j$ means that the j-th operator is missing. This structure is analyzed in Sect. 5.3.6 where the conservations laws (5.3.34) are also demonstrated

$$\mathcal{L}'\left(N(N-1)\dots(N-n+1)\right) = 0.$$

Complete positivity can still be proved for the time evolution restricted to these typical field structures having an equal number of creation and annihilation operators, whose indexes related to the normal modes are linked two by two by a condition of sufficient diagonality.

The generalized kinetic equation obtained in this chapter has already led to a Boltzmann equation with statistical corrections in the homogeneous case, but it can also be applied to the non-homogeneous one, making use of joint position-momentum effect observables, as we intend to do in the near future. This equation, as has been extensively shown in the case of particle-matter interaction where we obtained an expression with a similar structure, can account both for a typically quantum coherent behavior and an incoherent, kinetic regime. In fact a similar expression has been obtained [10] studying the problem of Bose Einstein condensation for alkali atoms, where starting from a kinetic regime one goes over to a macroscopically coherent behavior, and one can reasonably hope to successfully apply it to this utmost interesting field. An important generalization of this formalism would consist in overcoming the Markov approximation, thus keeping memory effects, which are often very relevant, into account.

Appendix A

Laws of Quantization

In this appendix we briefly sketch, referring mainly to [11, vol. I, Chap. VI], how axiom **QM**, which connects the general notion of microsystem as interaction carrier with the Hilbert space structure typical of quantum mechanics, may be replaced by other axioms bearing a physical interpretation, so that their validity can be checked by experience. On the basis of these axioms **QM** may be deduced as a theorem. Our starting point is the following theorem, which can be proved as a consequence of the properties of the function $\mu(w,g)$ on $\mathcal{K}\times\mathcal{L}$ enumerated in Sect. 2.2.3

Theorem *There exists a pair of Banach spaces $\mathcal{B}$, $\mathcal{B}'$ (where $\mathcal{B}'$ is dual to $\mathcal{B}$) such that $\mathcal{K}$ may be identified with a subset of $\mathcal{B}$ and $\mathcal{L}$ with a subset of $\mathcal{B}'$ and moreover:*

i) The canonical bilinear form $\langle w,g\rangle$ defined for the dual pair $\mathcal{B}$, $\mathcal{B}'$ is identical with $\mu(w,g)$ on $\mathcal{K}\times\mathcal{L}$: $\mu(w,g)=\langle w,g\rangle_{|\mathcal{K}\times\mathcal{L}}$

ii) $\mathcal{B}$ is a base norm space with basis K, where K is the norm-closed convex set generated by $\mathcal{K}$

iii) The linear span of $\mathcal{L}$ is $\sigma(\mathcal{B}',\mathcal{B})$ dense in $\mathcal{B}'$

$\mathcal{B}$ and $\mathcal{B}'$ are uniquely defined (up to isomorphisms) by (ii) and (iii).

Taking the "finiteness of physics" into account we may assume that the sets $M, \mathcal{Q}, \mathcal{R}$ are countable, so that $\mathcal{K}$ and $\mathcal{L}$ are also countable and $\mathcal{B}$ is separable. An immediate consequence of (*ii*) is the fact that $\mathcal{B}'$ is an order unit space. Being $0\le\mu(w,g)\le 1$ for $w\in\mathcal{K}$ and $g\in\mathcal{L}$ we also have $0\le\mu(w,g)\le 1$ for $w\in K$ and $g\in\mathcal{L}$, so that $\mathcal{L}\subset[\mathbf{0},\mathbf{1}]$, where $\mathbf{1}$ is the order unit of $\mathcal{B}'$. We will denote by L the $\sigma(\mathcal{B}',\mathcal{B})$ closure of $\mathcal{L}$ in $\mathcal{B}'$.

Even though we formulate the axioms as relations in K and L, so that they are mathematically much more concise, they express relations in $\mathcal{Q}, \mathcal{R}, \mathcal{R}_0$ and are therefore basic axioms for preparation and registration procedures. They may be considered as *main natural laws* of preparation and registration, necessary in order to specify the fundamental domain of the theory one is considering, and therefore characterizing the nature of microsystems to be described by quantum mechanics. All axioms are ultimately structure statements for the convex set K, hiding in itself the crucial features of quantum mechanics. They translate, in a way which is physically as intuitive as possible, the assumptions needed to get the usual representation of $\mathcal{B}$ and $\mathcal{B}'$ by spaces of operators in a separable Hilbert space. In the following a crucial role will be played by the notion of face.

If C is a closed convex set in a topological vector space, we say that a subset $F \subset C$ is a closed FACE provided it is a closed convex set which contains no point of any open line segment in C unless it contains the whole line segment ($x \in F, x = \lambda x_1 + (1-\lambda)x_2, 0 < \lambda < 1, x_1, x_2 \in C$ implies $x_1, x_2 \in F$). Faces are therefore subsets of convex sets invariant under mixtures and decompositions. To help intuition consider a closed, convex solid in $\mathbf{R}^3$ with the usual topology: then the faces of the solid coincide with the geometrical faces. Let A be the set of affine continuous functionals on C, with A_+ the subset of positive functionals. We say that F is an EXPOSED FACE provided there exists an $y \in A_+$ such that $F = \{x | x \in C, y(x) = 0\}$. If an exposed face consists of only one point, this is called an *exposed point* of C, and it is in particular an *extreme point* of C. Closed faces, ordered by set-theoretic inclusion, form a complete lattice (with C as unit element and $\emptyset$ as zero element), in which the lattice-theoretic intersection equals the set-theoretic one (the notion of closed face being stable under intersection). Given $w \in K$ there always exists a smallest norm-closed face generated by w, which we denote by $F(w)$. Conversely every norm-closed face F of K may be written as $F(w)$ for a suitably chosen w. In particular the sets $K_0(l) = \{w | w \in K$ and $\mu(w,g) = 0$ for all $g \in l \subset L\}$ and $K_1(l) = \{w | w \in K$ and $\mu(w,g) = 1$ for all $g \in l \subset L\}$ are norm-closed faces of K, while the sets $L_0(k) = \{g | g \in L$ and $\mu(w,g) = 0$ for all $w \in k \subset K\}$ are $\sigma(\mathcal{B}',\mathcal{B})$ closed faces of L. If $l = \{g\}$ we write $K_0(g)$ instead of $K_0(l)$.

The first law of measurement will rule the possibility of constructing more sensitive devices under given constraints. We say that the effect procedure $f_1 \in \mathcal{F}$ is more sensitive than $f_2 \in \mathcal{F}$ if $\mu(a, f_1) \geq \mu(a, f_2)$ for all those $a \in \mathcal{Q}'$ for which $\mu(a, f_1)$ and $\mu(a, f_2)$ are defined. This is equivalent to $\mu(w, \psi(f_1)) \geq \mu(w, \psi(f_2))$ for all $w \in K$, and with respect to the order in $\mathcal{B}'$ to $\psi(f_1) \geq \psi(f_2)$. Correspondingly an effect $g_1 \in L$ is called *more sensitive* than $g_2 \in L$ if $g_1 \geq g_2$. An experimentally useful registration procedure $b \in \mathcal{R}$ ($b \neq \emptyset$) is such that there exist interaction carriers which cannot trigger it. This means that there are some $a \in \mathcal{Q}'$ such that $a \cap b = \emptyset$ although some b_0 (with $b \subset b_0$) is combinable with a. The existence of such a means that b does not appear in the device b_0 by itself, but only by its interaction with a suitable preparing device. A $b \in \mathcal{R}$ ($b \neq \emptyset$) for which $K_0(\psi(b_0, b)) \neq \emptyset$ is an indication which can only be triggered by "real" interactions with interaction carriers, and $M_0(b_0, b) = \{a \in \mathcal{Q}' | \phi(a) \in K_0(\psi(b_0, b))\}$ is the set of all those interaction carriers which cannot trigger b. All other preparing procedures a' with $\phi(a') \notin K_0(\psi(b_0, b))$ must also generate such systems $x \in a'$ which make b occur. This raises the experimentally obvious problem of finding devices b_0 with signals $b \subset b_0$ such that the sets $M_0(b_0, b)$ are not decreased, while the response probability for (b_0, b) is made as large as possible, i.e., the problem of obtaining more sensitive effect procedures (b_0, b) without decreasing $M_0(b_0, b)$. The device must increase the sensitivity only with respect to the considered phenomenon. A positive answer to this experimental problem is indirectly given by (**L** standing for law)

L 1 For each pair $g_1, g_2 \in L$ there is a $g \in L$ with $g \geq g_1, g \geq g_2$ and $K_0(g_1) \cap K_0(g_2) = K_0(g)$

which we call the *law of increase in sensitivity of the first kind.* To clarify the physical situation with the aid of an example consider two linear polarization filters E_1, E_2, corresponding to two registration devices built by putting a photon counter after each filter. A positive result of the connected effect processes f_1, f_2 corresponds to the fact that photons have been reflected by the filter rather than detected by the photon counter. Calling $E_3 = E_1 E_2$ the filter obtained by putting E_2 behind E_1 we have f_3 more sensitive than f_1, corresponding to the fact that E_3 reflects more than E_1. Moreover $K_0(\psi(f_1)) \cap K_0(\psi(f_2)) = K_0(\psi(f_3))$ because the photons going through both E_1 and E_2 go through E_3. Nonetheless f_3 need not be more sensitive than f_2. Consider in fact photons prepared with a linear polarization along the y axis, together with a polarizer E_2 along the x axis and E_1 making an angle of 45 degrees between the two axes. Then E_2 reflects all photons, while E_3 only half of them. Taking instead the filter $E_3 = E_1 E_2 E_1 E_2 \ldots$, obtained putting an infinite series of filters $E_1 E_2$ one after the other, we have the desired device.

As a consequence of **L 1** each set $L_0(k)$ has a largest element $eL_0(k)$ which will be called *decision effect.* Let G be the set of all decision effects. If we call $\mathcal{U}$ the set of all faces of the form $L_0(k)$ with $k \subset K$ ($\mathcal{U} = \{L_0(k) | k \subset K\}$), it can be shown that $\mathcal{U}$ is a complete lattice with respect to the set-theoretic inclusion. Then the mapping $L_0(k) \to eL_0(k)$ is a lattice isomorphism and G is a complete lattice with respect to the order induced on $G \subset \mathcal{B}'$ by $\mathcal{B}'$. Moreover $G \subset \partial_e L$, where $\partial_e L$ denotes the set of extreme points of L.

We now analyze the problem of the increase in sensitivity of a single effect. For effects $g \in \mathcal{L}$ such that $\mu(w_0, g) \approx 0$, but $\sup_{w \in K} \mu(w, g) \not\approx 1$, one expects that it is possible to construct a more sensitive effect $g' \in \mathcal{L}$ with $\mu(w_0, g') \approx 0$ and with $\mu(w, g') \approx 1$ for those $w \in K$ for which $\mu(w, g)$ comes close to its supremum. We are thus led to

L 2 $L = [\mathbf{0}, \mathbf{1}]$

which we call *law of increase in sensitivity of the second kind.* To understand the meaning of such a law note that it implies the following statement: for each $g_0 \in L$ and $y \in [\mathbf{0}, \mathbf{1}]$ with $K_0(g_0) \subset K_0(y)$, there is a $g \in L$ with $K_0(g_0) \subset K_0(g)$ and $\mu(w, g) \geq 1 - \delta(\varepsilon)$ for all $w \in K$ with $\mu(w, y) \geq 1 - \varepsilon$, where $\delta(\varepsilon)$ can also be chosen so that $\delta(\varepsilon) \to 0$ as $\varepsilon \to 0$.

As we have seen the closed faces of K are exactly those closed subsets which are invariant under mixtures and decompositions. If F is a closed face of K we may therefore consider the set $M_F = \{a \in \mathcal{Q}' | \phi(a) \in F\}$, characterized by the fact that it is not physically possible to construct ensembles outside F by decompositions of M_F into subsets or by joining subsets in M_F. In this sense microsystems from M_F admit a uniform characterization, which can be called a "property". This intuitively suggests that it should also be possible to build an effect procedure f such that $\mu(\phi(\tilde{a}), \psi(f))$ noticeably differs from zero if $\tilde{a} \in \mathcal{Q}'$, $\phi(\tilde{a}) \notin F$, whereas $\mu(\phi(a), \psi(f)) \approx 0$ holds for all the $a \in \mathcal{Q}'$ with $\phi(a) \in F$. Such an effect procedure does not respond to systems from M_F, but it can be triggered by systems from $\tilde{a}$, since not all systems from $\tilde{a}$ can have the characterization belonging to F (if they could we would have $\tilde{a} \in M_F$). According to physical intuition, exploiting **L 2** one can show that for every exposed face F of K, for $w_0 \in F$, $\tilde{w} \in K$ and $\tilde{w} \notin F$ there is a sequence $g_\nu \in \mathcal{L}$ with $\mu(w_0, g_\nu) \to 0$ and $\mu(\tilde{w}, g_\nu) > \delta$ ($\delta > 0$ a fixed number).

As a consequence of **L 2** the set of exposed faces of K coincides with the set $\{K_0(g)$ with $g \in L\}$. Furthermore it can be shown that $\sup_{w \in K} \mu(w, e) = 1$ (that is to say $\|e\| = 1$) provided $e \in G$, $e \neq 0$. A mathematical idealization of this statement leads to

L 3 To each $e \in G$, $e \neq 0$ there exists a $w \in K$ for which $\mu(w, e) = 1$.

This is equivalent to: $e \in G$ implies $\mathbf{1} - e \in G$. Then the map $e \to e^\perp \equiv \mathbf{1} - e$ is an orthocomplementation in the lattice G and G is also orthomodular. Writing $K_1(e) = K_0(\mathbf{1} - e) = K_0(e^\perp)$ we have that the map $e \to K_1(e)$ is an isomorphism between G and the lattice of exposed faces of K.

The axioms introduced so far are also satisfied by classical systems, characterized by the fact that all decision effects are commensurable. We now introduce further laws which should restrict the domain of validity of the theory to microsystems. The next law to be introduced is connected with the existence of non-coexistent registrations and will be necessary in order to introduce the covering property for the lattice G. Consider three decision effects e_1, e_2, e_3 with $e_2 \perp e_3$. Being orthogonal e_2, e_3 are commensurable and there exists a registration method b_0 with $b_2, b_3 \in \mathcal{R}(b_0)$ and $\psi(b_0, b_2) = e_2$, $\psi(b_0, b_3) = e_3$. The relation $e_2 \perp e_3$ then implies $b_2 \cap b_3 = \emptyset$. Since e_1 need not necessarily be commensurable with e_2, e_3, we consider another registration method $\tilde{b}_0$ with $\tilde{b}_1, \tilde{b}_2 \in \mathcal{R}(\tilde{b}_0)$ and $\psi(\tilde{b}_0, \tilde{b}_1) = e_1$, $\psi(\tilde{b}_0, \tilde{b}_2) = e_1 \vee e_2$ ($e_1 \leq e_1 \vee e_2$ and $e_1, e_1 \vee e_2$ are therefore commensurable). In particular $\tilde{b}_1 \subset \tilde{b}_2$, $\psi(\tilde{b}_0, \tilde{b}_2 \backslash \tilde{b}_1) = (e_1 \vee e_2) - e_1$ and $\psi(\tilde{b}_0, \tilde{b}_0 \backslash \tilde{b}_2) = \mathbf{1} - (e_1 \vee e_2)$. There are of course important correlations between the responses of the two devices b_0 and $\tilde{b}_0$ for the different ensembles $w \in K$. We consider the response of the device b_0 to ensembles $w \in K_1(e_1 \vee e_2)$ (for which the indication $\tilde{b}_2$ on $\tilde{b}_0$ occurs with certainty) and that of the device $\tilde{b}_0$ to the $w \in K_1(e_3)$ (for which the indication b_3 on b_0 occurs with certainty). This response is easily ascertained if $e_1 \perp e_2 \vee e_3 = e_2 + e_3$, that is $\mu(w, e_2 + e_3) = 0$ for all $w \in K_1(e_1)$ and $\mu(w, e_1) = 0$ for all $w \in K_1(e_2 + e_3)$. In that case $\mu(w, \psi(b_0, b_3)) = 0$ for all $w \in K_1(e_1 \vee e_2)$ and $\mu(w, \psi(\tilde{b}_0, \tilde{b}_2)) = 0$ for all $w \in K_1(e_3)$. We now consider the case in which e_1 is no longer orthogonal to $e_2 + e_3$, and thus no longer commensurable with e_2, e_3, but also e_1 is not "close" to $e_2 + e_3$, in the sense that

$$\sup_{w \in K_1(e_1)} \mu(w, e_2 + e_3) \neq 1 \quad \text{and} \quad \sup_{w \in K_1(e_2+e_3)} \mu(w, e_1) \neq 1, \tag{A.1}$$

conditions that can be physically tested by means of the two devices $b_0, \tilde{b}_0$. For $F(w_3) = K_1(e_3)$, from $w_3 \in K_1(e_2 + e_3)$ due to (A.1) follows

$$\mu(w_3, \psi(\tilde{b}_0, \tilde{b}_0 \backslash \tilde{b}_1)) = \mu(w_3, \psi(\tilde{b}_0, \tilde{b}_2 \backslash \tilde{b}_1)) + \mu(w_3, \psi(\tilde{b}_0, \tilde{b}_0 \backslash \tilde{b}_2)) > 0$$

or equivalently

$$\mu(w_3, \mathbf{1} - e_1) = \mu(w_3, (e_1 \vee e_2) - e_1) + \mu(w_3, \mathbf{1} - (e_1 \vee e_2)) > 0.$$

In this expression one expects that the last summand cannot vanish: in fact due to $e_2 \perp e_3$ the ensemble w_3 is such that in its realization by preparation procedures only such systems are prepared that are "totally different" from e_2 (that is with certainty do not trigger the indication b_2 on b_0). Hence, at least some of these systems should trigger the indication $\tilde{b}_0 \backslash \tilde{b}_2$, since by (A.1) not all such systems trigger $\tilde{b}_1$. After some manipulations one sees that this requirement is equivalent to

L 4 If $e_1, e_2, e_3 \in G$ and if $e_2 \leq e_1 \leq e_2 \vee e_3$, $\Delta(e_1, e_3) \neq 0$ then $e_1 = e_2$

where $\Delta(e_1, e_3)$ is the distance between two elements of G defined by

$$\Delta(e_1, e_3) = \max \left\{ \inf_{w \in K_1(e_1)} \mu(w, \mathbf{1} - e_3), \inf_{w \in K_1(e_3)} \mu(w, \mathbf{1} - e_1) \right\}.$$

Note that $\Delta(e_1, e_3) \neq 0 \iff K_1(e_1) \cap K_1(e_3) \neq \emptyset$ and that $\Delta(e_1, e_3) = 1 \iff e_1 \perp e_3$. As an example consider two Stern-Gerlach devices into which an atomic beam of hydrogen atoms in the ground state falls in the z-direction. One device shall decompose the beam according to the x-component of spin, the other according to the r-component (with r in the xy-plane). Moreover let the two devices be equipped to measure the energy of the atoms in the outgoing beam. The first device measures:

- e_2: spin in the $+z$-direction, energy greater than ε;

- e_3: spin in the $+z$-direction, energy smaller than ε;
- $\mathbf{1} - (e_2 + e_3)$: spin in the $-z$-direction.

The second device measures:

- e_1: spin in the $+r$-direction;
- $e_1 \vee e_2$: spin in the $+r$-direction and spin in the $-r$-direction, energy greater than ε;
- $\mathbf{1} - e_1 \vee e_2$: spin in the $-r$-direction, energy smaller than ε.

If the r-direction is the $-z$-direction both devices act the same, $e_1 \perp e_2 + e_3$ and the requirement is trivially satisfied. If one slowly rotates the r-direction out of the $-z$-direction, $\mu(w_3, \mathbf{1} - e_1 \vee e_2)$ should not jump to zero but continuously vary away from 1. Very pictorially, $\Delta(e_1, e_2 + e_3)$ is a measure for the deviation of the r-direction from the z-direction, becoming zero as the r-direction approaches the z-direction. Then $\mu(w_3, \mathbf{1} - e_1 \vee e_2)$ can also tend to zero. Our requirement is therefore a sort of continuity law for the probability function μ. If all decision effects are commensurable, as in the classical case, **L 4** is automatically satisfied and has no meaning.

So far no axiom has been introduced which accounts for the typical peculiarity of microsystems, that of occupying discretely distinguishable states. The existence of such discrete states of atomic systems, expressed through the notion of preparation and registration, means that there are preparations, i.e., ensembles, which cannot be decomposed into arbitrarily many different subensembles: a simple example is the ground state of an atom. Contrary to classical mechanics, in which one never reaches a limit of maximal precision, in quantum mechanics one can easily produce ensembles which cannot be made more uniform. With reference to the set K and to the notion of face, in classical systems any face can be arbitrarily refined, while this is not true for quantum mechanics, where there are faces which can be distinguished by finitely many registrations, i.e., by finitely many effects. This leads to the following axiom, which will permit us to distinguish between microsystems and classical systems, an axiom we shall call the *main law of quantization*

L 5 Each exposed face F of K is the upper bound of a sequence of increasing exposed faces of finite dimension

to be extended by

L 6 Every finite-dimensional face F of K is exposed .

We are now in the position to clarify what we intend by microsystems: they are those interaction carriers for which the axioms **L 1** to **L 6** hold. On the other hand classical systems are recovered when for the interaction carriers **L 1** to **L 3** hold together with (**C** standing for classical)

C Any two decision effects are commensurable and each exposed face of K is infinite dimensional.

Thanks to **L 5** one can show that G is an atomic lattice having the covering property (its atoms being exactly the extreme points).

We are now ready to recover the Hilbert space structure of quantum mechanics. This can be done exploiting the representation theory already developed inside the lattice theoretic approach to quantum mechanics, according to which the lattice G of decision effects, with the above introduced properties, can be identified with the lattice of projection operators in a Hilbert space $\mathcal{H}$ over a field which, on the basis of physical arguments, can be taken as $\mathbf{C}$. Then the spaces $\mathcal{B}$ and $\mathcal{B}'$ are represented respectively by the space of trace-class operators with basis K and by the space of bounded operators with L as the order interval $[\mathbf{0}, \mathbf{1}]$.

Appendix B

List of Axioms

In this appendix we give a list of the axioms introduced in the presentation of Ludwig's approach to the foundations of quantum mechanics, together with the names used in Ludwig's books to denote the corresponding axioms

Thesis	*Ludwig's books*
S 1.1	**AS 1.1**
S 1.2	**AS 1.2**
S 2.1	**AS 2.1**
S 2.2	**AS 2.2**
S 2.3	**AS 2.3**
A 1	**APS 1**
A 2	**APS 2**
A 3	**APS 3**
A 4.1	**APS 4.1**
A 4.2	**APS 4.2**
A 5	**APS 5**
A 6	**APS 6**
A 7.1	**APS 7.1**
A 7.2	**APS 7.2**
A 8.1	**APS 8.1**
A 8.2	**APS 8.2**
A 9	**Axiom**
QM	**AQ**
L 1	**AV 1.1**
L 2	**AV 1.2s**
L 3	**AVid**
L 4	**AV 3**
L 5	**AV 4s**
L 6	**AV 2f**
C	**AVkl**

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