TIME SCALE AND COMPLETELY POSITIVE DYNAMICAL EVOLUTIONS

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It is argued that in the description of macroscopic systems inside quantum mechanics the study of the dynamics of selected degrees of freedom slowly varying on a suitable time scale, corresponding to relevant observables for the given reduced description, is particularly meaningful. A formalism developing these ideas in the more simple case of a microsystem interacting with a macroscopic system is briefly outlined, together with an application to the field of neutron optics. The obtained reduced description relies on a T-matrix formalism and has the property of complete positivity.

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. 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, through the phenomenon of entanglement (\textit{Verschränkung}) make the attribution of properties to part of a system problematic; the famous E.P.R. paradox; recent experiments in which the particle picture seems to lead to inconsistencies, e.g., the heavily debated superluminal photonic tunneling experiments. \(^2\) 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 \textit{event}. \(^3\) A possible alternative approach was elaborated by Ludwig \(^4\) (for a brief but self-consistent survey of Ludwig’s axiomatic approach see also \(^5\)): 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 \textit{event} is also introduced. \(^7\)

\section*{2 Time Scale and Macroscopic Systems}

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, \(^8\) 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 system-
atic 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 sub-dynamics 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.

A significant achievement for the concrete realization of this research program would be 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. A first elaboration of a formalism with these features has already been developed in the case of a microsystem interacting with a macroscopic system, and will be the object of the following paragraphs, paying particular attention to structural properties such as complete positivity. This formalism will prove suitable for the description of both coherent and incoherent interactions, as we shall see in the last paragraph, with reference to the case of neutron optics. The possibility of describing incoherent effects being strictly connected to the use of a statistical operator formalism. This formal approach has been pursued further in order to apply it to macroscopic systems (see also the contribution of Prof. L. Lanz to these Proceedings). 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. This could be a promising feature in connection with the description of many-body systems in which a coherent dynamics plays a relevant role, as it happens for the recently observed Bose-Einstein condensates of trapped alkali atoms. It appears that, considering slow variables, the time evolution satisfies a generalization of the complete positivity property.

3 Subdynamics and Complete Positivity

3.1 A Particle Interacting with Matter

To obtain a concrete realization of the previously introduced ideas in a tractable case we consider the simplest example of subdynamics of a macrosystem: a particle interacting with matter at equilibrium. This example can be of particular physical interest in connection with recent so called single particle experiments using massive particles. In this case the subdynamics of the microsystem may be extracted, as a selected degree of freedom, from the dynamics of the whole system. It can also be seen as the slightest disturbance to the equilibrium state, a first tiny step towards the study of non-equilibrium systems. We will briefly sketch here only the general scheme, referring the reader to the original paper. Before doing this however, we will introduce the definition of the property of complete positivity, so as to fully appreciate its appearance in the structure of the generator of the dynamical evolution.

3.2 Complete Positivity

The most general representation of the preparation of a physical system described in a Hilbert space $\mathcal{H}$ is given by a statistical operator, that is to say an operator in the space $\mathcal{TC}(\mathcal{H})$ of trace class operators on $\mathcal{H}$, positive and with trace equal to one. Consider now a mapping $\mathcal{U}$ defined on the space of trace class operators into itself $\mathcal{U} : \mathcal{TC}(\mathcal{H}) \rightarrow \mathcal{TC}(\mathcal{H})$, possibly corresponding to a Schrödinger picture description on the states. We say that the map $\mathcal{U}$ is completely positive, or equivalently has the property of complete positivity, if and only if the adjoint map $\mathcal{U}'$ acting on the space $\mathcal{B}(\mathcal{H})$ of bounded linear operators, dual to $\mathcal{TC}(\mathcal{H})$, $\mathcal{U}' : \mathcal{B}(\mathcal{H}) \rightarrow \mathcal{B}(\mathcal{H})$, and therefore corresponding to an Heisenberg picture description in terms of observables, satisfies the
Inequality

\[ \sum_{i,j=1}^{n} \langle \psi_i | U'(\hat{B}_i \hat{B}_j) | \psi_j \rangle \geq 0 \quad \forall n \in \mathbb{N}, \quad \forall \{ \psi_i \} \in \mathcal{H}, \quad \forall \{ \hat{B}_i \} \in \mathcal{B}(\mathcal{H}). \quad (1) \]

For \( n = 1 \) one recovers the usual notion of positivity, while for bigger \( n \) this is actually a nontrivial requirement. It is immediately seen that any unitary evolution is completely positive. In this sense one can see complete positivity as a property that is worth retaining when shifting from the unitary dynamics for closed systems to a more general dynamics for the description of open systems. In fact the general physical argument for the introduction of complete positivity is the following. Consider a system \( S_1 \) described in \( \mathcal{H}_1 \), whose dynamics is given by the family of mappings

\[ U : \mathcal{T} \mathcal{C}(\mathcal{H}_1) \to \mathcal{T} \mathcal{C}(\mathcal{H}_1) \]

and an \( n \)-level system \( S_2 \) described in \( \mathcal{H}_2 = \mathbb{C}^n \), whose dynamics can be neglected, so that \( \mathcal{H}_2 = 0 \). Because the two systems do not interact, the map \( \hat{U} \) describing their joint evolution

\[ \hat{U} : \mathcal{T} \mathcal{C}(\mathcal{H}_1 \otimes \mathbb{C}^n) \to \mathcal{T} \mathcal{C}(\mathcal{H}_1 \otimes \mathbb{C}^n) \]

will be simply given by the tensor product \( \hat{U} = U \otimes 1 \). But the dynamical map \( \hat{U} \) must of course be positive and this is equivalent to the requirement that \( \hat{U} \) be completely positive.

The property of complete positivity has already shown to be particularly relevant in the determination of quantum structures, for example in the field of quantum dynamical semigroups, used for the description of the irreversible dynamics of open quantum systems, typically the reduced dynamics of systems interacting with an external system, such as a heat bath or a measuring instrument. In Heisenberg picture quantum dynamical semigroups are given by collections of positive mappings

\[ U'_t : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H}) \quad t \geq 0, \quad U'_0 1 = 1 \]

which satisfy the semigroup composition property

\[ U'_s U'_t = U'_{s+t} \quad s, t \geq 0. \]

Under these conditions a generally unbounded generator \( \mathcal{L}' \) exists such that

\[ \frac{d}{dt} U'_t \hat{B} = \mathcal{L}' U'_t \hat{B} \]
for all $\hat{B}$ in the domain. If one further asks the semigroup to be norm continuous, so that the generator is a bounded map, it can be shown, as has been done by Lindblad, that complete positivity determines the general expression for the generator to be of the form

$$L'\hat{B} = \frac{i}{\hbar}[\hat{H}, \hat{B}] - \frac{1}{2}\left\{\sum_j \hat{V}_j \hat{V}_j^\dagger, \hat{B}\right\} + \sum_j \hat{V}_j^\dagger \hat{B} \hat{V}_j$$

$$\hat{V}_j, \sum_j \hat{V}_j \hat{V}_j^\dagger \in \mathcal{B}(\mathcal{H}), \quad \hat{H}_j = \hat{H}_j^\dagger \in \mathcal{B}(\mathcal{H})$$

This Lindblad structure of master equation, possibly allowing for unbounded operators or even quantum fields, appears in many applications in very different fields of physics and is often taken as starting point for phenomenological approaches. It accounts for a non-Hamiltonian dynamics and has been extensively used in the formulation of continuous measurement theory and especially in quantum optics.

### 3.3 Structure of the Generator

We now come back to the description of the dynamics of a particle interacting with a macroscopic system, typically matter at equilibrium, and consider the total Hamiltonian in the field formalism of second quantization. The Hamiltonian contains the term describing the free particle $H_0$, the contribution of matter at equilibrium $H_m$ and an interaction potential $V$

$$H = H_0 + H_m + V \quad H_0 = \sum_f E_f a_f^\dagger a_f \quad [a_f, a_g^\dagger] = \delta_{fg}$$

where $a_f$ is the destruction operator for the microsystem, either a Fermi or a Bose particle, in the state $u_f$. Having it in mind to describe situations in which only one particle is observed in each experimental run we assume for the statistical operator the form

$$\rho = \sum_{gf} a_f^\dagger \varrho^m a_f w_{gf},$$

where $\varrho^m$ is the statistical operator describing matter, while $w_{gf}$ is a matrix with positive entries and trace one, which can be considered as the representative of a statistical operator $\hat{w}$ in the one particle Hilbert spaces $\mathcal{H}^{(1)}$. To understand this choice consider the charge $Q = \sum_f a_f^\dagger a_f$. $\varrho^m$ is an eigenvector of this operator with eigenvalue zero, i.e., it contains no microsystems, while
\( \rho \) has eigenvalue one, corresponding to a single microsystem. To extract the subdynamics of the microsystem we consider observables bilinear in the field operators, \( A = \sum_{f,g} a_f^\dagger A_{fg} a_g \), and the following simple reduction formula

\[
\text{Tr}_\mathcal{H} (A \rho) = \sum_{f,g} A_{fg} w_{gf} = \text{Tr}_\mathcal{H} (1) (\hat{A} \hat{w}),
\]

connecting the expectation value of such observables with \( \rho \) to the expectation value in the one particle Hilbert space of the state and observable corresponding to the given matrices. To develop the calculations one goes over to the Heisenberg picture and exploits a superoperator formalism, so that to the T-matrix is associated the following superoperator \( \mathcal{T}(z) \), the prime denoting superoperators on \( \mathcal{B}(\mathcal{H}) \), the conjugate space of \( \mathcal{T}(\mathcal{H}) \)

\[
\mathcal{T}(z) \equiv \mathcal{V'} + \mathcal{V'}(z - \mathcal{H'})^{-1} \mathcal{V'}, \quad \mathcal{H'} = \frac{i}{\hbar} [\mathcal{H}, \cdot], \quad \mathcal{V'} = \frac{i}{\hbar} [\mathcal{V}, \cdot].
\]

As a result we obtain the following structure for the evolution mapping on a time \( t \) which is small with respect to the particle’s dynamics, though much larger than the relaxation time of the macrosystem

\[
\mathcal{U}'(t) (a_h^\dagger a_k) = e^{i\mathcal{H}' \tau} (a_h^\dagger a_k) = a_h^\dagger a_k + t \mathcal{L}' a_h^\dagger a_k
\]

where the generator restricted to this typical bilinear structure of field operators in the quasi-diagonal case is given by:

\[
\mathcal{L}' (a_h^\dagger a_k) = \frac{i}{\hbar} [\mathcal{H}_0 + \mathcal{V}, a_h^\dagger a_k] - \frac{1}{\hbar} \{ [\Gamma, a_h^\dagger] a_k - a_h^\dagger [\Gamma, a_k] \} + \frac{1}{\hbar} \sum_{\lambda} R_{hl}^\dagger R_{k\lambda}
\]

\( \mathcal{V} \) and \( \Gamma \) being linked respectively to the self-adjoint and anti-self-adjoint part of the T-matrix. Let us note that due to the presence of the minus sign the term between curly brackets cannot be rewritten as a simple commutator. Complete positivity of the mapping \( \mathcal{U}'(t) \) restricted to these simple bilinear field structures

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

can be seen from the decomposition which holds true for an infinitesimal positive time \( dt \)

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

One can also check that particle number conservations holds, so that \( L'(N) = 0 \), where \( N = \sum_f a_f^\dagger a_f \).

Exploiting the reduction formula (2) we recover a Lindblad equation for the time evolution of the statistical operator describing the microsystem, in which the effective Hamiltonian contains a contribution linked to the self-adjoint part of the T-matrix, averaged over the state of matter, the gamma operator being connected instead to its anti-self-adjoint part

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

(3)
The last contribution is typically incoherent, leading from a pure state to a mixture and can be introduced only in the formalism of the statistical operator. Particle number conservation implies \( \hat{\Gamma} = 1/2 \sum_{\xi\lambda} \hat{L}_{\lambda\xi}^\dagger \hat{L}_{\lambda\xi} \).

3.4 Neutron Optics as an Application

In recent years there has been a rapidly growing interest in the field of particle optics, especially neutron and atom optics, due to a spectacular improvement of the experimental techniques, connected to the introduction of the single crystal interferometer in the case of neutrons. Such new achievements provide very important tests verifying the validity of quantum mechanics, especially in that it predicts wavelike behavior 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 main interest is devoted to the coherent wavelike behavior of particles interacting with homogeneous samples of matter, as can be justified on the basis of the similarity between a Schrödinger equation with an optical potential and the Helmholtz wave equation. The very existence of such an optical description of the interaction is far from trivial and strongly depends on the experimental conditions. While the attention has been mostly devoted to exploiting the optical analogies, very 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
coh esent wave formalism, instead of a reduced density matrix description, as
usually adopted in quantum optics. We now want to address the question
of how to consistently describe both regimes applying the previously deduced
master-equation (3), mainly following, where the interested reader can find
further details. The operators 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.
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, the remaining incoherent part is related to the dynamic
structure function.

As a first step we want to consider the coherent interaction of neutrons
with matter and therefore we neglect in (3) 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. Adopting the Fermi pseudopo-
tential to describe the neutron nucleus interaction the T-matrix takes the
form
\[ \hat{T} = \frac{2\pi \hbar^2}{m} \int d^3r \psi^\dagger(r)\delta^3(\hat{x} - r)\psi(r) \]
a local potential parameterized by the coherent scattering length \( b \). If we
consider only pure states we come to the following stationary Schrödinger
equation
\[ \left\{ -\frac{\hbar^2}{2m} \Delta_x + \frac{2\pi \hbar^2}{m} \delta(\psi^\dagger(x)\psi(x)) \right\} \phi(x) = E\phi(x), \quad (4) \]
with a potential depending on the average particle density. If the medium can
be considered homogeneous, with density \( n_o \), Eq. (4) describes propagation
of matter waves with an index of refraction given by
\[ n \simeq [1 - (\lambda^2/2\pi)b n_o]. \quad (5) \]
This leads to the formula currently used to calculate phase shifts in neutron
interferometry experiments
\[ e^{ix} = e^{i(n-1)\frac{\Delta}{\lambda}D} = e^{-in_o b \lambda D}, \]
where \( D \) is the thickness of the sample.

We now come to the connection between the contributions other than
the commutator in (3) and the dynamic structure function, together with the
relevance of this relationship to the optical theorem. An expression of the form \( n(\xi) = \frac{1}{\pi} \sum_{\lambda, \zeta} \hat{L}_{\lambda \xi} \hat{L}^{\dagger}_{\lambda \zeta} \hat{w} \hat{L}^{\dagger}_{\lambda \xi} \) 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. To keep also the attenuation of the coherent wave into account we have to consider all contributions in \( n(\xi) \). 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

\[
- \frac{1}{\hbar} \left\{ \frac{1}{2} \sum_{\xi, \lambda} \hat{L}_{\lambda \xi} \hat{L}^{\dagger}_{\lambda \xi}, \hat{w} \right\} + \frac{1}{\hbar} \sum_{\xi, \lambda} \hat{L}_{\lambda \xi} \hat{w} \hat{L}^{\dagger}_{\lambda \xi}
\]

allow for the presence of a non-self-adjoint potential which is nevertheless not linked to real absorption. 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. In fact the trace of this term gives all the contributions to incoherent scattering, that is to say the total diffusion cross section; if the momentum distribution of the incoming particle is suitably peaked around \( p_0 \), this trace may be written in the static limit

\[
n_{\alpha} \delta^2 p_0 \int d\Omega_q \ S_c(q) = n_{\alpha} \frac{p_0}{m} \sigma_d
\]

where

\[
S_c(q) = \frac{1}{N} \int d^3x \ e^{i q \cdot x} \int d^3y \ \langle \delta N(y) \delta N(x + y) \rangle,
\]

and we have denoted in the structure function \( S_c(q) \) by \( q \) the momentum transfer and by \( \sigma_d \) the total diffusion cross section per particle. This is the result derived for the attenuation of the coherent beam due to incoherent scattering, usually obtained by an evaluation of the local field effects, neglected in the equation giving the optical neutron dynamics \( n(\xi) \). In this approach the incoherent contribution is already present in the equation giving the dynamics of the microsystem, thanks to the more general formalism adopted. The
correction to the optical potential can be read by

\[
\hat{\mathcal{U}} = \frac{2\pi \hbar^2}{m} n_o \left[ b - \frac{i\beta p_0}{4\pi \hbar} \int d\Omega_q S_c(q) \right]
\]

and is of second order in the small parameter \(b\).

The incoherent contribution is thus necessary to fulfill the optical theorem and take diffuse scattering, that attenuates the coherent beam, into account. Even though it introduces a smaller correction the incoherent contribution is very important from the theoretical point of view. 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 \(\hat{w}\), rather than by the wave function \(\psi\). 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.

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